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6. AUTHOR(S)
Diola Bagayoko, Ph.D., Southern University System Distinguished Professor of Physics and Chancellor's Fellow (Telephone: 225-771-2730)
Ella L. Kelley, Ph.D., Professor of Chemistry
Bagayoko@aol.com or Bagayoko@phys.subr.edu

7. PERFORMING ORGANIZATION NAME(S)AND ADDRESS(ES)
Southern University and A&M College, P. O. Box 11776
Department of Physics
Baton Rouge, Louisiana 70813

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9. SPONSORING/MENTORING AGENCY NAME(S) AND ADDRESS(ES)
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13. SUPPLEMENTARY NOTES
We urge the reader to consult the web site of the Timbuktu Academy for a scientific approach to the creation of educational, research, and professional value-added (http://www.phys.subr.edu/timbuktu.htm). We believe Publications singled out in the summary report are necessary readings—in physics and in mentoring.

14. ABSTRACT

We present the objectives, approach, and accomplishments of the Timbuktu Academy. We claim to have established a scientific approach to systemic mentoring. Our accomplishments include the production of 106 SEM Bachelor's degree holders (61 from 1994 to 1998 and 45 from 1998 to 2001). 104 of them are African Americans. Well over half of our 106 alumni earned or are successfully pursuing advanced degrees, including the Ph.D. We published well over 50 articles (20 in physics and 11 in mentoring from 1999 to 2001). We made over 100 presentations (58 from 1993 to 1998 and 55 from 1999 to 2001). We utilized our scientific approach to produce 10 National Merit/National Achievement, minority, pre-college scholars in 2000 and 11 in 2001! We submit that ONR and the Naval Research Laboratory (NRL) should pay attention to the Bagayoko, Zhao, and Williams procedure for the prediction of properties of materials, including molecules, clusters, semiconductors, and nuclei (in the shell model).

15. SUBJECT TERMS
THE SCIENCE OF SYSTEMIC MENTORING. THE 10-STEP SYSTEMIC MENTORING MODEL OF THE TIMBUKTU ACADEMY. THE BAGAYOKO, ZHAO, AND WILLIAMS (BZW) METHOD FOR DESCRIPTIVE AND PREDICTIVE CALCULATIONS OF PROPERTIES OF MATERIALS.

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PROGRESS REPORT

GRANT#: N00014-98-1-0748

PRINCIPAL INVESTIGATOR: Diola Bagayoko, Ph.D.

INSTITUTION: Southern University and A & M College

GRANT TITLE: Science, Engineering and Mathematics at the Timbuktu Academy

AWARD PERIOD: August 1, 1998 – July 31, 2001

OBJECTIVE: As per the proposal funded by **the Department of the Navy, Office of Naval Research (ONR)**, the objectives of Science, Engineering, and Mathematics at the Timbuktu Academy were

- **(a)** To produce highly qualified and technically trained SEM graduates—fifty (50) undergraduate students were to be supported per year with preference given to physics, chemistry, mathematics, computer science, and engineering (ME, EE, CE);
- **(b)** To guide a significant percentage of these graduates, beyond average national percentages, to the successful pursuit of advanced degrees in science, mathematics, and engineering (SEM) disciplines and related ones, with emphasis on the Ph.D. degree;
- **(c)** To provide first-rate summer enrichment for hundreds of pre-college students, from middle to high school with emphasis on mathematics, English and reading skills, and SMET careers; and
- **(d)** To deliver extensive educational services to 5000 pre-college and college students, their teachers, counselors, parents, and members of the greater community, including seventy (70) pre-college students to be engaged in academic enrichment activities in the summer.

APPROACH: The essential characteristics of our approach are listed below.

- **(1)** We established, through research and publications, *a paradigm for the creation of educational and research value-added.* This paradigm, known as the Paradigm of the Timbuktu Academy, rests on a current, dynamic sum of knowledge in education and related disciplines, including cognitive and behavioral sciences. The law of performance (LP) plays a role similar to that of the "Rosetta Stone" in our deciphering of the creation of educational, research, and professional value-added.
- **(2)** We utilized this paradigm to design and redesign the programs and comprehensive, *systemic mentoring* activities of the Timbuktu Academy [Education, Vol. 115, No. 1, pp. 31-39, pp.11-18 (1994); and to appear in Inter. Journal of Materials Science. Education, 2001].
- **(3)** Our implementation of the systemic mentoring activities, including research participation for undergraduates, and of the academic, enrichment activities for pre-college students strictly adhered to the paradigm that guided them. The details of the paradigm, programs, activities, and results (including some publications) of the Timbuktu Academy are available at its web site **(http://www.phys.subr.edu/timbuktu.htm).**
- **(4)** In particular, the following **subprograms** are described in the brochure of the Academy (available at the above web site): Getting Smarter at the Timbuktu Academy (GeSTA, 20 - 30 students), Summer Science Institutes for middle school (SSI-M, 60-100 students) and high school students (SSI, 20 11th graders); Summer Enrichment at the Timbuktu Academy (SETA, 20 9th graders); Challenge 2000 for twenty (20) high school students of varying levels of academic preparedness; the Summer Bridge Institute (SBI) for 20 high-achieving, high school graduates; the Undergraduate Research Program (URP) for fifty (50) college students in engineering, physics, and chemistry; and the Educational Service Program (ESP) that publishes extensively and disseminates empowering, factual, educational knowledge to the larger community. A Saturday Academy, also known as the *Learning Olympiads*, is a part of ESP. There are different Olympiads for students with vastly different levels of academic preparedness.

ACCOMPLISHMENTS

The Production of BS Degree Holders in Physics, Chemistry, and Engineering and Graduate School Attendance by and Success of Alumni

From 1998 to July 2001, forty-five (45) Academy scholars earned bachelor degrees: 18 in Physics, 11 in Chemistry, and 16 in Engineering. These numbers show that our key objective, relative to the production of graduates, has been met and surpassed. Sixty-one percent (61%) of Physics alumni have successfully enrolled in graduate school. Our graduate school attendance rates are 56% for Chemistry and 44% for Engineering from 1998 through 2001. The National average for graduate school enrollment of Physics BS holders is around 55% as per the annual, enrollment reports of the American Institute of Physics (AIP).

The Production and Dissemination of New Knowledge

We placed the creation of educational value added on a rigorous, scientific basis (Education, Vol. 115, No. 1, pp. 31-39, 1994). We introduced the Bagayoko, Zhao, and Williams (BZW) procedure in ab-initio calculations and ushered in the era of *predictive* computations of excitation-related properties of atoms, molecules, clusters, semiconductors, and insulators (Bulletin, American Physical Society, Vol. 43, No. 1, p. 846, 1998; Journal of Physics: Condensed Matter, Vol. 10, No. 25, pp. 5645-5655, 1998; and the paper in Physical Review B60, pp. 1563-1572, 1999). *Over the last three years, the director of the Academy authored or co-authored twenty (20) refereed publications in physics and eleven (11) scholarly publications on the creation of educational value-added and on mentoring.* Over the last three years, the Academy director made *fifty-five (55) presentations*, twenty-three (23) of which were devoted to mentoring, with one (1) international, eleven (11) national, and seven (7) statewide presentations.

Direct Results: Educational Services Rendered to the Pre-college Community and Others

The Timbuktu Academy reaches over 5,000 pre-college and college students, teachers, parents and others, per year, with printed materials, motivational speeches, workshops, etc. The following table shows the number of pre-college students *directly and significantly* affected by the summer programs (SSI-M, SETA, SSI, Challenge, and SBI) of the Timbuktu Academy. (The Learning Olympiads/Saturday Academies are year round.)

Summer Pre-College Program Participants of the Timbuktu Academy (TA)

Program	1994	1995	1996	1997	1998	1999	2000	2001	Total
Getting Smart at the TA-GesTA	--	--	--	--	--	--	20	34	**54**
Summer Science Institute–Mid. School-SSI-M	39	40	80	80	70	60	63	100	**532**
Summer Enrich. At the TA-SETA	0	0	0	24	22	18	27	20	**111**
Summer Science Institute (SSI)	40	53	39	23	21	19	20	8	**223**
Challenge 2000 at the TA	--	--	--	20	19	22	23	27	**111**
Earth Science at the TA-ESTA	--	--	--	--	--	28	21	13	**62**
Summer Bridge Institute (SBI)	25	25	24	13	14	13	19	13	**146**
GRAND TOTAL									**1239**

The *average increase in ACT scores,* as attributable only to the summer programs, ranged from 2.5 to 3.0 points from the summer of 1994 to the summer of 1997. Building upon our acquired expertise in creating educational value added, we made appropriate changes to the 1998 summer programs and increased the English practice time. For that summer (1998), we had increases in the ACT English and composite score of five (5) and four (4) points, respectively. *These quantum leaps were directly caused, for the most part, by the six-week, residential, academic enrichment program of the Timbuktu Academy (i.e., SSI and Challenge 2000).*

Academic Excellence by Design: National Merit/National Achievement Scholars

The Timbuktu Academy helped to produce an average of five (5) National Merit/National Achievement Finalists in 1998 and in 1999. In 2000, it helped to produce **ten (10)** National Merit/National Achievement Finalists. In 2001, the Timbuktu Academy helped to produce **eleven (11)** National Merit/National Achievement Semifinalists. Please see the approach described above to for the clear-road map that led to this feat.

Direct Results: Outcomes of Systemic Mentoring Activities for 50-100 Undergraduate Scholars

Summer Research	**1994**	**1995**	**1996**	**1997**	**1998**	**1999**	**2000**	**2001**	**Totals**
No. of Scholars Placed	18	21	28	40	43	47	39	50	286*
Number of Research Sites	6	12	20	32	33	32	22	32	189*

*Not necessarily distinct students or research sites

Conference Participation	**1994**	**1995**	**1996**	**1997**	**1998**	**1999**	**2000**	**2001**	**Totals**
Number of conferences	5	8	10	9	5	6	5	6	54
No. of student attendees	58*	34*	126*	67*	11	65*	97*	89*	547*
No. of student presentations	12*	5	9	14*	0	1	3	16*	60*

*Not necessarily distinct students as some students attend more than one conference.

Description	**1994**	**1995**	**1996**	**1997**	**1998**	**1999**	**2000**	**2001**	**Totals**
Physics Alumni	12*	6	10	8	10	8	4	5	63
Enrolled in/ finished Grad. Sch	11	3	8	7	8	6	1	5	49
Chemistry Alumni	--	--	3	2	6	5	2	1	19
Enrolled/completed graduate school	--	--	2	0	5	2	0	1	10
Engineering Alumni	2	1	1	2	5	7	4	2	24
Enrolled/completed graduate school	0	0	0	1	3	2	1	2	9

**Includes 1992 and 1993 graduates*

-- Not Applicable, Chemistry students were admitted into the Academy starting in 1993-94.

SEM Infrastructure Development Activities and Results

Previous reports provided detailed information on the infrastructure Development activities of the Timbuktu Academy and on related results at the departmental, university, state, and national levels. While we avoid reiterating these accomplishments, their summary listing provided below.

- *A dramatic increase in the number and the quality of students majoring in physics and in other SEM disciplines; over 25% increase in the Graduate Record Examination scores of physics graduates.*
- *Significant and positive impact on student retention rate, on time graduation rate, and graduate school going and success rates.*
- *The establishment of the MS degree in program in Physics in the fall of 1996 was made possible by the above increased enrollment at the undergraduate level and the high quality of the scholars.*
- *Institution-wide and Statewide Replication of the Timbuktu Academy by the Louis Stokes Louisiana Alliance for Minority Participation.*
- *Development of partnerships and collaborations with federal, industrial, and university laboratories.*

SIGNIFICANCE: Our research findings have far-reaching applications for creating educational value-added and (b) for predictive calculations of properties of materials. The Timbuktu Academy has made significant contributions to meeting the technical and research personnel need of this country. It also added measurably to the knowledge base not only in theoretical condensed matter physics but also in education.

PATENT INFORMATION: None (Not quite applicable for a formalism)

AWARD INFORMATION

- In the fall of 1999, Dr. Diola Bagayoko, the Director of the Timbuktu Academy, was appointed Southern University System Distinguished Professor of Physics. He is currently the only one with this title.
- As noted in previous report, Dr. Diola Bagayoko received **one of the first US Presidential Awards for Excellence in Science, Mathematics, and Engineering Mentoring (US-PAESMEM) in 1996.** Previous reports also noted the that the Timbuktu Academy won the Quality Education for Minority (QEM) Network's ***National Exemplary Mathematics, Science and Engineering Undergraduate Program Award*** *in 1996.*
- The Timbuktu Academy scholars (from middle school to graduate school) have won more scholastic awards, internships, graduate fellowships, etc. than we have space to list. Please visit the web site of the Academy for details or contact the Academy.

PUBLICATIONS

Twenty (20) Refereed Publications in Theoretical Physics (1999-7/2001) [6 illustrative ones are below]
These publications are included in an attachment to this final report. The 22 physics publications, from 1993 to 1998, were submitted in an attachment to the fall, 1998 report.

1. *"Ab-Initio Description and Prediction of Properties of Carbon-Based and Other Non-Metallic Materials."* D. Bagayoko, G. L. Zhao, and S. Hasan. Proceedings of the Sixth Applied Diamond Conference/Second Frontier Carbon Technology Conference (ADC/FCT) 2001, Auburn University, August 4-8, 2001. Pages 544-549, 2001. ISBN# 0-9710327-0-X, NASA/CP-2001-210948.
2. "*Predicted Electronic Properties of Cubic Silicon Nitride (c-Si_3N_4)*, D. Bagayoko and G. L. Zhao. Accepted for Publi. in Physica C, 2001.
3. "Predictive Ab-Initio Computations of Properties of Ferroelectric Materials." D. Bagayoko and G. L. Zhao, International Journal of Modern Physics B Vol.13 Nos. 29, 30 & 31, pp 3767-3773, 1999.
4. *"Ab-Initio Calculations of Superconducting Properties of $YBa_2Cu_3O_7$."* G. L. Zhao and D. Bagayoko, International Journal of Modern Physics B Vol. Nos.29, 30 & 31 pp. 3579-3581, 1999.
5. *"Electronic Structure and Charge Transfer in 3C- and 4H-SiC,"* G. L. Zhao and D. Bagayoko. New Journal of Physics 2, 2000, 16.1-16.12. entirely available on the web, free of charge.
6. *"Local-Density-Functional Prediction of Electronic Properties of GaN, Si, C, and RuO_2"* G. L. Zhao, D. Bagayoko, and T. D. Williams. Physical Review B60, 1563, 1999.

Eleven (11) Scholarly Publications on Mentoring, Teaching, and Learning From 1999 to 2001 [4 illustrative ones are listed below]

1. *"The Law of Performance and the Excellence in Research."* D. Bagayoko. Proceedings of the 15th Annual High Technology Student Expo of the National Association for Equal Opportunity (NAFEO) in Higher Education, 2001.
2. October 18, 2000. Recording of a 30 Minute Video Tape on *"A Rosetta Stone for Competitive Education."* This media publication (Video Tape) has been shown in the fall of 2000 for a full month, several times per week, so as to reach 99% of Louisiana households. Audience: tens of thousands.
3. *"A Problem Solving Paradigm,"* D. Bagayoko, Saleem Hasan, and Ella L. Kelley. College Teaching, Vol. 48, No. 1, pp. 24-27, 2000.
4. *"Misconceptions and the Certainty of Response Index (CRI),"* Saleem Hasan, D. Bagayoko, & Ella L. Kelley. Phys. Education (UK) 34 (5), pp. 294-299, 1999.

PRESENTATIONS

Fifty five (55) were presentations on theoretical physics, teaching, mentoring from 1999 to 2001. Twenty three (23) were on mentoring with one(1) international, eleven (11) national, and seven (7) statewide presentations.

SOUTHERN UNIVERSITY And Agricultural & Mechanical College

THE TIMBUKTU ACADEMY
P. O. BOX 11776

MATTER - ENERGY FUNDAMENTAL TIMBUKTUACADEMY 1990 INTERACTION(S) SPACE - TIME

DEPARTMENT OF PHYSICS
Southern University and A&M College
Baton Rouge, Louisiana 70813

Telephone: (225) 771-2730 Fax: (225) 771-4341

http://www.phys.subr.edu/timbuktu.htm
bagayoko@aol.com

Diola Bagayoko, Ph.D., Director
bagayoko@phys.subr.edu

MEMORANDUM

TO: Dr. Laura Petonito
Office of Naval Research

FROM: Diola Bagayoko Ph.D. Bagayoko
Southern University System Distinguished Professor of Physics

DATE: October 2, 2001

SUBJECT: Progress Report for Grant No. N00014-98-1-0748: SEM-Timbuktu Academy

This communication comes to submit to you the progress report of the Timbuktu Academy pursuant to the significant and long term funding afforded to it by the Department of the Navy, Office of Naval Research. This report cumulatively addresses the period from the fall of 1998 to the end of the summer of 2001.

The report is in accordance with the guidelines previously provided to us by the Department of the Navy, Office of Naval Research. Consequently, the narrative portion of the report is limited to four (4) pages as required by the guidelines. An attachment provides a complete listing of the thirty-one (31) publications made in the last three years (1999-2001) and full copies of eighteen (18) of these publications.

Copies of the report have been distributed in accordance with the aforementioned guidelines as confirmed by my recent conversation with you. Specifically, the following offices or individuals were sent a copy: the Director of the Naval Research Laboratory (NRL), Mr. Anthony Junior, the Atlanta Office of ONR, and the Defense Technical Information Center (DTIC).

I would like to take this opportunity to thank you and your colleagues at ONR for the long-standing funding and support. We hope that this report attests to the wisdom of the investment made in the Science, Engineering, and Mathematics (SEM) at the Timbuktu Academy.

xc: Dr. Mildred R. Smalley, Vice Chancellor for Research
Southern University and A & M College, Baton Rouge, Louisiana

LIST OF PUBLICATIONS (from 1999 to 2001)
Progress Report of Grant No. N00014-98-1-0748
SEM Timbuktu Academy, Southern University and A&M college
Baton Rouge, Louisiana 70813
Project Director: D. Bagayoko (bagayoko@aol.com)

Twenty (20) Refereed Publications in Condensed Matter Theory (1999-7/2001)

1. *"Electronic Structure, Charge Transfer, and Optical Properties of Magnesium Diboride."* D. Bagayoko and G. L. Zhao. To be submitted to the New Journal of Physics.

✓2. *"Ab-Initio Description and Prediction of Properties of Carbon-Based and Other Non-Metallic Materials."* D. Bagayoko, G. L. Zhao, and S. Hasan. Proceedings of the Sixth Applied Diamond Conference/Second Frontier Carbon Technology Conference (ADC/FCT) 2001, Auburn University, August 4-8, 2001. Pages 544-549, 2001. ISBN# 0-9710327-0-X, NASA/CP-2001-210948.

✓3. *"The Band-Gap and Optical Absorption Edge of Wurtzite AlN,"* Y. X. Lou, G. L. Zhao, and D. Bagayoko. To be submitted to the New Jour. in Physics, 2001.

4. *"Superconducting Gap Symmetry from Repulsive Interaction in a Spin Singlet Channel,"* Yuri Malozovsky, J. D. Fan, and D. Bagayoko. Accepted for Publication in Physica C, 2001.

5. *"Predicted Electronic Properties of Cubic Silicon Nitride (c-Si_3N_4)*, D. Bagayoko and G. L. Zhao. Accepted for Publication in Physica C, 2001.

6. *"Anomalous Isotope Effect in Narrow Band Superconductors."* G. L. Zhao and D. Bagayoko. Accepted for Publication in Physica C, 2001.

✓7. *"The BZW Method and Calculations of Electronic and Related Properties of Zinc Oxide (ZnO)."* D. Bagayoko and G. L. Zhao. To be submitted to the New Journal of Physics (UK).

8. "Temperature Dependence of the Anisotropic Gap in Yba$_2$Cu$_3$O$_7$," G. L. Zhao and D. Bagayoko, Physica C 341-348,161-162, 2000.

8. *"Electronic Structure and Fermi Surface of CrO_2,"* N. E. Brener, J. M. Tyler, J. Callaway, D. Bagayoko, and G. L. Zhao, Physical Review B61, No. 24, 16582-16588, 2000.

✓10. *Description et Prédiction des Propriétées Electroniques des Matériaux."* D. Bagayoko, Refereed Proceedings, Fist Mali Symposium on Applied Sciences (MSAS). University of Mali, Bamako, Mali, West Africa.. Pages 185-192. Editor: Dr. Seydou Fad; Publisher: Oulu University Press, 2001. ISBN: 951-42-6403-7.

11. *"Predicted Electronic and Related Properties of Cubic Silicon Nitride (c-Si_3N_4)."* D. Bagayoko and G. L. Zhao. Accepted for Publ.in the Physica C, 2001.

✓12. *"Polaronic Effect in Materials with Ferroelectric Phase Transitions."* Y. M. Malozovsky, J.D. Fan, D. Bagayoko and J. T. Wang International Journal of Modern Physics B, Nos. 29, 30 & 31, pp. 3555- 3559, 1999.

✓13. *"How can an Atom or Ion Remember its Initial State?"* J. T. Wang, F. Tang, and D. Bagayoko, International Journal of Modern Physics B, Vol. 13, Nos. 29, 30, 31, pp. 3830-3834, 1999.

✓14. *"Predictive Ab-Initio Computations of Properties of Ferroelectric Materials." D. Bagayoko and G. L. Zhao, International Journal of Modern Physics B Vol.13 Nos. 29, 30 & 31, pp 3767-3773, 1999.*

15. *"Ab-Initio Calculations of Superconducting Properties of $YBa_2Cu_3O_7$."* G. L. Zhao and D. Bagayoko, International Journal of Modern Physics B Vol. Nos.29, 30 & 31 pp. 3579-3581, 1999.

Dup 16. *"Ab-initio Calculations for the Superconducting Properties of Yba2Cu3O7"*, G. L. Zhao and D. Bagayoko. The International Journal of Modern Physics B Vol.13, Nos. 29-31, pages 3579-3581 (1999).

✓17. *"Electronic Structure and Charge Transfer in 3C- and 4H-SiC,"* G. L. Zhao and D. Bagayoko. New Journal of Physics 2, 2000, 16.1-16.12. entirely available on the web, free of charge.

18. *"Predictive Calculations of Properties of Molecules, Clusters, and Semiconductors,"* D. Bagayoko, G. L. Zhao, and Troy D. Williams. Proceedings, 1999 Meeting of the National Society of Black Physicists (NSBP '99), Atlanta, Georgia, March 21 (1999).

19. *"Local-Density-Functional Prediction of Electronic Properties of GaN, Si, C, and RuO_2"* G. L. Zhao, D. Bagayoko, and T. D. Williams. Physical Review B60, 1563, 1999.

20. *"Monte-Carlo Simulation of Coarsening in a Model of Submonolayer Epitaxial Growth"* Pui-Man Lam, Diola Bagayoko and Isiaka Aknabi, Physical Review B59, 5871 (1999).

Eleven (11) Scholarly Publications on Mentoring, Teaching, and Learning (including refereed ones)

1. *"Correlations Between the Global Learning and Observations to Benefit the Environment (GLOBE)and the Louisiana Science Content Standards."* D. Bagayoko and Deborah Muhammad. A 37 page book published by the Timbuktu Academy. Printed in Baton Rouge, Louisiana, USA. ISBN# 0-9704609-8-8.

2. *"The Law of Performance and the Excellence in Research."* D. Bagayoko. Accepted for Publication in the Proceedings of the 15th Annual High Technology Student Expo of the National Association for Equal Opportunity (NAFEO) in Higher Education, 2001.

3. October 18, 2000. Recording of a 30 Minute Video Tape on *"A Rosetta Stone for Competitive Education."* This media publication (Video Tape), has been shown in the fall of 2000 for a full month, several times per week, so as to reach 99% of Louisiana households. Estimated audience in tens of thousands.

4. *"Le Montage ou developpement de Projets Sponsorisés," D. Bagayoko and M. Diarra,* Refereed Proceedings, First Mali Symposium on Applied Sciences. University of Mali, Bamako, Mali, West Africa.. Pages 185-192. Editor: Dr. Seydou Fad; Publisher: Oulu University Press, 2001. ISBN: 951-42-6403-7.

5. *"A Problem Solving Paradigm,"* D. Bagayoko, Saleem Hasan, and Ella L. Kelley. College Teaching, Vol. 48, No. 1, pp. 24-27, 2000.

6. *"Misconceptions and the Certainty of Response Index (CRI),"* Saleem Hasan, D. Bagayoko, & Ella L. Kelley. Phys. Education (UK) 34 (5), pp. 294-299, 1999.

7. August 9, 2000. One hour video recording on *"The Genesis of Genius."* This media publication (video tape) has been shown in the fall of 2000 for a full month, several times per week, so as to reach 99% of Louisiana households. Estimated audience in tens of thousands.

8. *"Expanding GLOBE Participation: An Emerging Model for Diversification."* Robert L. Ford and Diola Bagayoko, International Conference of the Global Learning and Observations to Benefit the Environment (GLOBE), Annapolis, Maryland, July 19, 2000.

9. *"Avoiding or Closing the Academic Achievement Gap."* D. Bagayoko, S. Hasan, and R. L. Ford, Department of Energy and Louis Stokes Louisiana Alliance for Minority Participation (LS-LAMP) Annual Conference, February 12, 2001, Radisson Hotel, New Orleans, Louisiana. ISBN No. 0-970460-4-5.

10. *"Fundamentals of Mentoring and Networking."* D. Bagayoko, Robert L. Ford, and Ella L. Kelley; a chapter in a monograph entitled "Scholarly Guideposts for Junior Faculty Members," Published by Quality Education for Minority (QEM) Network. Washington, D.C., February, 2000.

11. "Perspective of a US Presidential Awardee on Workforce Development." US Science, Engineering, and Technology Workforce of the Future: National Strategy, National Portfolio, National Resource Base. Publication Number: NSF 99-132.

International Journal of Modern Physics B Vol. 13 Nos. 29, 30 & 31 (1999) 3579–3581

AB-INITIO CALCULATIONS OF SUPERCONDUCTING PROPERTIES OF $YBa_2Cu_3O_7$

G. L. ZHAO and D. BAGAYOKO
Physics Department, Southern University and A & M College,
Baton Rouge, Louisiana 70813 USA

Received (31 May 1999)
Revised ()

We present ab-initio calculations for the electronic structure and superconducting properties of $YBa_2Cu_3O_7$ (YBCO). The electronic structure was calculated using a self-consistent ab-initio LCAO method. We solved the anisotropic Eliashberg gap equation numerically. The strong coupling of the high energy optical phonons around 60 - 73 meV, with the electrons at the Fermi surface, leads to a high T_c in YBCO. The calculated T_c is about 89 K for $\mu^* = 0.1$. The good agreement of the calculated results with experimental measurements and the ab-initio nature of the calculations support the scenario of an anisotropic s-wave superconductor for YBCO.

Because of the complexity of the material structures, the condition of the surfaces of the ceramic samples and the strong anisotropy, the experimental results for high T_c cuprates, including $YBa_2Cu_3O_7$ (YBCO), are far more difficult to understand than that of the conventional low T_c superconductors of simple structures.[1] As a result, it has been difficult to provide experimental confirmation for any of the large number of theoretical models that have been proposed to explain these materials. It is our view that many experimental results cannot be understood without careful and reliable ab-initio calculations to account for the complex electron structures as well as a realistic electron-phonon coupling effect and the large number of phonon modes in these materials.

Ab-initio calculations for the superconducting properties of high T_c cuprates are very difficult task. Such studies require reliable ab-initio computations for the electronic structure (including the electron energy levels and the wave functions), the phonon properties (including the phonon frequencies and the eigen-vectors), and the electron-phonon coupling matrix elements. Ultimately, we need to solve the anisotropic Eliashberg gap equations, which are the basis for the calculations of T_c and the superconducting gap functions.

Through the effort of Zhao, Callaway, Browne, and Bagayoko, some substantial progress has been achieved.[2,3,4] We used a self-consistent ab-initio linear-combination-of-atomic-orbitals (LCAO) method to calculate the electronic structure of YBCO. This method has been tested by others and found to give results whose accuracy is comparable to that obtained using other ab-initio methods.[5,6,7,8,9] We employ the phonon dispersions and eigenvectors from a shell-model calculation employing parameters determined by Humlicek et al[10] from a fitting to the observed Raman spectrum, infrared data, and inelastic neutron scattering results. The electron-phonon interaction matrix elements for YBCO are calculated using a non-orthogonal tight-binding method.[3] The non-orthogonal tight-binding method has been used by Zhao and Harmon[9] to predict the phonon anomalies in β-phase NiAl along the [100] and [111] directions. The predicted phonon anomalies in NiAl have been confirmed by inelastic neutron scattering measurements.[11]

We followed the well-established strong-coupling (Eliashberg) theory in calculating T_c and the gap function.[12,13] In these calculations, we only considered the case that pairing occurs between electrons in states with opposite linear momentum and opposite spins. Then, the total angular momentum for the pairing electrons is $\vec{J} = 0$. A full consideration of anisotropy is allowed throughout the calculations. Therefore, we only calculated a case in which the pairing electrons are in an anisotropic s-wave state.

In the following, we summarize the major results from our calculations for YBCO.

(i). Our calculated electronic structure for YBCO agrees with other ab-initio computations. In particular, the calculated Fermi surface for YBCO agrees well with photoemission measurements.[14]

(ii). We have calculated the superconducting transition temperature T_c using the anisotropic Eliashberg equations on the imaginary axis. The calculated T_c for YBCO is about 89 K for $\mu^* = 0.1$. This calculated T_c is very close to experimental observations.

(iii). The smallness of the isotope effect in YBCO could be understood when calculations include the electron-phonon interactions that are not limited to the Fermi surface, but are within the phonon energy near the Fermi surface. The optical phonon energies (up to 80 meV) in YBCO are not small, as compared to the energy scale on which the electron band structure varies significantly. Especially, the narrow bands near E_f can make a very significant contribution to the interaction.

(iv). Our calculation found that the phonons with an energy near about 60-73 meV have a strong interaction with the electrons around the Fermi surface. This finding is consistent with the experimental results of a strong instability for the phonons in the same energy range.[15]

(v). We obtained the superconducting gap function for YBCO by solving the temperature-dependent Eliashberg gap equation on the real axis for an anisotropic superconductor. The calculated superconducting gap clearly shows a strong anisotropy on the Fermi surface, but without nodes. The superconducting gap does not change much along k_z (or c) direction. We associate this property with the approximate two-dimensional nature of the material.[2] Carefully examining the electronic structure of YBCO, we found that the narrow-band electronic states are associated with large gaps.

(vi). From the calculated gap function for YBCO, we further calculated the quasiparticle spectrum and compared with experimental results. We found that the quasiparticle spectrum is strongly momentum and band dependent. The broad structure in the tunneling spectrum[16] for YBCO is due to a large variation of the pairing gap function.

In conclusion, we have performed ab-initio computations for the superconducting properties of YBCO based on density functional theory for the electronic structure and the strong-coupling Eliashberg theory for anisotropic superconductors. The good agreement of the calculated results with experimental measurements and the ab-initio nature of the theoretical calculation support the scenario of an anisotropic s-wave superconductor for YBCO. Other experimental results claimed as evidence for *d*-wave pairing[17,18] in YBCO should be reexamined to see if they can be explained with an anisotropic *s*-wave pairing state.

Acknowledgements

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The Band-Gap and Optical Absorption Edge of Wurtzite AlN

Y. X. Lou, G. L. Zhao, and D. Bagayoko

Department of Physics, Southern University and A & M College

Baton Rouge, Louisiana 70813

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Abstract

We employed the recently developed, ab-initio, Bagayoko-Zhao-Williams (BZW) method to calculate the electronic structure of AlN, including the optical absorption edge. We employed a local density potential and the linear combination of atomic orbitals (LCAO) formalism. Our calculated principal absorption edge agrees with experimental measurements. We found that the tail structure near the principal absorption edge, which was frequently ascribed to sample contaminations, is partly due to the intrinsic properties of the low energy conduction band of AlN.

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I. INTRODUCTION

III-V nitride semiconductor AlN, along with GaN, attracted an extensive interest in recent years. The large band-gap energy of the material makes it suitable for applications in electronic and optic devices in short wavelength regions.[1–3] Substantial efforts in experimental and theoretical studies have been made to understand the electronic, optical, and structural properties of this important group of materials and considerable progress has been achieved in the last several years.[1–7] However, there remain some questions regarding the understanding of the optical absorption edge of AlN and related problems. The interpretations of the experimentally measured results of the optical absorption spectra led to a wide range of conclusions. Optical experiments identified the band-gap energy of AlN to be in a range from 3.9 to 6.2 eV.[3,5–7] The aim of this report is to address the issue of the electronic structure and the optical absorption edge of AlN, using ab-initio computations that employed the Bagayoko, Zhao, and Williams (BZW) procedure. Recently, we have applied the BZW procedure to calculate the electronic structures and the optical properties of wurtzite GaN, Si, diamond, 3C and 4H-SiC, and ferroelectric semiconductor BaTiO3.[8–10] Our calculated electronic and optical properties of semiconductors, including the band gaps, agree well with experimental results. This agreement partly suggested our current study of AlN for which there are outstanding issues relative to the optical absorption edge and the band gap.

II. COMPUTATION DETAILS

Our computational method has been discussed in some recent publications.[8,9] We utilized density functional theory and the linear combination of atomic orbital (LCAO) formalism for the self-consistent ab-initio calculation of the electronic structure of wurtzite AlN.[11,12] We employed the Ceperley-Alder[13] local density functional potential as parameterized by Vosko, Wilk, and Nusair,[14] to describe the exchange-correlation interaction of the many-body electron system. We utilized the newly developed BZW procedure[8,9] throughout the calculations. A description of the BZW procedure has been presented in previous publications.[8–10] Our calculations are non-relativistic.

The ground-state structure of AlN is wurtzite. There are four atoms in its unit cell in a hexagonal lattice. The two Al atoms are in (0, 0, 0) and (1/3, 2/3, 1/2), and the two N atoms are in (0, 0, u) and (1/3, 2/3, 1/2+u), where $u = 0.385$ is the dimensionless internal parameter. The lattice constants a and c used in our calculations are 3.11 and 4.98 $\AA$, respectively.

We began the calculation with self-consistent, ab-initio computations for the atomic wave functions of neutral Al and N atoms. The radial parts of the atomic wave functions were expanded in terms of Gaussian functions. A set of even tempered Gaussian exponents was employed with a minimum of 0.12 and a maximum of 0.15×10^6, in atomic unit. In the calculation of atomic orbitals of Al and N, we employed the BZW procedure. The calculated energy levels of the occupied electron states of Al and N were converged to the order of 1 mRy.

We then performed self-consistent calculations for wurtzite AlN and obtained an estimate of the charge transfer to be Al^{2+} and N^{2-}. Gabe et al[1,15] used x-ray techniques to measure the AlN valency and obtained a value of -1.8±0.8e which agrees well with our calculated charge transfer of AlN. We subsequently performed self-consistent calculations for free Al^{2+} and N^{2-} ions to obtain the atomic functions that served as the input for the solid state calculations.

In the self-consistent calculations of the electronic structure of wurtzite AlN, we took the Al(1s) and N(1s) as the core states. Other states such as Al(2s3s 2p3p) and N(2s3s 2p) are included as valence states in the self-consistent calculations. We used 60 k-points with proper weights in the irreducible Brillouin zone in the self-consistent calculations. The computational error for the valence charge was about 0.007 for 32 electrons. The computation for the exchange-correlation potentials was done in real space with a mesh of points around each of the atoms. The numbers of mesh points per atomic site varied from 6736 to 6758, depending on the local structure of the atom. The self-consistent potentials converged to a difference around 10^{-5} after about sixty iterations. The total number of iterations varies with the input potentials.

III. RESULTS

We present the calculated electronic band structure of wurtzite AlN in Fig. 1, where the Γ, K, H, A, M, and L are the high symmetry points in the Brillouin zone. The zero of the energy is set at the top of the valence band. The low energy bands from -16 to -12 eV are mainly attributed to the nitrogen 2s levels. They are separated from the upper bands that are mainly the contribution of nitrogen 2p and aluminum 3s and 3p states. The calculated band structure in Fig. 1 indicates that AlN has a direct band gap occurring at the Γ point with a theoretical minimum value of 5.5 eV.

We have calculated the effective electron mass of AlN. The effective mass is a measure of the curvature of the electron energy bands. The effective mass of the n-type carriers near the Γ-point shows a moderate anisotropy. The calculated effective masses of the n-type carriers of AlN are 0.26 m_0 in the c-direction and 0.30 m_0 in the direction perpendicular to the c-direction. The average effective masses of the n-type carriers is 0.28 m_0. Here m_0 is the free electron mass. Our calculated effective mass of the n-type carriers agree well with the reported values by Suzuki et al.[16]

We present the calculated total density of states (DOS) of wurtzite AlN in Fig. 2. The zero of the energy is again set at the top of the valence band. The occupied valence bands arise mainly from the nitrogen p-states with a minor contribution from aluminum s- and p-states. The low energy conduction bands have a dominant contribution from aluminum s- and p-states. Noteworthily, the density of states of the conduction bands has a long tail in the low energy region. The inset of Fig. 2 presents a fine structure of the tail of the density of states around the top of the valence band and the bottom of the conduction band. The diminutively low density of states of the low energy conduction band leads to a tail structure in the optical absorption spectrum as observed experimentally. Previously, the tail structure of the optical absorption spectrum was frequently ascribed to the effects of sample contaminations. A large band-gap of 6.2 eV was derived from some optical measurements.[7,5] Our calculated electronic structure of AlN shows the need to re-examine the previous interpretation of some experimental results from the optical measurements.

For a semi-quantitative discussion of the dependence of the absorption spectra on the electronic structure, we calculated the joint density of states (JDOS) as follows.

$$J(\nu) = \sum_{\epsilon_1,\epsilon_2} \rho_v(\epsilon_1)\rho_c(\epsilon_2)\delta(\epsilon_2 - \epsilon_1 - h\nu) \tag{1}$$

where $\rho_v(\epsilon_1)$ is the DOS of the valence bands at energy ϵ_1; $\rho_c(\epsilon_2)$ refers to the DOS of the conduction bands at energy ϵ_2; the δ-function ensures the energy conservation law. The summation includes all possible transitions.

The transitional probabilities of the optical excitations strongly depend on the joint density of states, in addition to the transition matrix elements. Within the assumption of slowly varying transition matrix elements, in a narrow region near the absorption edge, the JDOS provides a picture of the absorption spectrum. We present the calculated JDOS of AlN near the principal absorption edge in Fig. 3. The joint density of states in Fig. 3 is in a unit of $(1/eV^3)$. The inset of Fig. 3 clearly shows a sharp increase of the JDOS near 6.2 eV and a tail from 5.5 eV to 6.2 eV. Our calculated properties of the JDOS of AlN is similar to the experimentally measured spectrum of the optical absorption.[5–7] We previously introduced the concept of "practical band gap" to describe semiconductors in which the lowest lying conduction band has a strong parabolic feature. The parabolic nature of this lowest lying conduction band results in effective masses of n-type carriers significantly less than the free electron mass (i.e., an average of 0.28 m_0 for AIN). This feature of semiconductors leads to discrepancies between experimental values of the band gaps, particularly when they are determined by optical means. Indeed, the reported experimental values depend not only on the sensitivity of measurement devices but also on the quality of the samples and of subsequent analytic interpretations. Hence, the electron band structure in Fig. 1, the DOS in Fig. 2, and the JDOS in Fig. 3 illustrate the reason that measured band gaps of AlN fall in the wide range from 5.5 to 6.2 eV. While features near the optical absorption edge of AlN, at energies up to 5.5 eV, are likely due to sample contaminations[1,5,7], the above discussion ascribes the tail from 5.5 eV to 6.2 eV to intrinsic properties of AlN.

IV. CONCLUSION

We have calculated the electronic structure and the optical properties of AlN near the principal absorption edge. Our calculated electron bands of AlN indicates a theoretical band-gap to be 5.5 eV. The calculated effective mass of the n-type carriers near the Γ-point shows a moderate anisotropy. The average effective mass of the electrons is 0.27 m_0. Our calculated density of states and the joint density of states identify the "practical" band-gap of wurtzite AlN to be from 5.5 to 6.2 eV. Our calculated results suggest that the tail structure near the principal absorption edge, which was frequently ascribed to sample contaminations, is partly due to the intrinsic properties of the low energy conduction band of AlN.

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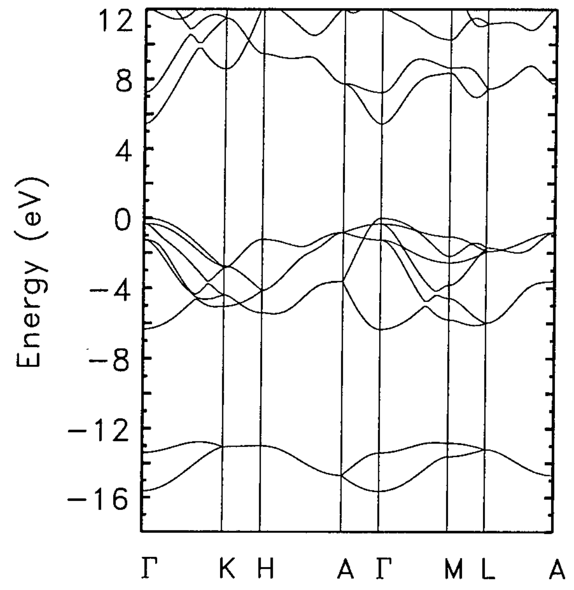

FIG. 1. The calculated electronic energy bands of wurtzite AlN along the high symmetry directions, as obtained with the optimal basis set of the BZW method.

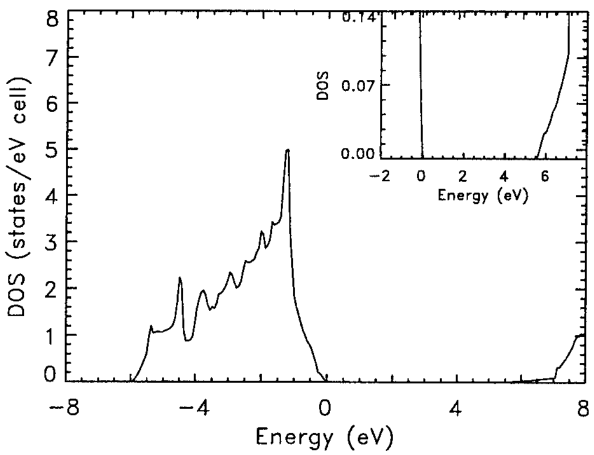

FIG. 2. The calculated total density of states of wurtzite AlN. The inset shows the fine structure of the tail of the density of states around the top of the valence band and the bottom of the conduction band.

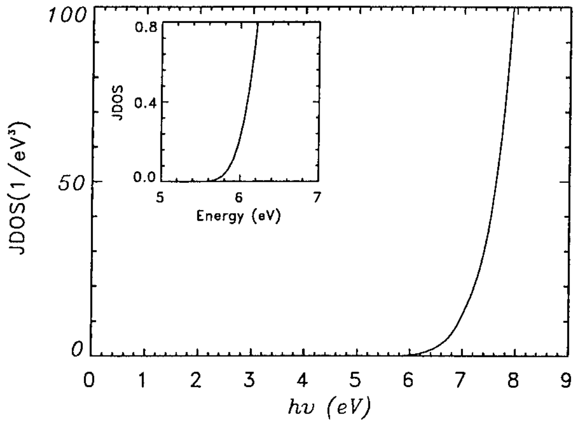

FIG. 3. The calculated joint density of states of wurtzite AlN, as defined in Equation (1). The inset of the figure clearly shows a sharp increase of the JDOS near 6.2 eV and a tail that extends to the lower energy of 5.5 eV.

The BZW Method and Calculation for the Electronic and Related Properties of ZnO

D. Bagayoko and G. L. Zhao
Department of Physics, Southern University and A & M College
Baton Rouge, Louisiana 70813

ABSTRACT

We used the newly developed BZW method to calculate the electronic and structural properties of ZnO. With optimal basis set as per the BZW method, we found the theoretical minimum band-gap of ZnO to be 3.2 eV. The calculated effective masses of the n-type carriers, near the bottom of the conduction band at the Γ point, is $0.26\pm0.02m_0$. The calculated total energy curves yield the theoretical lattice constants a and c to be 3.27 ± 0.02 $\AA$ and 5.18 ± 0.02 $\AA$, respectively. The calculated internal parameter u of hexagonal ZnO is 0.381 ± 0.002. The calculated charge transfer leads to the ionic formula of ZnO as $Zn^{1.8+}O^{1.8-}$. Our calculated results agree well with experimentally measured data.

I. Introduction

Ab-initio density functional computations are well established at present as a very powerful tool to study properties of materials, including semiconductors, metals, surfaces, interfaces, and others.[1, 2, 3, 4, 5, 6, 7] However, previous density functional calculations in local density approximation (LDA) for semiconductors or insulators often underestimated the band-gaps by 30-50 %. Closely related to the band-gap problem, the calculated low energy conduction bands and optical properties of semiconductors –from previous LDA computations– also disagree with experimental results. In the cases of previous LDA calculations for ZnO, the theoretical band structures found a nearly closed band gaps,[8, 6, 9] contrary to experimental results. There have been some theoretical efforts intended to address these issues, including calculations that utilize nonlocal, energy-dependent, non-Hermitian self-energy operators.[10, 11, 12, 13] Aryasetiawan and Gunnarson reviewed several computational approaches, including the GW method, aimed at describing excited state properties.[14]. Johnson and Ashcroft utilized some simplified applications of the GW method to make scissors-type corrections to the band gaps of semiconductors.[15]

In previous publications,[16, 17, 18] Bagayoko et al introduced a new ab-initio computational method based on mathematical properties of variational calculations of the Rayleigh-Ritz type. In this article, we report the calculated electronic and related properties of ZnO, as obtained by applying the Bagayoko, Zhao, and Williams (BZW) procedure. We found electronic and structural properties of ZnO that agree well with experimental results. In the next section, we summarize our computational method. The calculated results are presented in Section III. They are followed by a short conclusion in Section IV.

II. Method

Our ab-initio calculations utilized the linear combination of atomic orbital (LCAO) method. These self-consistent LCAO calculations included all electrons and full potentials, without shape approximations. Details of the general computational method are available in previous publications.[5, 19, 20] We employed the Ceperley-Alder local density potential[21] of the local density functional potential as parameterized by Vosko, Wilk, and Nusair[22]. The newly developed BZW procedure[16, 17, 18] is employed throughout the calculations.

The BZW method utilized the criterion, which is derived from the theory of variational calculation as discussed in previous publications, to identify the optimal basis set in ab-initio, LCAO calculations. Essentially, this procedure requires the performance of three or more self-consistent calculations, beginning with the minimal basis set. The minimal basis set is that required to account for all the electrons of the atomic or ionic species in a material (molecules, clusters, or solids). Every subsequent calculation is carried out with a basis set including that for the previous calculation plus one (or more) orbital of the atomic or ionic species that are present in the material under study. These orbitals are added in the order of increasing energy. Several self-consistent calculations are done until the energies of the occupied states, for calculation N, are the same as those for calculation (N+1). Then, the material is studied using the basis set from calculation N, known as the optimal basis set. Physically, the BZW procedure defines a new form of convergence, i.e., that of the occupied states (or charge density) with respect to the size of the basis set.

ZnO (or zincite) possesses a hexagonal lattice in the space group C_{6v}^4. The experimentally measured lattice constants at room temperature are $a = 3.249 - 3.253\AA$, and $c = 5.207 - 5.213\AA$, respectively.[23, 24] There are four atoms per unit cell, in the (2b) positions as following. Zn: (0, 0, 0), (1/3, 2/3, 1/2); O: (0, 0, u), (1/3, 2/3, 1/2 + u).

In our LCAO calculations, the atomic orbitals of Zn and O are constructed from results of ab-initio atomic computations. In the first step of the calculations for ZnO, the wave functions of the atomic orbitals for Zn and O atoms in the neutral state are calculated. Subsequently, the electronic structure and charge transfer of ZnO solid were calculated. The calculated charge transfer for ZnO indicated that Zn and O atoms would be in an ionic state in the ZnO solid environment. The atomic orbitals of Zn^{2+} and O^{2-} would be more appropriate for the calculation of ZnO solid. In the self-consistent calculations for ZnO, we used a mesh of 24 k-points, with proper weights in the irreducible Brillouin zone. The self-consistent potentials converged to a difference around 10^{-5} in the last iteration. The computational error for the valence charge was about 0.0002 for 52 electrons.

III. Results

We calculated the electronic and structural properties of ZnO using the BZW procedure.[16, 17, 18] The implementation of the BZW procedure consisted of carrying out completely self-consistent calculations to identify the optimal basis set for the LCAO calculation. The criterion is based on the discussion in the last section.

The first self-consistent LCAO calculation utilized the atomic orbitals of Zn(1s2s3s4s 2p3p 3d) and O(1s2s 2p). We then repeated the self-consistent calculation using the above basis set augmented by the orbitals describing the first excited state of Zn. Hence, Zn(4p) orbitals were added to the basis set of the first calculation. We then plotted the electronic energy bands obtained from those two distinct self-consistent calculations. In Fig. 1, the solid and dashed lines represent the calculated energy bands of ZnO from the first and second calculations, respectively. Fig. 1 shows that the occupied bands of ZnO from the first calculation are substantially different from the ones from the second calculation. It indicates that the larger basis set of the second self-consistent calculation is preferred to that of the first calculation. This preference is based on physical considerations, i.e., the calculated charge density is not converged in the first calculation.

The next step was to perform another self-consistent calculation, for a third time, with a new basis set that includes O(3s) orbital. The calculated electron energy bands of this third calculation (dashed lines) and that of the second calculation (solid lines) are shown in Fig. 2. This figure shows that the calculated occupied states are fully converged. In particular, the changes in occupied energies, from calculation II to III, are in the range of computational errors that are due to other factors, including rounding errors. In contrast to the unchanged nature of the occupied states, the lowest unoccupied states at the Γ point is shifted downward by approximately 2.2 eV. Fig. 2 shows that the differences for the conduction bands from calculation II and III are not a rigid shift and cannot be corrected by a "scissors" operation.

The drastic changes in the unoccupied states of the conduction bands, in going from calculation II to III, can be understood from variational theory and related theorems. As discussed in the last section, the iteration procedure in the self-consistent calculations only includes the wave functions of occupied states in the reconstruction of the charge density, potential, and Hamiltonian. Therefore, the optimal basis set is that of calculation II, as previously explained by Zhao and Bagayoko[16]. The total absence of a difference between the corresponding, occupied energies in calculations II and III indicates that the charge density and the potential for the two calculations were the same. The Rayleigh theorem, however, is a possible reason for the lowering of some unoccupied energy levels from calculations III as compared to calculation II. Additionally, the ground state requirements of density functional theory suggest that the physical solution is that provided by calculation II. From the calculated electron bands (the solid lines of Fig. 2), the theoretical minimum band-gap of ZnO is 3.2 eV. It agrees with experimental data of about 3.4 eV, within the experimental uncertainty.[23]

The effective mass is a measure of the curvature of the calculated bands. The agreement between calculated and measured effective masses indicates an accurate determination of the shape of the bands. We calculated the effective masses of the n-type carriers of ZnO, using the electronic structure from calculation II (the solid line of Fig. 2). The calculated effective masses of the n-type carriers near the bottom of the conduction band at the Γ-point is $0.26 \pm 0.02 m_0$. It agrees well with the experimental value of 0.275 m_0.[23] Here, m_0 is the free electron mass. We also calculated the effective mass of the n-type carriers in three different directions, i.e., Γ-A, Γ-K, and Γ-M directions. The resulting effective mass of the n-type carriers of ZnO is quite isotropic, as the differences of the calculated effective masses in the three directions are within our computational uncertainty.

We computed the structural properties of ZnO from the electron charge density obtained with the optimal basis set of calculation II. We calculated the total energy of ZnO by varying the structural parameters in the hexagonal lattice. Fig. 3 shows the calculated total energy at various values of the lattice constant c, where the lattice constant a is kept at 3.25 $\AA$. The calculated equilibrium lattice constant c of ZnO, i.e., the value at the minimum of the total energy curve, is 5.18 ± 0.02 $\AA$. It agrees well with experimentally measured values of 5.207- 5.213 $\AA$.[23, 24] The uncertainty in the calculated lattice constant is due to the shallow minimum in Fig. 3. Fig. 3 also shows that there is an abrupt increase of the total energy when the lattice constant c is increased beyond 5.35 $\AA$, when the lattice parameter a is kept constant. This behavior might be an indication of the brittleness of the material.

A similar behavior can also been seen in Fig. 4 that shows the calculated total energy of ZnO versus the lattice constant a with the lattice constant c kept at 5.18 $\AA$. The calculated equilibrium lattice constant a of ZnO from Fig. 4 is 3.27± 0.02 $\AA$, which agrees well with experimental value of 3.249 - 3.253 $\AA$.[23, 24] We also calculated the internal parameter, u, of Zno in the hexagonal lattice. The calculated internal parameter u, at the minimum of the total energy, is 0.381 ± 0.002. It also agrees well with the experimental value of 0.3817.[25]

We calculated the effective charge and charge transfer in ZnO, using the electronic wave functions from the optimal calculation (calculation II). Our method for calculating the effective charge and charge transfer has been discussed in a previous publication.[26] We found that zinc atoms in ZnO give about 1.8 electrons/atom that are gained per oxygen atom. The ionic formula for zincite may be written as $Zn^{1.8+}O^{1.8-}$. The calculated charge transfer for ZnO indicates a strong ionic character of the Zn-O bonds.

IV. Conclusion

In summary, we have utilized the LCAO method, a local density potential, and the BZW procedure to calculated the electronic and structural properties of ZnO. The calculated theoretical minimum band-gap of ZnO is about 3.2 eV. Our total energy calculations found the theoretical lattice constants a and c to be 3.27± 0.02 $\AA$ and 5.18 ± 0.02 $\AA$, respectively. The calculated internal parameter u of the hexagonal ZnO is 0.381 ± 0.002. The effective masses of the n-type carriers, near the bottom of the conduction band at the Γ point, is $0.26\pm0.02m_0$. The calculated properties of ZnO agree well with experimental data.

Acknowledgment: This work was funded in part by the Department of the Navy, Office of Naval Research (ONR), through the Timbuktu Academy [Grant No: N00014-98-1-0748].

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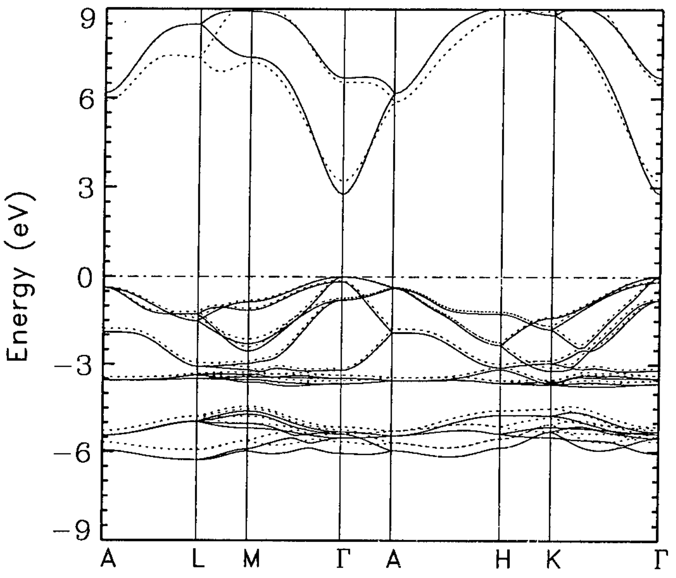

Figure 1: The electronic energy bands of ZnO from calculation I and II. The solid lines show the results of calculation I, and the dashed lines represent the bands from calculation II. The Fermi levels in the two calculations are superimposed. Consequently, some bands from calculation I may "appear" to be lower than their counterpart from calculation II, even though they are not – as per the Rayleigh theorem.

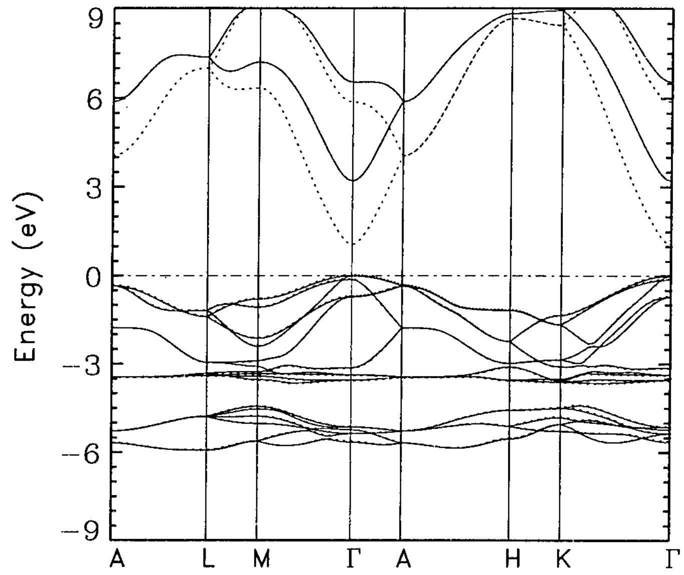

Figure 2: The electronic energy bands of ZnO from calculation II and III. The solid lines show the results of calculation II, and the dashed lines represent the bands from calculation III. Calculation II gives the final electronic structure of ZnO with the optimal basis set. The Fermi levels from the two calculations are superimposed.

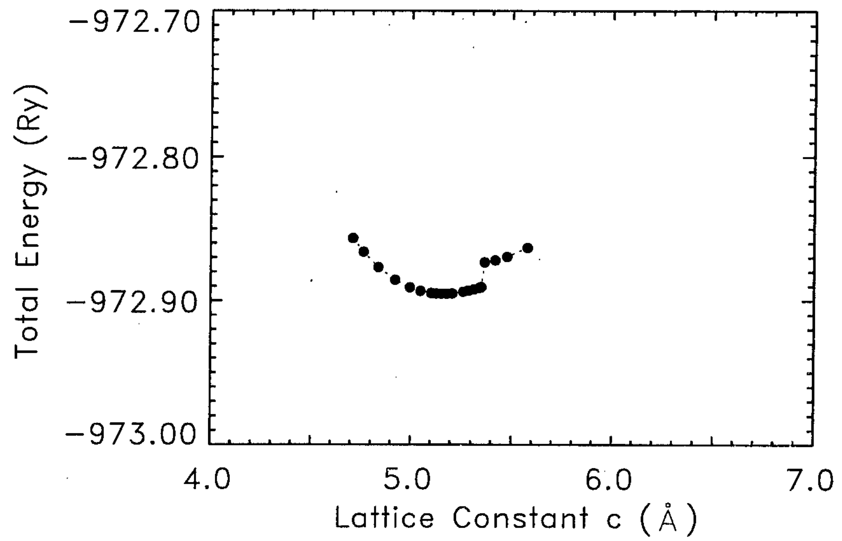

Figure 3: The calculated total energies of ZnO in the hexagonal lattice at various values of the lattice constant c – as obtained with the optimal basis set.

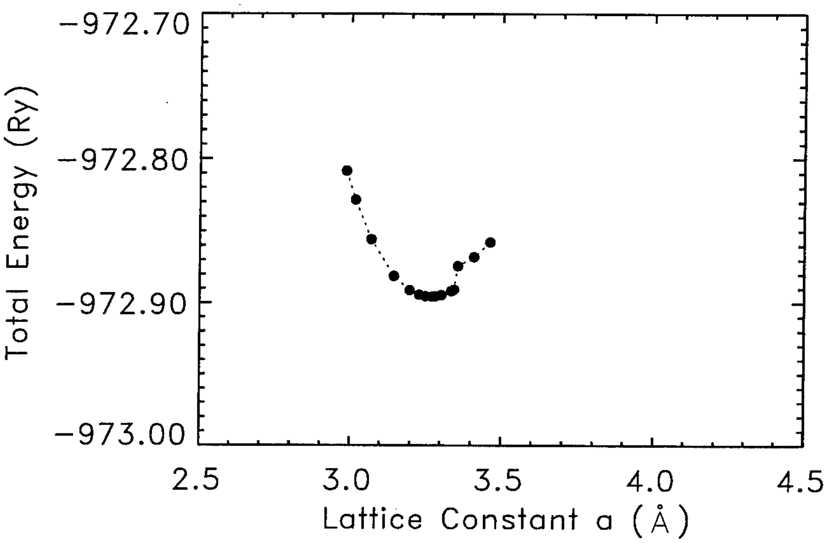

Figure 4: The calculated total energies of ZnO in the hexagonal lattice versus the lattice constant a – as obtained with the optimal basis set.

Proceedings of the first Mali Symposium on Applied Sciences

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DESCRIPTION ET PREDICTION DES PROPRIETES ELECTRONIQUES DES MATERIAUX

Par

Diola Bagayoko, Ph.D.
(Bagayoko@aol.com)
Professeur Distingué de Physique et Directeur de l'Académie de Tombouctou
Département de Physique, Southern University and A&M College
Baton Rouge (SUBR), Louisiane, USA

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CONTENU SOMMAIRE

Nous adressons le problème consistant des différences persistantes (de 20% à 50% ou plus) entre les valeurs calculées et les valeurs mesurées des **niveaux vides** d'énergie des semiconducteurs et autres matériaux (1900-98)! La méthode générale pour nos calculs de mécanique quantique est la combinaison linéaire d'orbitales atomiques. Nous utilisons un potentiel local.
La distinction de ce travail réside dans l'emploi de la nouvelle procédure de Bagayoko, Zhao, et Williams (BZW). Nos resultats, en accord avec l'expérience, sont en partie publiés sur les matériaux et dans les journaux suivants: BaTiO$_3$, *J. Phys.: Condens. Matter 10, 5645;* GaN, Si, et C, *Phys. Rev. B60, 1563, 1999;* 3C-SiC and 4H-SiC, *New Journal of Physics, 2, pages 16.2 - 16.12, 2000; c-*Si_3N_4*).* La procédure ou méthode BZW rend possible la prédiction des matériaux et de leurs propriétés electroniques. En particulier, elle permet la prédiction des fosses d'énergie des semiconducteurs et des insulateurs.

REVUE & MOTIVATIONS

Au début du siècle dernier, la mécanique quantique émergea comme la synthèse de plusieurs contributions, parmi lesquelles celles de I. Schr◇dinger, W. Heisenberg, L. de Broglie, N. Bohr, M. Planck, P.A. M. Dirac, et d'autres. Cette branche de la physique décrit ou, si possible, prédit les propriétés électroniques, optiques, magnétiques, structurelles, etc. des atomes, molécules, et solides. (Propriétés microscopiques). Vu que l'atome d'hydrogène est le seul pour lequel nous avons résolu, analytiquement, l'équation de Schr◇dinger (et de Dirac), on utilise des calculs souvent longs et compliqués pour étudier les matériaux (atomes, molécules, solides, etc.). Pour toute la durée du siècle dernier, les physiciens n'ont pas réussi ℂ résoudre totalement le problème suivant: **comment calculer les niveaux excités d'énergie des noyaux, atomes, molécules, et solides de mannière qu'ils soient en accord avec l'expérience?**

En 1998, mes collègues et moi avons découvert un effet qui causait les niveaux excités calculés à être généralement plus bas que les niveaux réels (i.e., mesurés par l'expérience). Voir Bagayoko, Zhao, et Williams, Bulletin de la Société Américaine de Physique [Bull., APS., **Vol. 43**, No. 1, p. 846, 1998]. Cette contribution adresse cet effet et la nouvelle méthode ou procedure de

Bagayoko, Zhao, et Williams (BZW) qui permet de l'éviter. *En ce faisant, nous avons résolu le problème noté ulterieurement.* Nous discutons des résultats obtenus avec cette méthode, *y compris la description et prédiction des valeurs correctes des "fossés d'énergie (band-gaps en Anglais)" des semiconducteurs.* **En particulier, nous présentons des résultats pour une phase cubique nouvelle du nitride de zinc pour laquelle il n'y a pas encore de valeurs mesurées expérimentalement** [Prière de voir Zerr et al qui ont découvert cette phase récemment ($c\text{-}Si_3N_4$), Nature, 400, pages 340-342, 1999]. **Ceci constitue un cas très clair de prédiction par la méthode BZW.**

METHODE GENERALE DE CALCUL

A. LA COMBINAISON LINEAIRE D'ORBITALES ATOMIQUES (LCAO)

L'EQUATION A VALEURS PROPRES, $H\Psi = E\Psi$, EST RESOLUE PAR LA METHODE AUTO-CONSISTANTE EN UTILISANT: $\Psi = \sum_{i=1}^{N} a_i \Phi_i$, i = 1 N.

Les orbitales (fonctions Phi) Φ_i sont obtenues des calculs pour les atomes (ou ions) qui apparaissent dans les systèmes à étudier (Si et N pour Si_3N_4). Les Φ_i comprennent les parties radiales et angulaires. Les a_i sont des coefficient numériques de développement de la fonction d'onde Psi.

B. LE POTENTIEL

Nous utilisons un potentiel qui est une fonctionelle locale de la densité électronique (Local Density Functional Theory). Les détails sont dans les publications (fournies au project TOKTEN et au Symposium Malien des Sciences Appliquées, 2000)

C. LE THEOREME DE RAYLEIGH ET LA METHODE BZW

Soit $H\Psi = E\Psi$. La combinaison linéaire des orbitales atomiques (LCAO) donne: $\Psi = \sum_{i=1}^{N} a_i \Phi_i$, i = 1 à N. Soient E_i^N les valeurs propres auto-consistantes, **ordonnées de la plus petite à la plus grande** E_N^N. Ayons la même équation résolue en employant une base de *(N+1) orbitales atomiques. Nous obtenons cette nouvelle base en ajoutant une orbitale atomique à la base de N orbitales utilisée dans le premier calcul.* Soient $E_i^{(N+1)}$ les valeurs propres auto-consistantes résultant du second calcul, ordonnées de la plus petite à la plus grande ($E_{(N+1)}^{(N+1)}$). **Alors, le théorème de Rayleigh dit que** $E_i^{(N+1)} \leq E_i^N$ **, pour chaque** $i \leq N$. (Pour plus de détails, prière de voir D. Bagayoko dans Inter. Jour. Quant. Chem. 17, 527, 1983)

Utilisant le théorème de Rayleigh, Bagayoko, Zhao, et Williams (BZW) **ont identifié un effet** qui est inhérent à l'utilisation de bases d'orbitales dans une approche variationnelle du type de Rayleigh-Ritz. Cet effet vient du fait que **seules les fonctions d'onde des niveaux occupés d'énergie** entrent dans la reconstruction de la densité de charge, du potentiel, et du hamiltonien quand on va d'une "iteration" (étape) à la suivante dans le formalisme d'auto-consistance. (Le hamiltonien est la somme des interactions physiques réelles.) *Si plusieurs calculs auto-consistants sont faits avec des bases d'orbitales de tailles croissantes, en commençant par la base minimale de taille N,* alors il arrivera que les niveaux occupés d'énergie d'un calcul avec

(N+p) orbitales seront identiques (en valeur numériques, plus courbure et branchement pour les bandes) à ceux du calcul suivant avec (N+p+1) orbitales. P est un nombre entier (1, 2, 3, ...)

Une base minimale est telle qu'elle rend tout juste compte de tous les électrons dans les espèces atomiques (atomes ou ions) présents dans le système à étudier--sans pourvoir pour la polarisation angulaire ou la "diffusion." L'effet en question consiste de la décroissance de certain niveaux vides, dans les calculs avec des bases de (N+p+1), (N+p+2), etc. orbitales. Cette décroissance est dictée par le théorème de Rayleigh et ne correspond pas nécessairement à la manisfestation d'interactions physiques réelles! Cet effet, parfois connu comme l'effet BZW, est évident seulement si on comprend le contenu du dernier paragraphe sur la page précédente. La méthode ou procédure BZW de calcul, décrite sur les pages suivantes, évite cet effet tout en guarantissant que la base d'orbitales est complète (au sens quantique). Pour détails, prière de voir Inter. J. Quant. Chem., 17, page 527, 1983; J. Phys. Condens. Matter 10, page 5645, 1998; and Phys. Rev. B60, page 1563, 1999.

L'EXECUTION DE LA METHODE BZW

Trois (ou plus) calculs auto-consistants sont généralement nécessaires pour exécuter proprement la méthode BZW. Le calcul I (auto-consistant) emploie la base minimale d'orbitales. Soit N le nombre d'orbitales dans cette base minimale. Le calcul (auto-consistant) II emploie une base obtenue en ajoutant à la base minimale l'orbitale (ou les orbitales) représentant le niveau excité le plus bas dans les espèces atomiques du système. *(Si deux de ces niveaux sont très proche en énergie, on peut ajouter plus d'une orbitale à la fois.)* On compare (numériquement et graphiquement) les **niveaux occupés** d'énergie résultant des calculs I et II [calculs avec des bases de N et (N+1) orbitales] Le calcul auto-consistant III utilise une base obtenue en augmentant la base du calcul II avec l'orbitale (ou les orbitales) représentant les niveaux excités immédiatement au-dessus du plus bas niveau excité dans les espèces atomiques. On compare les résultats, pour les niveaux occupés, des calculs II et III. On continue ce processus jusqu'au point où les niveaux occupés d'un calcul [avec (N+p) orbitales] sont identiques à ceux du calcul suivant [avec (N+p+1) orbitales]. Alors, la méthode BZW dit que, *en vue du théorème de Rayleigh et du fait que seules les fonctions des niveaux occupés entrent dans la construction du potentiel et du hamiltonien,* le calcul avec (N+p) orbitales donne **la solution physique** du problème.

Une décroissance supplémentaire de certains niveaux vides, dans les calculs avec plus de (N+p) orbitales dans la base, n'est pas nécéssairement la manisfestation d'interactions physiques réelles. Elle peut être une conséquence du théorème de Rayleigh. La méthode BZW introduit une nouvelle convergence dans les calculs: celle des niveaux occupés d'énergie par rapport à la taille de la base d'orbitales (ou de fonctions). Cette convergence vérifie que la base d'orbitales est complète.

NOUVEAUX RESULTATS EN ACCORD AVEC L'EXPERIENCE (pour $BaTiO_3$, GaN, Si, C, 3C-SiC, ZnO, 4H-SiC, c-Si_3N_4 et autres)

Propriétés Electroniques Des Semiconducteurs: Résultats Obtenus avec la Méthode BZW (i.e., les bases optimales d'orbitales ont été déterminées et utilisées). *(Voir J. Phys., Condens. Matt. 10, 5645, 1998, Phys. Rev. B60, 1563, 1999, et et New J. Phys., 2, 16.2-16.12, 2000.)*

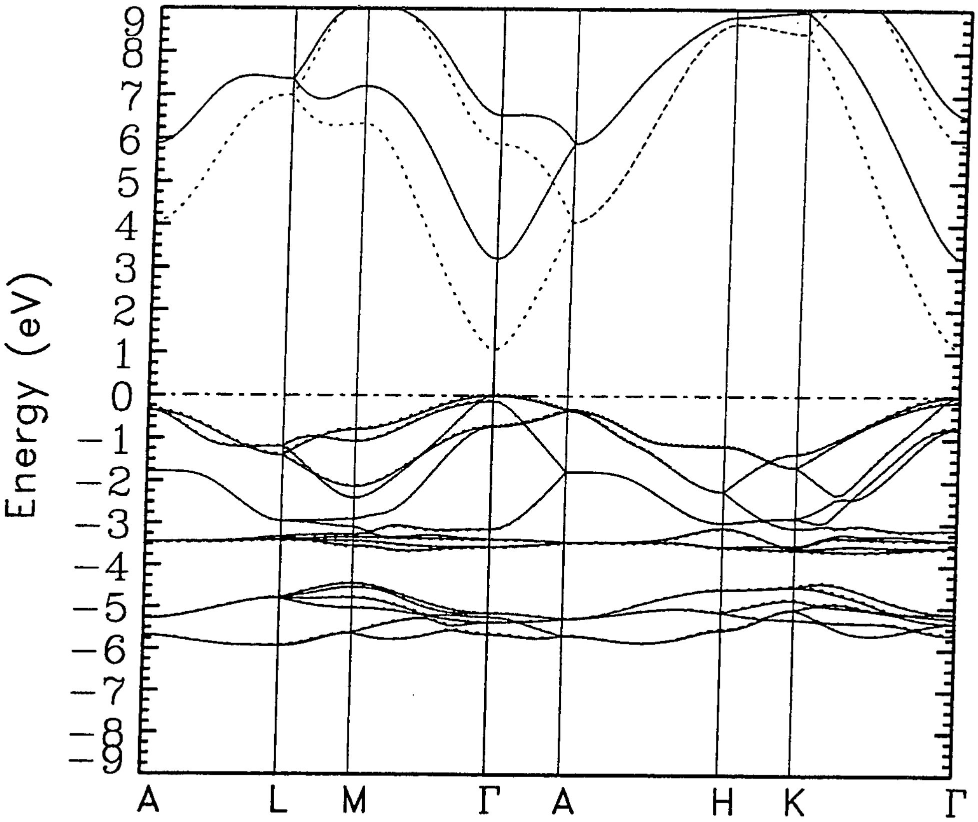
	Valeurs Calculées	**Valeurs Mesurées**
BaTiO$_3$ (Barium Titanate)		
Eg (Fossé d'énergie)	2,6 eV	2,8; 3,0 eV
$M^*_{p,\parallel}$	7,5 m_0	anisotropique
$M^*_{p,\perp}$	1,2 m_0	
$M^*_{n,\parallel}$	3,4 m_0	
$M^*_{n,\perp}$	1,2 m_0	1,0-1,5 m_0
GaN (Nitride de Gallium)		
Eg (Fossé d'énergie)	3,2, 3,4* eV	~3,4 eV
M^*_n	0,22 ± 0,03 m_0	0,2 ± 0,02 m_0
Si (Silicium, solide)		
Eg (Fossé d'énergie)	1,02 eV	1,14; 1,17 eV
W(valence)	12,1 eV	12,5 eV
M^*_{nt}	0,20 ± 0,03 m_0	0,19 m_0
M^*_{nl}	0,93 ± 0,03 m_0	0,98 m_0
C (diamant, solide)		
Eg (Fossé d'énergie)	5,05 eV	5,3; 5,48 eV
W_v	21,35 eV	21 ± 1 eV
$M^*_{n,\parallel}$	1,1 ± 0,2 m_0	1,4 m_0
$M^*_{n,\parallel}$	0,30 ± 0,03 m_0	0,36 m_0
3C-SiC (Etat solide à très basses températures)		
Eg (Fossé d'énergie)	2,24 eV	2,2; 2,4 eV
$M_{X\square}$	0,72 ± 0,04 m_0	0,677 ± 0,015 m_0
M_{XW}	0,22 ± 0,02 m_0	0,247 ± 0,011 m_0

Il est critique de noter qu'avant la procedure ou méthode de Bagayoko, Zhao, et Williams (BZW), les valeurs calculées des fossés d'énergie étaient de 20 à 50 % plus petites que les valeurs mesurées: **La méthode BZW rend la prédiction possible.**

LES BANDES D'ENERGIES ELECTRONIQUES DE L'OXIDE DE ZINC OBTENUES PAR LA PROCEDURE DE BAGAYOKO, ZHAO, ET WILLIAMS (BZW)

Les courbes pleines (____) représentent les résultats du second calcul, avec une base augmentée d'orbitales atomiques, et les autres courbes (….) montrent les résultats du troisieme calcul, avec une base d'orbitales atomiques plus large que la précedente.

NOTEZ BIEN QUE LES ENERGIES OCCUPEES ONT ATTEINT LA CONVERGENCE ALORS QUE LES ENERGIES DES ETATS VIDES CONTINUENT, PAR LE THEOREME DE RAYLEIGH, A DECROITRE! **LE SECOND CALCUL EST FINAL, PAR LA PROCEDURE BZW.**



Les bandes électroniques d'énergie de c-Si_3N_4 sont pourvues au site Internet (http://www.phys.subr.edu/faculty/bagayoko). Nous (D. Bagayoko et G. L. Zhao) prédisons un fossé d'énergie de 3,68 eV et un "bulk modulus" de 330 GPa. Nous avons obtenu un paramètre du réseau cristallin de 7,72 ± 0,02 Å, en accord avec l'expérience (7,80 ± 0,08 Å). *Nous attendons les expériences pour la comparaison!*

CONCLUSION

LA PROCEDURE BZW OUVRE LA VOIE POUR

- **La prédiction de nouvelles molécules** (larges ou petites, inorganiques ou organiques),
- **La prediction des fossés d'énergie des bandes (band gaps) des matériaux** (pour guider le dessin et la fabrication d'instruments électroniques divers--des plus simples aux plus complexes),
- **Une compréhension approfondie de la structure des noyeaux atomiques;**
- **L'amélioration des simulations** en fournissant des paramètres pour les formes d'énergie potentielle utilisées par les simulations de la dynamique moléculaire (DM or MD) ou de la méthode de Monte Carlo (MC), et
- **Un avancement fondamental de notre connaissance de la matière (nucléaire, atomique, moléculaire, et condensée)** – et des limitations réelles de la théorie de la fonctionelle de la densité.

Prière de bien réfléchir sur les implications immédiates et futures de la méthode BZW pour les industries (des semiconducteurs, du noyau atomique, de la biotechnologie, etc.—y compris la nanotechnologie naissante).

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POLARONIC EFFECT IN MATERIALS WITH FERROELECTRIC PHASE TRANSITIONS

Y. M. MALOZOVSKY, J. D. FAN, D. BAGAYOKO and J. T. WANG
Department of Physics, Southern University,
Baton Rouge, Louisiana 70813, USA

We studied polaron effects due to the interaction of an electron with optical phonons in ferroelectrics with a layered crystal structure. We evaluated the polaron self-energy using the effective T-matrix. We showed that transition from the large radius polaron to the small radius polaron is controlled by the interlayer interaction or interlayer spacing. We also found that the polaron interaction with the fluctuations of polarizability near the Curie temperature causes polaron localization.

1. Introduction

It is well-known that the majority of the materials with ferroelectric phase transitions[1] show extremely low conducting properties (for example, KDP, $BaTiO_3$, $PbNbO_3$, etc.). Most materials with ferroelectric phase transition can surely be classified as insulators. Excited or injected electrons become localized or trapped in ferroelectrics. Such an effect of localization can find a natural explanation in terms of the strong electron–phonon interaction — polaronic effect. There are several reasons to believe this explanation. First, for the materials with ferroelectric phase transitions, electrons have quite narrow electronic bands which are separated by large forbidden gaps (for example perovskites $BaTiO_3$, $PbHbO_3$, $LiTiO_3$, etc.). Second, due to the strong ionic nature of the crystal lattice, all the ferroelectric materials have optical branches of phonon excitations. Third, ε_∞ and ε_s the high frequency and the static dielectric lattice permeabilities are greatly different in magnitude, i.e. $\varepsilon_s \gg \varepsilon_\infty$, which results in the large electron–phonon coupling constant. Moreover, $\varepsilon_s(T) = C/(T - T_c)$, the static dielectric permeability, greatly increases near the temperature of the ferroelectric phase transition. It also increases the electron-phonon coupling constant. Another effect which also contributes to the polaron formation is the dimensionality of the lattice. For example, in two-dimensional case, the polaron formation can be achieved at much less constraints than that in three-dimensional case. Moreover, the anisotropy of the lattice also favors the polaron formation. A layered nature of the crystal lattice (like perovskites $BaTiO_3$, $PbNbO_3$, $LiTiO_3$, etc.) is one of the ways to consider the effect of anisotropy on the polaron formation. In ferroelectrics, fluctuations of polarizabilty become large at the temperature of transition to the ferroelectric phase. In this case, it is also important to consider the effect of fluctuations of polarizability on polaron properties. In this paper we consider only the polaron effect in a layered crystal.

2. Polaronic Effect in a Layered Crystal

We consider a model of ferroelectrics as a layered crystal consisting of ionic (cations and anions) layers with the interlayer lattice constant c. For simplicity we assume that the electrons can freely move along layers while the motion of electron between the layers can be described by the tight-binding approximation. The energy for electrons in a layered crystal can be written as $\varepsilon_{\mathbf{k}} = (\mathbf{k}^2/2m_b) + t[1 - \cos(ck_z)]$, where m_b is the longitudinal band mass, t is the hopping integral between the layers.[2,3]

The polaron self-energy part, taking into account the multiphonon processes, satisfies the equation[4,5]

$$\Sigma(P) = -\sum_{p'} t(P,P';P',P)G(P')\,, \tag{1}$$

where $t(P,P';P',P)$ is the effective four points T-matrix describing the multiphonon interactions of an electron with the lattice, $G(P)$ is the polaron Green's function which satisfies the Dyson equation $G^{-1}(P) = G_0^{-1} - \Sigma(P)$, with $G_0(p) = G_0(p,\omega_n) = 1/(i\omega_n - \varepsilon_{\mathbf{p}})$ being the bare electron Green's function in the temperature technique. The equation for the T-matrix can be written as follows

$$\begin{aligned} t(P,P';P',P) = D_{\mathrm{ph}}(P-P') - \sum_k D_{\mathrm{ph}}(P-K)G(K) \\ \times G(P+P'-K)t(K,P+P'-K;P',P)\,, \end{aligned} \tag{2}$$

where $D_{\mathrm{ph}}(Q)$ is the phonon Green's function including electron–phonon interaction constant. For brevity, in Eqs. (1) and (2), we have used four-dimensional notations $P = (\mathbf{p}, i\omega_n)$, $K = (\mathbf{k}, i\omega_n)$, and $Q = (\mathbf{q}, i\Omega_n)$, where ω_n/Ω_n are odd/even Matsubara frequencies, and $\Sigma_P = T\Sigma_{\omega_n,\mathbf{p}}$ with T being the temperature. The diagram representation of Eqs. (1) and (2) is shown in Fig. 1.

The phonon Green function in Eq. (2) can be written in the conventional form

$$D_{\mathrm{ph}}(\mathbf{q},\omega) = \frac{2g^2(\mathbf{q})\omega_l}{\omega^2 - \omega_l^2 + i\delta} \tag{3}$$

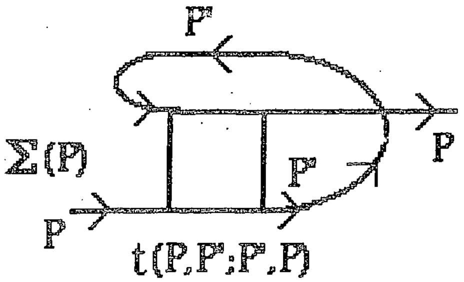

Fig. 1. Polaron self-energy in terms of the T-matrix.

where $g(\mathbf{q})$ and ω_l are the matrix element of the electron-phonon interaction and the longitudinal optical phonon frequency, respectively. For a layered Coulomb lattice, $g(\mathbf{q})$ can be written as[2,3]

$$g^2(\mathbf{q}) = \frac{V(\mathbf{q})\omega_l}{2}[\varepsilon_\infty^{-1} - \varepsilon_s^{-1}], \tag{4}$$

where ε_∞ is the high frequency lattice dielectric permeability of the crystal, $\varepsilon_s(T)$ is the static lattice dielectric permeabilities of the crystal and is a function of temperature; $V(\mathbf{q})$ is the Coulomb matrix element in a layered crystal,

$$V(\mathbf{q}) = \frac{2\pi e^2}{q}\frac{\sinh(cq)}{\cosh(cq) - \cos(cq_z)}. \tag{5}$$

The matrix element of the electron–phonon interaction in the long wavelength limit, $c|\mathbf{q}| \ll 1$, is $g^2(\mathbf{q}) = M^2\alpha/(c\mathbf{q}^2)$, which is exactly the isotropic three-dimensional case, where M is the Frohlich matrix element of the electron–phonon interaction ($M^2 = 4\pi\alpha(\omega_l)^{3/2}/(2m_b)^{1/2}$), and $\alpha = e^2(m_b/2\omega_l)^{1/2}[\varepsilon_\infty^{-1}\varepsilon_s^{-1}(T)]$ is the dimensionless polaron coupling constant.[4,5] The situation changes for a momentum transfers in the short wavelength limit, $qc > 1$ (and $|q_z| \leq \pi/c$). The matrix element of the electron–phonon interaction in this limit becomes two-dimensional in character, $g^2(\mathbf{q}) = M^2\alpha/(2q)$, when $qc > 1$. In Eq. (4), the static dielectric permeability is a function of temperature and becomes very large at the Curie temperature $\varepsilon_s(T) = 1 + 4\pi\chi(T) = 1 + 4\pi C/(T - T_c)$, where $\chi(T) = C/(T - T_c)$ is the lattice susceptibility for $T > T_c$, C is the Curie constant, and T_c is the Curie temperature for the ferroelectric phase transtiton.

The solution to Eqs. (1) to (3) shows that, in the weak coupling, the well-known results for the weak coupling polaron are reproduced,[4,5] i.e. $m^* = m_b/(1 - \alpha/6)$, the polaron effective mass, and $\tau_{\rm pol}^{-1} = 2\alpha\omega_l N_B \propto \alpha\omega_l \exp(-\omega_l/T)$, where $\tau_{\rm pol}$ is the polaron lifetime. In the strong coupling, we are able to estimate the polaron lifetime as follows

$$\tau_{\rm pol}^{-1} - A\alpha\Delta \exp\left(-\frac{\Delta}{T}\right), \tag{6}$$

where $\Delta \propto \omega_l$ is the characteristic polaron binding energy, and A is some constant. The polaron effective mass in the strong coupling seems to be in agreement with Miyake result,[6] i.e. $m^* \approx 0.227\alpha^4 m_b$.

3. Interaction of a Polaron with Fluctuations Of Polarizability in a Ferroelectric Crystal

The generalized polarizability of the ferroelectrics in the approximation of the hydrodynamic fluctuations of polarizability for, $T > T_c$, can be written[7]

$$\chi(\mathrm{k}, \omega) = \frac{\gamma}{-i\omega + \tau_0^{-1} + 2\gamma g \mathrm{k}^2}, \tag{7}$$

where γ is the rate of the relaxation of polarizability, $g > 0$ is the coefficient describing the fluctuations of polarizability, $\tau_0^{-1} = (\gamma/C)(T - T_c)$ for $T > T_c$, where

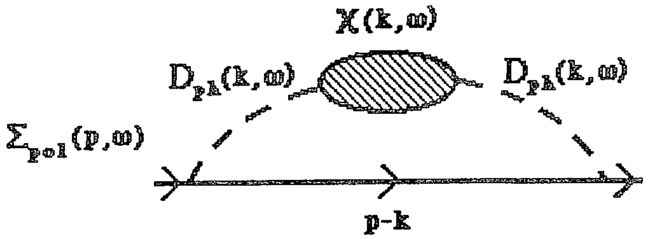

Fig. 2. Polaron self-energy describing the interaction of a polaron with fluctuations of polarizability. The hatched bubble represents $\chi(\mathbf{k},\omega)$, the generalized susceptibility of the ferroelectric. The dashed lines stand for $D_{\text{ph}}(\mathbf{k},\omega)$, the phonon Green's function.

C is the Curie constant. It follows from Eq. (7) that the generalized polarizability contains a diffusion pole which corresponds to the hydrodynamical fluctuations of the polarizability at the transition to the ferroelectric phase.

Now, we consider the effect of the interaction of a polaron with the fluctuations of polarizability. The self energy part $\Sigma_{\text{pol}}(\mathbf{p},\omega_n)$ representing the interaction of polaron with the fluctuations of polarizabiltity in the RPA can be written as

$$\Sigma_{\text{pol}}(\mathbf{p},\omega_n) = -T\sum_{\mathbf{k},\omega_{n'}} D^2_{\text{ph}}(\mathbf{k},\omega_{n'})G(\mathbf{p}-\mathbf{k},\omega_n-\omega_{n'})\chi(\mathbf{k},\omega_{n'})\,, \tag{8}$$

where $D_{\text{ph}}(\mathbf{k},\omega)$ is the electron-phonon Green's function, $\chi(\mathbf{k},\omega)$ is the generalized polarizability of the ferroelectric and is given by Eq. (7), $G(\mathbf{p},\omega_n)$ is the polaron Green function in the temperature technique. The diagram representation for Eq. (10) is shown in Fig. 2.

The contribution to $\tilde{m}^*$ from the exchange with the fluctuations of the polarizability in the RPA can be represented by

$$\frac{\tilde{m}^*}{m^*} \approx 1 + \alpha^2\gamma\tau_0 B\,, \tag{9}$$

where $\tilde{m}^*$ is the polaron effective mass, and B is a some constant. From Eq. (9) we can see that for the temperatures far form the ferroelectric phase transition, $\gamma\tau_0 \ll 1$, the polaron effective mass enhancement due to the interaction of a polaron with the fluctuations of polarizability is small.

Near the ferroelectric phase transition the situation is completely different. In this case, $\gamma\tau_0 \propto 1/(T-T_c^*)$ and

$$\frac{\tilde{m}^*}{m^*} \approx 1 + \frac{\alpha^2 CB}{T-T_c^*}\,. \tag{10}$$

Thus, the interaction of a polaron with the fluctuations of the polarizability near the temperature for the transition to the ferroelectric state leads to the extremely large effective mass of polaron, and thus, causes the polaron to become localized.

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HOW CAN AN ATOM OR ION REMEMBER ITS INITIAL STATE?

J. T. Wang, F. Tang and D. Bagayoko
Department of Physics, Southern University and A & M College,
Baton Rouge, Louisiana 70813 USA

T.-P. Chen
Department of Physics, University of North Dakota, Grand Forks, ND 58202, USA

The experiment has found that in order to form the thin film of certain compound by deposition, the same compound should be used for the target material. A stoichiometric mixture of components for forming the compound by solid reaction as the target material won't do the work. It seems that the particle emitted from the target remembers its initial state, the state when it is in the compound. By perturbation approximation, we estimated the life time of the initial state of the emitted particle, if the states of the particle are represented only by the states of outer shell electrons. To elucidate the experimental finding, other factors regarding the states of the emitted particle may have to take into consideration.
Keywords: Atom or Ion, Memory

1. Introduction

It is found that in order to form the thin film of a certain chemical compound by sputtering or laser ablation or other deposition techniques, the target used in the process should be the same compound as the one of the film to be formed. One question arising is that if the material in the target is the mixture of the chemical components used to form the desired compound of the film, the film of that compound can also be formed? For example, by laser ablation, we fabricated $YBa_2Cu_3O_{6+x}$ superconductor thin film on $LaAlO_3$ substrate. If the target material is $YBa_2Cu_3O_{6+x}$, the film on the substrate is $YBa_2Cu_3O_{6+x}$. If the target materiel is the mixture of $Y_2O_3 + BaCO_3 + CuO$, the film on the substrate is also a mixture of those components. The $YBa_2Cu_3O_{6+x}$ will not be formed on the substrate.[1] Why? There are several possibilities. The whole molecule may be emitted, when the target is bombarded by other particle, for example, laser photons, electrons or ions. Most likely, the particles emitted from the target bombarded by other particles are atoms or ions. From the experimental findings mentioned above, it seems that the particles (atoms or ions) ejected from the target of compound or mixture of components behave differently from each other and the differences are remained for a period of time till they reach the substrate. We studied the life time of the initial state (before emission) of the particles emitted from targets by perturbation theory.

2. Transition Probability

The mechanism of the sputtering technique using different target is schematically shown in Fig.1a, and 1b. The dots represent the particles emitted from targets. They are the same element but in different compounds in the different target. Th states of particles (atoms or irons) are represented by the states of the electrons on the outer shell of the atoms. The electron in a compound occupies a state in the electronic bands of that compound . When a particle bombards the target, an interaction (perturbation) is imposed on the atom for a short period of time and then the atom (or ion) is ejected to the free space and the valence electron is in the field of a single atom (or ion).

Assuming that at time t_0, the electron is in the state of the electronic band and the Hamiltonian is H_0, the interaction Hamiltonian due to the bombarding particle is $H_1(t)$ and the final Hamiltonian, when the particle is in the free space, is H_f The Hamiltonians versus time are plotted schematically in Fig.2.

If the initial wavefunction is $| \varphi_0 >$ and the final wavefunction is $| \varphi_f >$ The transition probability from the initial state $| \varphi_0 >$ to the final state $| \varphi_f >$ is $|< \varphi_0 | \varphi_f >|^2$. The wavefunction of the initial state can be written as,

$$| \varphi_0 >= \sum_k a_k | \phi_k >,$$

and similarly the wavefunction of the final state

$$| \varphi_f >= \sum_k b_k | \phi_k > .$$

By perturbation theory the coefficient b_k can be calculated as^2

$$b_k \approx \sum_n a_n < \phi_k | [1 - i\frac{t_0}{h}(H_1 - H_f)] | \phi_n > .$$

For simplicity we can assume

$$| \varphi_0 >=| \phi_k >,$$

then

$$|< \varphi_0 | \varphi_f >|^2=|< \phi_k | \sum_n b_n | \phi_n >|^2=| b_k |^2.$$

The total transition probability of the final state

$$P = \int_0^\infty | b_k |^2 \rho(k,T)dk.$$

If the time period of each strike by the incident particle is t_0, the life time of the initial state would be

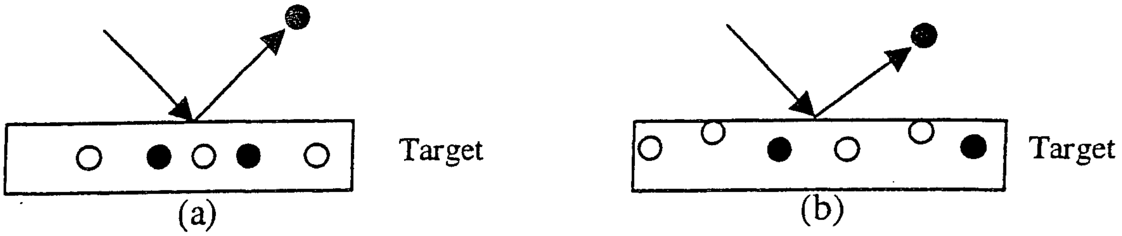

Fig. 1. Sputtering Technique.

$$t \propto \frac{t_0}{P}.$$

The time t calculated above could be characterized as the memory time of the initial state. When the bombarding particle hits the target, the emitted particle gains kinetic energy as the energy that the incident particle possesses, ϵ_0, i.e.

$$\frac{1}{2}mV^2 = \epsilon_0.$$

The velocity of the emitted particle can be found as

$$V = \sqrt{\frac{2\epsilon_0}{m}},$$

where m is the mass of the emitted particle. The time that needed for the emitted particle to travel from the target to the substrate can be evaluated as

$$t' = \frac{d}{V},$$

where d is the distance from the target to the substrate. If the life time of the initial state of the emitted particle in the target substance t is longer the travel time of the emitted particle t', the possibility that the deposition has the same chemical composition as in the target would be greater. For a approximation, let $H_1 = constant$, $H_f = constant$. Then

$$\begin{aligned} b_k &= \sum_n a_n[1 - i\frac{t_0}{h}(H_1 - H_f)] < \phi_k \mid \phi_n > \\ &= a_k[1 - i\frac{t_0}{h}(H_1 - H_f)], \end{aligned}$$

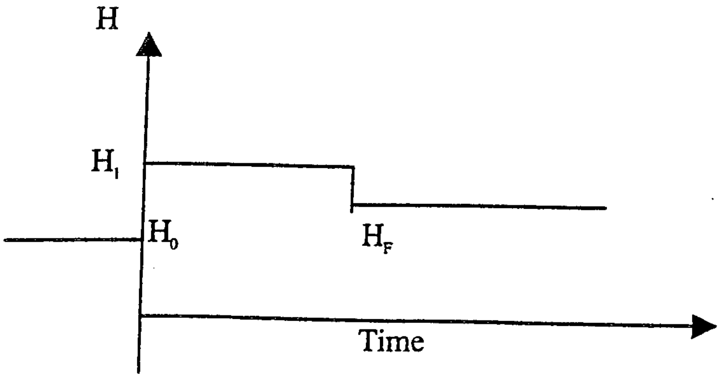

Fig. 2. Hamiltonian versus Time.

and

$$|b_k|^2 = |a_k|^2 \left(1 + \frac{t_0^2 (H_1 - H_f)^2}{h^2}\right).$$

Approximately

$$H_1 - H_f = h\omega,$$

hence

$$|b_k|^2 \approx |a_k|^2 \left[1 + \frac{t_0^2 (h\omega)^2}{h^2}\right] \approx |a_k|^2 \left[1 + 4\pi^2 t_0^2 f^2\right].$$

If the initial state is a single eigen state k, the total transition probability

$$P = |b_k|^2 \approx 1 + 4\pi^2 t_0^2 f^2,$$

then

$$t = \frac{t_0}{|b_k|^2} = \frac{t_0}{1 + 4\pi^2 t_0^2 f^2}.$$

Since

$$1 + 4\pi^2 t_0^2 f^2 \geq 1,$$

hence the life time t is in the same order of magnitude of t_0 In any cases, the travel time of the emitted particle should be longer than the interaction time t_0 Therefore, the travel time seems always to be longer than the life time. The travel time can be estimated as the following:

$$\frac{1}{2}mV^2 = \epsilon_0 = h\omega.$$

The travel time of the emitted particle

$$t' = \frac{d}{V} = \frac{d\sqrt{m}}{2\pi\varpi} \approx \frac{10\sqrt{10^{-24}}}{\sqrt{10^{-27} \times 10^{14}}} \approx 10^{-5}s.$$

From this estimation it doesn't seem that the memory of the emitted particle comes from the outer shell electrons. The core electrons or even the nucleus of the emitted particle (atom or ion) may have contribution to the memory of its initial state, the state when the particle is still in the target compound. More experimental as well as theoretical studies are necessary to resolve this issue.

Acknowledgements

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PREDICTIVE AB-INITIO COMPUTATIONS OF PROPERTIES OF FERROELECTRIC MATERIALS

D. BAGAYOKO and G. L. ZHAO
Physics Department, Southern University and A & M College, Baton Rouge, Louisiana 70813 USA

We present a newly developed, ab-initio, self-consistent procedure for predictive calculations of electronic and related properties of ferroelectric materials. Known as the Bagayoko, Zhao, amd Williams (BZW) procedure, this approach resolves the long-standing disagreement between experimental and theoretical conduction bands, in general, and band gaps, in particular, for ferroelectrical materials and other semiconductors. We discuss applications to tetragonal $BaTiO_3$ and implications for molecules and band-gap engineering as well as the nuclear shell model.

1. Basis-Set in Self Consistent Variational Calculations

In typical self-consistent calculations, particularly the ones that employ a density functional potential, trial wave functions are constructed using basis sets often derived from atomic calculations.[1,2] Charge densities and potentials are constructed. The Hamiltonian matrix is generated and diagonalized. Key output quantities are energy levels or bands, for clusters[1] and solids[2] respectively, and related wave functions. The resulting output wave functions –for the occupied states– are employed to generate a new charge density and the computations are repeated. The process of using the output of iteration (n) –for occupied states– to construct the input for iteration (n+1) continues until self-consistency is reached. Various measures are utilized to define self-consistency, i.e., when the input and output energies, charge densities, potentials, etc. are respectively unchanged.

The trial basis sets are found by various authors by augmenting the atomic orbitals with polarization and diffuse orbitals [1,2] whose numbers, until now, had no particular limit. In fact, from a variational standpoint, the larger these numbers the better, provided no 'catastrophic sinking of energy levels' or negative Millican population numbers occur for occupied states.[1]

The extensive restructuring of the electronic clouds in molecules, cluster and solid environments, as compared to those of isolated atoms, compounds the difficulties in the selection of an expansion basis set. For this reason, polarization and diffuse orbitals are added to basis sets that are adequate for the description of the ground states of the isolated atoms.[1] The need for supplementary diffuse orbitals is dramatically illustrated by the case of metallic copper[2] where the neck of the Fermi surface at the L-point is not reproduced in the absence of these orbitals.

The aim of this article is to identify a basis-set and variational effect and to provide a first principle approach that circumvents this effect. We apply this approach to produce the electronic energy bands of $BaTiO_3$ using the LCGO (linear combination of Gaussian orbitals) formalism.[3] We show that a local density functional potential can accurately describe this material. Unlike in the case of most of the previous computations, this calculated band gap agrees with experimental findings.

2. A Basis-Set and Variational Effect

This basis set and variational effect consists of an extra-lowering of low unoccupied energy levels or bands, for molecules and clusters or solids, respectively. The effect is caused by the combination of (a) the use of large basis sets to meet completeness requirements, (b) a mathematical theorem, and (c) the use of the wave functions –for occupied states only– in reconstructing the charge density and the potential in going from one iteration to the next. The restriction of the iterative procedure to the occupied states physically defines an optimum basis set as one that reproduces the same occupied energy levels or bands as larger basis sets obtained by adding more orbitals. Such a basis set is "converged in size" or "complete" with respect to the description of occupied states. An essential result here is that the lowering of unoccupied states with a basis set larger than the optimum basis set does not need to represent any physical interactions. It is an unavoidable consequence of the theorem enunciated below.

The variational theorem[4,5] states that when a variational eigenvalue problem is solved with N and N+1 basis functions, by augmenting the set of N functions with an additional one, then the eigenvalues from the calculations with N and N+1 satisfy the inequalities: $E_i^N \geq E_i^{N+1}$, where i varies from 1 to N and the eigenvalues are ordered from the lowest (E_1) to the highest. In this inequality, the superscripts stand for the numbers of the basis functions. Bagayoko[2] utilized this theorem to explain the rigid upward shift of energy levels obtained with contracted basis sets of smaller sizes as opposed to the ones obtained with larger basis sets of uncontracted orbitals. Bagayoko, Zhao, and Williams (BZW)[6,7], developed a computational procedure, known as the BZW procedure, that methodically circumvents the extra-lowering of some unoccupied energy levels or bands on account of the above theorem.

The above effect directly leads to the need for multiple test-computations, using basis sets methodically increased or decreased in size, in order to obtain an optimum basis set for a given computational study. We describe below a basis set optimization method that utilizes the energy levels of the atomic species that are represented in a molecule, a cluster, or a solid.

Our calculations utilized an expanded version of the band structure calculation program package from Ames Laboratory of the US Department of Energy (DOE) in Iowa.[10,11] Details of the computational method are available in several previous publications.[8,9,10,11,12] We employed the Ceperly-Alder form[13] of the local density functional potential. We implemented the linear combination of Gaussian orbitals in accordance with the approach described below.

3. The BZW Procedure

Succinctly stated, this implementation of the BZW procedure first consisted of carrying out completely self-consistent calculations for $BaTiO_3$ using a minimal basis set. Namely, the initial charge density for $BaTiO_3$ was calculated using the occupied, atomic orbitals for Ba, Ti, and O, as obtained by self-consistent atomic calculations, to account for all the electrons.

We repeated the calculations using a basis set augmented by orbitals describing the first excited states (i.e., the lowest in energy) for Ba, Ti, and O. Hence Ba($5d^o$), Ti($4p^o$), and O($3s^o$) orbitals were added to the basis set. Superscript indices of zero indicate that these states are unoccupied in the free atoms (ions). We then plotted the energy bands obtained from these two distinct self-consistent calculations. In Figure 1, the solid and dashed lines represent the calculated results from the first and second calculations, respectively. Figure 1 shows that calculated bands varied significantly and in a non-rigid fashion. Hence, as noted above, the larger basis set for the second self-consistent calculation is preferred to that from the first. This preference is based on physical and variational considerations.

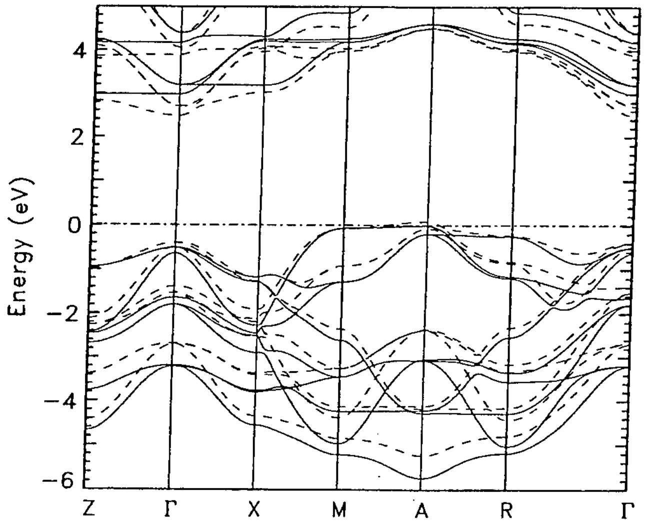

Figure 1: Comparison of the calculated, electronic band structures for ferroelectric tetragonal $BaTiO_3$ from computations using a minimum basis (first calculation, solid lines) and an extended basis (second calculation, dashed lines). The Fermi levels from the two calculations are superimposed in this graph.

A third self-consistent calculation was performed with a basis set that included orbitals for excited states immediately above the ones considered in the second calculation. The calculated energy levels of the excited Ba($6p^o$) and O($3p^o$) are much lower than that of Ti($5s^o$), in relative terms. Hence, the new basis set had ($5d^o$,$6p^o$) on Ba, $4p^o$ on Ti, and ($3s^o$,$3p^o$) on O as input orbitals beyond the minimum set. Figure 2 shows the energy bands from the second calculation (solid lines) and this third one (dashed lines). Again, we clearly observed a non-rigid variation of some occupied energy bands from the third calculation as compared to those from the second.

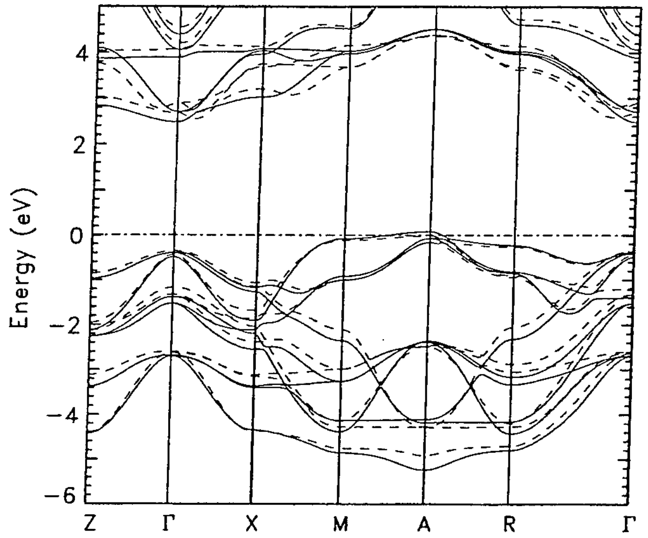

Figure 2: Calculated, electronic band structures from the second calculation (solid lines) and the third calculation (dashed lines). The Fermi levels are superimposed in this graph.

The next natural step was to repeat our procedure, for a fourth time, with a new basis set that includes $5s^o$ and $4d^o$ orbitals on Ti. The results of this fourth calculation (dashed lines) and of the third calculation (solid lines) are shown in Figure 3. Unlike in the cases of Figure 1 and Figure 2, there is no significant change in the bands for occupied states. *In particular, the changes in occupied energies, from calculation three to four, are in the range of computational errors due to other factors including rounding errors and approximation.* In contrast to the unchanged nature of occupied states, the lowest unoccupied states at the Γ, X, and Z symmetry points are shifted downward by more than 1 eV.

By virtue of the ground state nature of density functional theory[14,15,16,17,18] and in light of the iteration procedure described above and that only includes the wave functions of occupied state in the reconstruction of the charge density, potential, and Hamiltonian, the preferred basis set is that in calculation three. The drastic changes in the unoccupied states, in going from calculation three to four, are attributed to manifestations of the effect described above. The increase of the size of the basis set and the subsequent lowering of some eigenvalues inextricably link the basis set and the variational calculation to this effect. While no other graphs are shown here, we continued to add orbitals of higher and higher excited states to the basis set for calculation five and six. As expected, these calculations did not lead to changes in the occupied states. They led, expectedly, to drastic changes in higher and higher excited electron energy levels.

It should be noted that the effect of the variational theorem, consisting of a

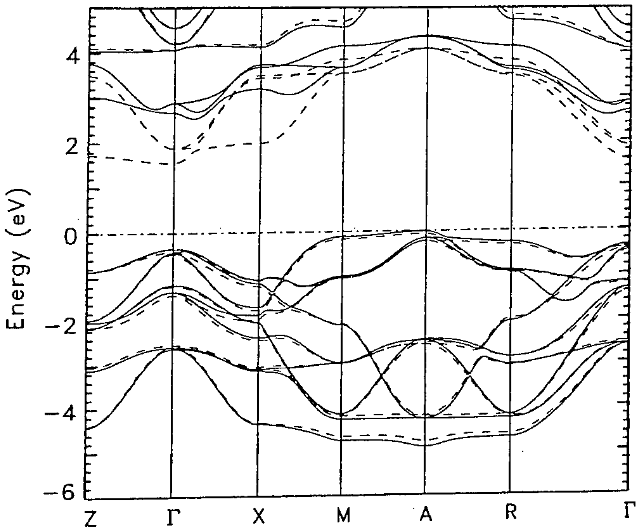

Figure 3: Comparison of the calculated, electronic band structure for tetragonal $BaTiO_3$ from the third calculation (solid lines) with that from the fourth calculation (dashed lines). The basis set in calculation three was found to be "optimum," i.e., increases of the size of this basis, by adding more polarization and/or diffuse orbitals, lead to no improvement in the occupied energy bands. The Fermi levels are superimposed in this graph.

possible lowering calculated energies with increases of the size of the basis set, is not apparent in Figures 1-3, for the occupied states. The Fermi levels are superimposed in these graphs. Simple plots of the data in Figures 1-3, without this superposition, clearly show the variational lowering of the calculated energies when the size of the basis set (or of the Hamiltonian matrix) increases. This is true for occupied and unoccupied states for the cases of Figures 1 and 2.

4. Prediction of Properties of Ferroelectric Material: $BaTiO_3$

The electronic band structure from the optimum basis set of calculation three is shown with solid lines in Figure 3. The zero of the energy is set at the top of the valence band. The calculated band gap (see the solid lines of Figure 3) is about 2.6 eV. This value is quite close to the experimental values of 2.8 to 3.0 eV.[19,20,21] The calculated effective mass of the holes along the c-direction is about 7 - 8 m_0. The effective mass on the plane perpendicular to the c-direction is only about 1.1 - 1.3 m_0. This is consistent with the experimental findings of a strong anisotropy in the hole drift mobility in this material.[22]

The lowest energy states of the conduction bands are not exactly at the Γ point. There are shallow minima near the Γ-point along the [100] and equivalent directions. The shallow minima may be smeared out by effects due to thermal or static disorders or other impurity effects. The effective mass along the [100] direction is then quite sensitive to the smearing effect. For a perfect crystal, the effective mass of the tetragonal phase of $BaTiO_3$ along the [100] direction is about 1.1 m_0. The effective mass for n-type carriers along the [001] direction (c-direction) is much higher than that in the [100] direction and was calculated to be about 3.5 m_0. The calculated properties from the predicted conduction band agree well with the electron transport measurements in single-domain, n-type, ferroelectric barium titanate in the tetragonal phase.[23] Experimental measurements found a strongly anisotropic effective mass along [100] and [001] directions as confirmed by our calculation. The conduction band with many-valleyed structures was also suggested from the experimental data.

The agreement between our computational findings and experiments, as reported elsewhere[3] and here, raised the question whether or not the BZW procedure can yield the correct description of semiconductors, including ferroelectric materials. Recent applications of the BZW procedure to GaN, silicon, diamond, and RuO_2 unambiguously show[6,7] that the procedure indeed leads to the correct description and prediction of properties of other semiconductors, including ferroelectric materials. Conduction bands, band gaps, optical transitions, dielectric functions, and effective masses are among the properties correctly reproduced or predicted by our procedure. The work of Williams showed[24] that the procedure does not lead to an appreciable difference for metals. Presumably, due to the crossing of the Fermi level by at least one band, the occupied bands and the lowest unoccupied bands converge simultaneously with respect to the size of the basis set.

Further, it is expected that the BZW procedure will be needed for variational computations for molecules, clusters, semiconductors, insulators, and for the nuclear shell model, i.e., systems for which there is an energy gap between the highest occupied and the lowest unoccupied levels. While the computations discussed to this point mainly employed a local density potential, this procedure is needed in calculations that employ basis sets of the LCAO or LCGO types, and that reconstruct intermediate quantities, (i.e., charge density, potentials, – in going from one iteration to the next – using only the wavefunctions of the occupied states.

5. Summary

We have identified a spurious basis set and variational effect in self-consistent calculations of the electronic structure of molecules, clusters and solids. The avoidance of the effect in self-consistent calculations basically require the execution of three or more calculations with different basis sets that are selected methodically, following the BZW procedure. Essentially, self-consistent calculations that employ basis sets and the Rayleigh-Ritz variational procedure have to avoid this effect. The need to do so is underscored by the role played by unoccupied energy levels and bands in the determination of the band gap in semiconductors and in the calculation of optical properties and related quantities. While many previous calculations may still remain valid in the absence of an implementation of the BZW procedure described above, the case of $BaTiO_3$ suffices to demonstrate that some will have to be revisited. Our procedure eliminates an element of guessing in the selection of an optimum basis set and clearly points to a predictive feature of self-consistent variational calculations.

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Electronic structure and charge transfer in 3C- and 4H-SiC

G L Zhao and D Bagayoko

Department of Physics, Southern University and A & M College, Baton Rouge, Louisiana 70813, USA

E-mail: `zhao@grant.phys.subr.edu` and `bagayoko@grant.phys.subr.edu`

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Abstract. We utilized a local density functional potential, the linear combination of atomic orbital (LCAO) method, and the BZW procedure to study the electronic structure of 3C- and 4H-SiC. We present the calculated energy bands, band-gaps, effective masses of n-type carriers, and critical point transition energies. There is good agreement between the calculated electronic properties and experimental results. Our preliminary total energy calculations for 3C-SiC found an equilibrium lattice constant of $a = 4.35$ Å, which is in agreement with the experimentally measured value of 4.348 Å. The calculated charge transfers indicate that each silicon atom loses about 1.4 electrons that are gained by a carbon atom in both 3C- and 4H-SiC.

1. Introduction

Due to its superior electronic, mechanical and chemical properties, silicon carbide (SiC) has become one of the most promising materials for high-temperature and high-power device applications [1, 2]. The large Si-C bonding energy makes SiC resistant to chemical attack and radiation and ensures its stability at high temperature. SiC is probably the most prominent material that exhibits a wide range of polytypism. More than 200 SiC polytypes have been determined. Among the SiC polytypes, 3C and 4H polytypes are attracting more attention for their favourable electronic properties.

In this paper, we report *ab initio* studies of the electronic structure and charge transfer in 3C- and 4H-SiC. *Ab initio* approaches based on density functional theory, in the local-density approximation (LDA) [3, 4], are well established as very powerful tools for studying properties of semiconductors, metals, surfaces, or interfaces [5, 6, 7, 8, 9]. In these *ab initio* calculations, the exchange–correlation interactions for the many-body electron system are expressed as a functional of the electronic charge density [3, 4, 5].

However, many LDA calculations for semiconductors or insulators often underestimated the band-gaps by 30–50%. Closely related to the band-gap problem, the calculated low energy conduction bands and optical properties of semiconductors—from many LDA computations—also disagree with experimental results. In the case of previous LDA calculations for Ge, several theoretical band structures are metallic [8, 10, 11], in contrast to experimental results. There have been some theoretical efforts intended to address these issues, including calculations that utilize nonlocal, energy-dependent, non-Hermitian self-energy operators [12, 13, 14, 15, 11]. Aryasetiawan and Gunnarsson reviewed several computational approaches, including the GW method, aimed at describing excited state properties [16]. These authors have shown that with converged basis sets and improved exchange and correlation, the calculated band-gap becomes generally correct. Johnson and Ashcroft utilized some simplified applications of the GW method to make scissors-type corrections to the band-gaps of semiconductors [17].

In previous reports [18, 19], Bagayoko and co-workers identified an effect inherent to the variational calculations that utilize a basis set, as done in the LCAO method. This effect is concomitantly due to basis sets and to intrinsic properties of the Rayleigh–Ritz variational approach as explained below. The Rayleigh theorem [20, 23] states that when an eigenvalue equation is solved by the LCAO method, using a basis set of N orbitals and one of $(N + 1)$ orbitals, where the larger set of size $(N + 1)$ is obtained by augmenting the smaller one of size N, then the calculated eigenvalues satisfy the following inequalities: $E_1^N \geq E_1^{N+1}$, $E_2^N \geq E_2^{N+1}$, $E_3^N \geq E_3^{N+1}, \ldots$. Succinctly, and provided the above conditions are met, a given eigenvalue is never increased by an increase of the size of the basis set; it either remains unchanged (i.e. if it is equal to the exact value) or is lowered to approach the exact eigenvalue from above. This theorem clearly dictates the use of large basis sets to ensure the convergence of calculated eigenvalues to the corresponding exact ones. Further, completeness consideration requires that the basis sets be as large as possible. Consequently, variational calculations generally place a needed emphasis on ensuring convergence by utilizing large basis sets. The method described below recognizes this requirement and the fact that only the wavefunctions of occupied states are used in the iterative procedure to reconstruct the charge density and the potential. This last fact provides a possible criterion for determining an optimum basis set, i.e. the convergence of the eigenvalues of all the occupied states. This criterion essentially defines the Bagayoko, Zhao and Williams (BZW) procedure that adds to the available approaches for first-principle calculations of properties of materials, with emphasis on the description of excited states and band-gaps.

This procedure has been applied to describe, within the local density approximation, the electronic and optical properties of $BaTiO_3$ [19], wurtzite GaN, Si, diamond (C) and RuO_2 [24]. In this paper, we report our calculations of the electronic properties and charge transfer for 3C- and 4H-SiC, employing the BZW procedure [18, 19, 24].

In the next section, we summarize our computational method. The calculated results are presented in section 3. They are followed by a short conclusion in section 4.

2. Method

Our self-consistent calculations utilized the *ab initio* linear combination of atomic orbital (LCAO) method. These self-consistent LCAO calculations included all electrons and full potentials, without shape approximations. Details of the general computational method are available in previous publications [7, 25, 26, 27, 28, 29]. We employed the Ceperley–Alder type [30] of the local density functional potential as parametrized by Vosko *et al* [31]. The newly developed BZW procedure [18] is employed throughout the calculations. Our calculations are non-relativistic.

Bagayoko, Zhao and Williams (BZW) utilized the criterion discussed above to introduce an *ab initio* procedure for identifying optimal basis sets in variational calculations. Essentially, this procedure requires the performance of three or more self-consistent calculations, beginning with the minimal basis set. The minimal basis set is that required to account for all the electrons of the atomic or ionic species in the material (molecules, clusters, or solids). Every subsequent calculation is carried out with a basis set including that for the previous calculation plus one (or more) orbital of the atomic or ionic species that are present in the material under study. These orbitals are added in the order of increasing energy. Several self-consistent calculations are done until the energies of the occupied states, for calculation N, are the same as those for calculation $(N+1)$. Then, the material is studied using the basis set from calculation N, known as the optimum basis set. Physically, the BZW procedure defines a new form of convergence, i.e. that of the occupied states (or charge density) with respect to the size of the basis set.

In these calculations for 3C- and 4H-SiC, the atomic wavefunctions were constructed from results of self-consistent *ab initio* atomic calculations. The radial parts of the atomic wavefunctions were expanded in terms of Gaussian functions. Even-tempered sets of Gaussian exponents were employed for both Si and C. The minimum and maximum Gaussian exponents for Si are 0.16 and 0.65×10^5, in atomic units, respectively. The minimum and maximum exponents for C are 0.1 and 0.65×10^5. We included 22 Gaussian orbitals for the expansion of the atomic wavefunctions of the s and p states for Si and C. For the extra atomic wavefunction of Si(3d), we used 18 Gaussian orbitals. We found that the optimal basis set [18, 19, 24] for the LCAO calculations of the electronic structures of 3C- and 4H-SiC consists of the atomic orbitals of Si(1s2s3s4s 2p3p 3d) and C(1s2s3s 2p). Here, Si(4s 3d) and C(3s) represent empty shells in free atoms or ions. They are used to augment the basis set to account for charge redistribution in the solid environment.

3C-SiC (or β-SiC) is the only type of the cubic structure of silicon carbide with a zinc-blende arrangement. In our studies of the electronic structure of 3C-SiC, we used a lattice constant of $a = 4.35$ Å, which is the experimentally measured value. Our calculations of the total energy led to this value as the theoretical one. In the self-consistent calculations of 3C-SiC, we included 28 general k-points in the irreducible Brillouin zone, with proper weights. The computational error for the valence charge was about 0.00056 for 16 electrons. The self-consistent potential converged to about 10^{-5}.

4H-SiC belongs to the C_{6v}^4 group. The atoms of its four 'molecules' are all on the trigonal axes in the special positions of the C_{6v}^4 group:

$$(2a) \quad (0,0,u); (0,0,u+1/2);$$
$$(2b) \quad (1/3,2/3,v); (2/3,1/3,v+1/2)$$

with u(Si) = 3/16, v(Si) = 7/16, and u(C) = 0, v(C) = 1/4. We used the experimental lattice constants of $a = 3.073$ Å, and $c = 10.053$ Å. In the self-consistent calculations of 4H-SiC, we included a mesh of 24 k-points, with proper weights, in the irreducible Brillouin zone. The computational error for the valence charge was about 0.25 for 64 electrons. The self-consistent potentials converged to a difference around 10^{-5} after about 50 iterations. The total number of iterations varies with the input potentials.

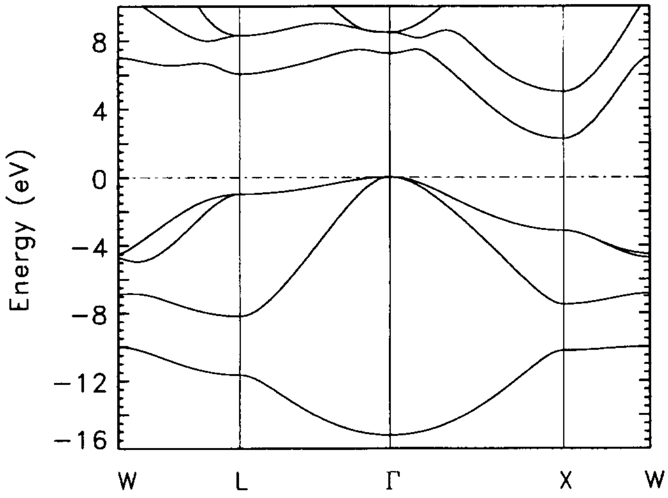

Figure 1. The calculated electronic energy band structure of 3C-SiC along high-symmetry directions, as obtained with the optimal basis set from the BZW procedure.

3. Results

3.1. Electronic structure and total energy of 3C-SiC

The electronic energy bands of 3C-SiC, calculated with the optimal basis set, are shown in figure 1. The zero of the energy is set at the top of the valence band. The top of the valence band of 3C-SiC is at the Γ-point and the lowest conduction band is at the X-point. Our calculated valence bands of the occupied states of 3C-SiC, figure 1, are very close to the previously reported results of *ab initio* LDA calculations [11, 33, 34, 35, 36, 37, 38]. Such agreements are expected from the BZW procedure, since the optimal basis set is the smallest basis set that leads to the same occupied eigenvalues or charge density as all the larger basis sets. The extra lowering of the unoccupied states of the conduction bands, as noted above, is avoided methodologically by the BZW procedure. Comparing our calculated conduction bands in figure 1 with previously reported results for 3C-SiC shows differences that are not a rigid shift of a set of bands with respect to another. These differences between our calculated conduction bands and previous LDA results directly affect the band gap and electron transition energies. Our calculated indirect band-gap of 3C-SiC is 2.24 eV, which is very close to the experimental value of about 2.2–2.4 eV [1, 32]. The previous LDA calculations obtained a theoretical band-gap of about 1.3 eV [33, 11], which was much smaller than experimental results.

Table 1 lists our calculated critical point transition energies of 3C-SiC, along with experimental results. In this table, the indexes v and c refer to the valence and conduction bands, respectively. The experimental transition energies are deduced from the decomposition analysis of the $\epsilon_2(\omega)$ spectrum [41]. Our calculated optical transitions, without any shift, agree well with experimental results. The previously calculated critical point transition energies of 3C-SiC differ with experimental results by about 1 eV [41]. We ascribe the difference between previous LDA results and experiments to the effect circumvented by the BZW procedure as noted above.

Table 1. Comparison of the calculated critical point transition energies (in eV) for 3C-SiC with experimental results. The experimental data are from [41] except where noted otherwise.

3C-SiC	Calculation	Measurements
E_g	2.24	2.2[1] 2.4[32]
$\Gamma^v_{15} \rightarrow \Gamma^c_1$	7.23	7.4
$L^v_3 \rightarrow L^c_1$	7.02	7.5
$X^v_5 \rightarrow X^c_1$	5.39	5.8
$X^v_5 \rightarrow X^c_3$	8.14	8.3±0.1
$\Gamma^v_{15} \rightarrow \Gamma^c_{15}$	8.46	9.0±0.2
$L^v_3 \rightarrow L^c_3$	9.27	9.4

Table 2. The effective masses (in m_0) of the n-type carriers at the lowest conduction band of 3C- and 4H-SiC. The theoretical $m_\perp$ of 4H-SiC was calculated as the geometric average of $\sqrt{m_{M\Gamma}.m_{MK}}$.

	Calculation	Measurements
3C-SiC		
$m_{X\Gamma}$	0.72±0.04	$0.677 \pm 0.015(m_{nl})$[42]
m_{XW}	0.22±0.02	$0.247 \pm 0.011(m_{nt})$[42]
4H-SiC		
$m_\perp$	0.41±0.02	0.42[40]
$m_\parallel(m_{ML})$	0.31±0.02	0.33 ± 0.01[46] 0.29[40]
$m_{M\Gamma}$	0.62±0.03	0.58 ± 0.01[46]
m_{MK}	0.27±0.02	0.31 ± 0.01[46]

The effective mass is a measure of the curvature of the calculated bands. The agreement between calculated and measured effective masses indicates an accurate determination of the shape of the bands. Our calculated effective masses of the n-type carriers are listed in table 2. The calculated electron effective mass around the conduction band minimum of 3C-SiC near the X-point is $m_{nl} = 0.72 \pm 0.04 m_0$ for the Γ–X direction, and is $m_{nt} = 0.22 \pm 0.02 m_0$ for the X–W direction. Here, m_0 is the free electron mass. The calculated, anisotropic effective masses are in good agreement with the reported experimental data of $m_{nl} = 0.677 \pm 0.015 m_0$, and $m_{nt} = 0.247 \pm 0.011 m_0$ [42]. The good agreements of the calculated effective mass and the band-gap with corresponding experimental results indicate that the lowest conduction band in figure 1 is reasonably reliable. Our calculated effective masses are not much different from those of previous LDA calculations, indicating that the extra lowering of the conduction bands, in the absence of the BZW procedure, does not seriously affect the shape of these low-energy conduction bands.

The calculated total and partial density of states (DOS) of 3C-SiC are shown in figure 2 and figure 3. From figures 1, 2 and 3, we can see that the lower valence band ranging from -15.2

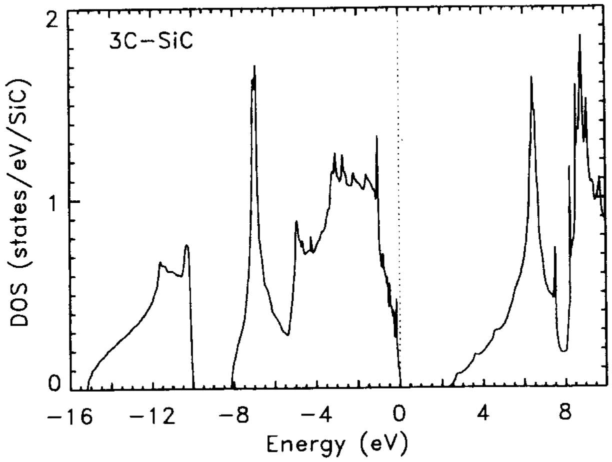

Figure 2. The total density of states (DOS) of 3C-SiC.

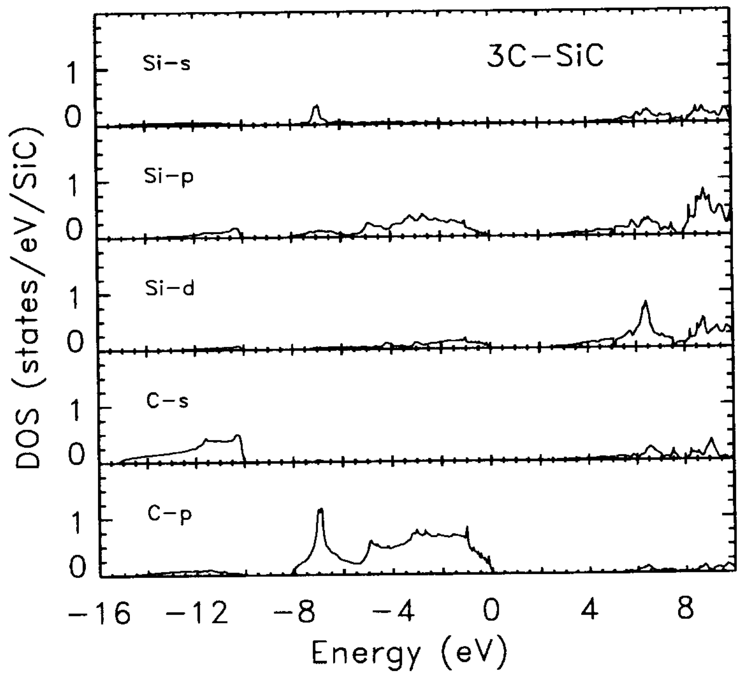

Figure 3. The partial density of states (PDOS) of 3C-SiC.

eV to -10.0 eV is dominated by the C(2s) states that are hybridized with the Si(3p) and C(2p) components. The upper valence bands are dominated by the C(2p) states and strongly hybridized with the Si(3p) states. The Si(3d) bands are highly extended and contribute also to the occupied valence bands in the solid-state environment. The conduction band of 3C-SiC has a long tail, ranging from 2.24 eV to about 5 eV, which is attributed to the wide conduction band around the X-point. In figure 2, the extended tail from the conduction band leads to some experimental complications in determining the exact band gap, including the optical absorption edge which can extend to several tenths of an eV. The total DOS curve in figure 2 shows that the 'practical'

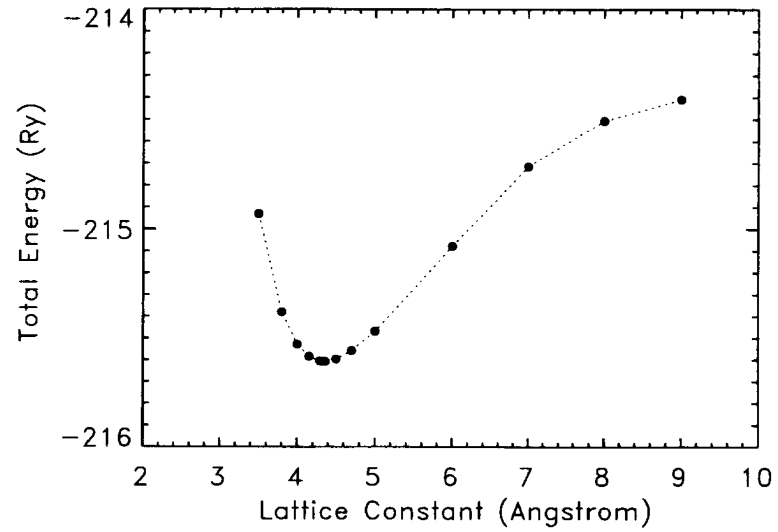

Figure 4. The calculated total energies of 3C-SiC at different lattice constants in the zinc-blende structure. The minimum total energy is located at a lattice constant of 4.35 Å.

An essential, physical quantity in density functional theory is the ground-state total energy of the system. Recently, we have performed preliminary total-energy calculations for the cubic structures of SiC. The calculated total energies for 3C-SiC at different lattice constants are shown in figure 4. The total energies in figure 4 are computed from the electron charge density using the optimal basis set that is identified by the BZW procedure. The calculated equilibrium lattice constant of 3C-SiC, i.e. the value at the minimum of the total energy curve, is 4.35 Å. This value is in excellent agreement with the experimentally measured lattice constant of 4.348 Å[43]. The calculated bulk modulus of 3C-SiC, from the total energy curve in figure 4, is 2.2 Mbar, which also agrees very well with the experimental value of 2.24 Mbar [44].

3.2. Electronic structure of 4H-SiC

The electronic bands of 4H-SiC along some high symmetry lines are shown in figure 5. The notation of the symmetry points in the Brillouin zone follows the convention used by Koster [39]. The highest occupied state of the valence band is at the Γ-point. The conduction band minimum is at the M-point. There is a second minimum of the conduction band at the M-point, which is only 0.18 eV above the lowest unoccupied state. These results are consistent with the ballistic electron emission microscopy study by Kaczer *et al* [45] who observed the second minimum of about 0.15 eV above the lowest conduction band minimum in 4H-SiC. The slight difference between these two minima is attributed to both computational and experimental limitations. These limitations include uncertainties introduced in the fit procedure in the analysis of the experimental data and computational uncertainties that include rounding errors. The indirect band-gap from our calculated electron structure of 4H-SiC is 3.11 eV, which is very close to the experimental data of about 3.2–3.3 eV [1, 32].

The calculated effective masses of the n-type carriers around the conduction band minimum of 4H-SiC are also listed in table 2. Our calculated electron effective mass in the plane

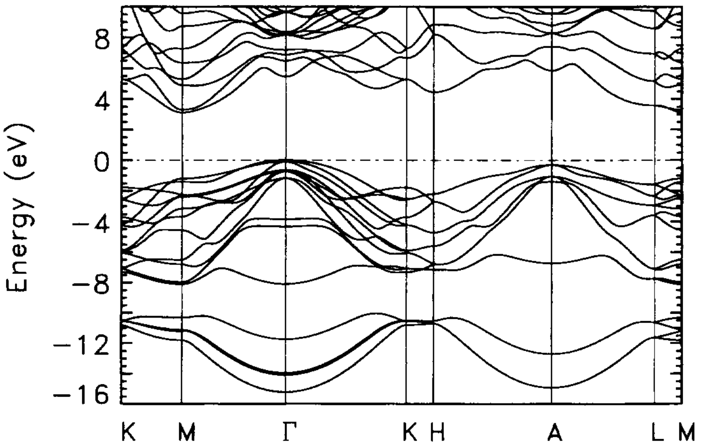

Figure 5. The electronic energy band structure of 4H-SiC along high-symmetry directions, as obtained with the optimal basis set from the BZW procedure.

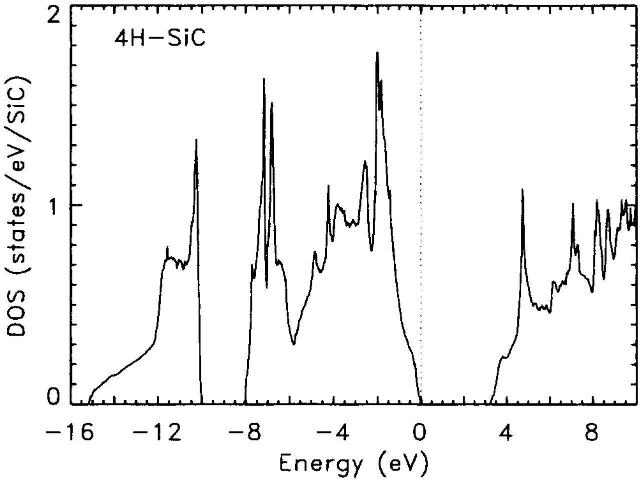

Figure 6. The total density of states of 4H-SiC.

experimentally measured result of 0.42 m_0 [40]. Here, $m_\perp$ is calculated as the geometric average of $\sqrt{m_{M\Gamma}.m_{MK}}$. The calculated effective masses of the n-type carriers in the direction parallel to the c-direction is $m_{ML} = 0.31 \pm 0.02 m_0$, which also agrees well with the experimental results of 0.29–0.33 m_0 [40, 46].

The calculated total and partial density of states (DOS) of 4H-SiC are shown in figures 6 and 7. The density of states of 4H-SiC is very similar to that of 3C-SiC. However, the conduction band edge of 4H-SiC does not have the long tail that that of 3C-SiC does.

3.3. Charge transfer in 3C- and 4H-SiC

Both the silicon and carbon atoms have four valence electrons and prefer a four-fold tetrahedral bond arrangement in the formation of compounds. Charge-transfer properties in SiC are consequently not trivial. We calculated the effective charges and charge transfer for 3C- and

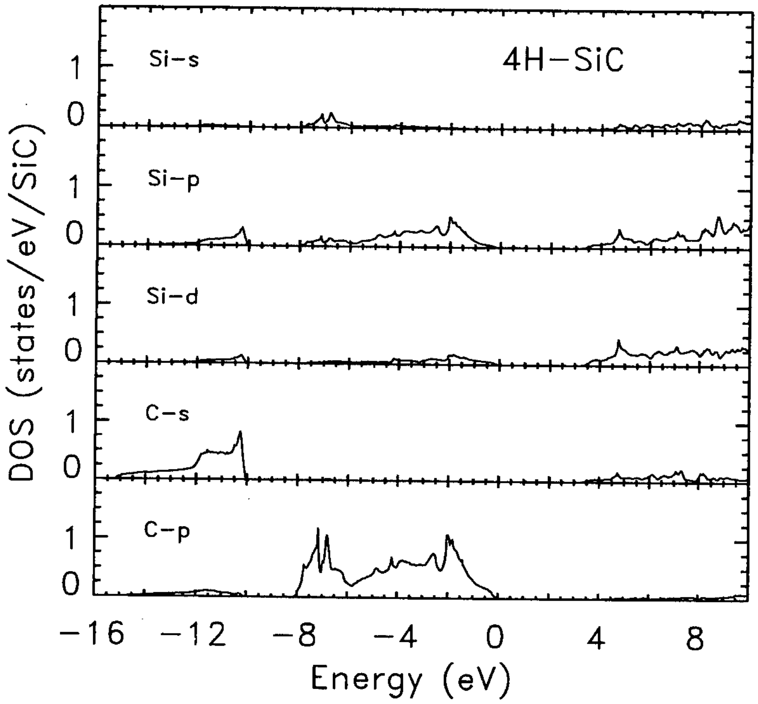

Figure 7. The partial density of states of 4H-SiC.

for calculating the effective charge and charge transfer has been discussed in a previous publication [47].

Our calculated results suggest that the charge transfer in 3C-SiC is very close to that in 4H-SiC, with a difference in the range of computational uncertainty. We found that silicon atoms, in 3C and 4H silicon carbides, give about 1.4 electrons/atom that are gained per carbon atom. The ionic formula for 3C and 4H silicon carbides can be written as $Si^{+1.4}C^{-1.4}$. This result, in retrospect, is understandable in the light of more effective shielding of the nucleus in Si as compared with C. The calculational error for the charge transfer was estimated at about ±0.1 electrons.

The charge transfer in 3C- and 4H-silicon carbides occurs mainly in the formation of the Si-C bond. In the formation of the Si-C bond in 3C- and 4H-SiC, the charge transfer is about 0.35 electrons/bond, which is very close to the so-called ‘one third rule’ suggested in the studies of silicon nitride [48, 47].

We also studied the dependence of the charge transfer on the Si-C distance or bond length in 3C-SiC. This dependence is relevant to understanding or simulating the formation of the Si-C bond. We performed *ab initio* self-consistent calculations for several values of the lattice constant. The calculated results for the charge transfers are listed in table 3. Here, we define the bond length as the distance between Si and C when they are the first nearest neighbours. Table 3 shows that the calculated charge transfer, from Si to C atoms in 3C-SiC, remains nearly constant for a substantially large range of the lattice constant or of the bond length. These results support the practice of assuming that the charge transfer in silicon carbides is a constant, as done in molecular dynamical simulations or in calculations of mechanical properties.

Table 3. The calculated charge transfer, from Si to C atoms in 3C-SiC, at different lattice constants and bond lengths.

Lattice constant (Å)	Bond length (Å)	Charge transfer (electrons)
4.35	1.884	1.4
4.50	1.949	1.4
5.00	2.165	1.5
6.00	2.598	1.4
7.00	3.031	1.4
8.00	3.464	1.2
9.00	3.897	1.1

4. Conclusion

We have calculated the electronic structures of 3C- and 4H-SiC, using the *ab initio* LCAO method and the newly developed BZW procedure. Our calculated valence band structures of 3C- and 4H-SiC agree with previous results from first-principle calculations. Our calculated band-gaps, effective masses of n-type carriers, and critical point transition energies agree well with experimental results. Our preliminary total energy calculations for 3C-SiC led to an equilibrium lattice constant of a= 4.35 Å, which is in an excellent agreement with experiment. Our calculated results suggest that the charge transfer in 3C-SiC is very close to that in 4H-SiC. The silicon atoms, in 3C and 4H silicon carbides, give about 1.4 electrons/atom to the carbon atoms. For a substantially large range of the bond length, the calculated charge transfer from Si to C atoms remains nearly constant in 3C-SiC.

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I

Local-density-approximation prediction of electronic properties of GaN, Si, C, and RuO_2

G. L. Zhao, D. Bagayoko, and T. D. Williams
Department of Physics, Southern University and A & M College, Baton Rouge, Louisiana 70813

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G. L. Zhao, D. Bagayoko, and T. D. Williams
Department of Physics, Southern University and A & M College, Baton Rouge, Louisiana 70813

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We present calculated electronic properties of gallium nitride (GaN), silicon (Si), diamond (C), and ruthenium dioxide (RuO_2). We implemented a simple computational procedure that avoids a recently identified basis set and variational effect. This effect, inherent to the use of basis sets in variational calculations, is believed to have affected *ab initio* calculations of electronic properties of semiconductors since their inception. We employed *ab initio*, density-functional calculations using a local-density-approximation potential and the linear combination of atomic orbital formalism. There is an excellent agreement between our findings and experimental results. In particular, the calculated, direct, minimum band gap of GaN, for low temperatures, is 3.2 eV, while the practical band gap, as per the calculated density of states, is 3.40 eV. Band gaps and excitation energies for silicon and diamond compare favorably with experimental results.

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I. INTRODUCTION

Local-density approximation (LDA) calculations for semiconductors, until very recently,[1,2] often led to band gaps that are typically 30–50% smaller than the experimental values.[3,4] The discrepancies between LDA and experimental results have been mostly ascribed to limitations of the local-density approximation. The quasiparticle calculations of Rubio *et al.*[3] provide energy bands and a band gap for wurtzite GaN that agree with experiment. The dressed Green function (G) and screened Coulomb interaction (W) approach of these authors, i.e., the GW method, used nonlocal, energy-dependent, non-Hermitian operators, which are beyond density-functional theory. The essential differences between the GW results and those of previous LDA calculations are mainly between the conduction (unoccupied) energy bands obtained by the two approaches. There is a reported, surprising agreement, however, between LDA and GW results for the wave functions of the valence (occupied) bands. A recent attempt to remedy the reported failure of LDA for the conduction bands of semiconductors consists of the work of Vogel *et al.*[4] These authors employed pseudopotentials that included self-interaction corrections (SIC) and self-interaction and relaxation corrections (SIRC) in an otherwise local-density potential calculation. They obtained wurtzite GaN band gaps of 1.7 and 4.0 eV with a standard LDA pseudopotential calculation and a new pseudopotential, LDA calculation with self-interaction and relaxation corrections, respectively. Vogel *et al.* utilized the Ceperley and Alder form of local-density approximation as parametrized by Perdew and Zunger.[5]

Recently, Bagayoko and co-workers identified[1,2,6] a basis set and variational effect inherently associated with the use of the linear combination of atomic orbital (LCAO) or linear combination of Gaussian orbital (LCGO) formalism in variational calculations of the Rayleigh-Ritz type. Essentially, the effect consists of a possible lowering of some unoccupied energy levels or bands for molecules, clusters, or solids, on account of a mathematical fact.[7,8] This fact is stated in the theorem[7] that describes the lowering or unchanged feature of any variational eigenvalue as the size of the basis set, i.e., the dimension of the matrices in the eigenvalue equation, increases. The theorem simply asserts that a given variational eigenvalue upon an increase of the size of the basis set is never increased, and that it remains either unchanged (i.e., if it is equal to the corresponding exact eigenvalue of the matrix) or it is lowered to approach the exact eigenvalue from above. The extent to which such exact eigenvalues are close to their corresponding eigenenergies of the physical system under study depends on the basic theory and the approximations utilized in the process of generating the matrix. Bagayoko and co-workers[1,2] identified the basis set and variational effect that consists of any lowering of unoccupied energy levels or bands beyond that which occurred before the "convergence" of the occupied levels with respect to the size of the applicable basis set. The possible, unphysical nature of such a lowering, they stated, stems from the use of the wave functions—of occupied states only—in constructing the charge density and the potential from one iteration to the next.

Bagayoko *et al.*[2] successfully applied the Bagayoko, Zhao, and Williams (BZW) procedure,[1] described below, to circumvent methodically the above basis set and variational effect while avoiding any possible "incomplete" nature of the basis set. Their calculated electronic and optical properties of $BaTiO_3$ agree very well with experimental results. The universal nature of the above mathematical theorem naturally raised the question whether or not the reported limitations of LDA, particularly as they pertain to the description of unoccupied energy levels or bands, are due to LDA or to the manifestation of the above basis set and variational effect.

To partly answer this question, we applied the BZW procedure to study the electronic properties of GaN, Si, diamond (C), and RuO_2. In what follows, we first describe our method, with emphasis on the BZW procedure. We subsequently present the electronic energy bands, density of states, charge transfer, and related physical properties for gallium nitride. This is followed by our findings for silicon, diamond, and RuO_2. These results are obtained with the optimal basis sets as determined by the BZW procedure. We compare our results to experimental and previous theoretical findings. A discussion of the implications of our work follows. The last section provides a brief conclusion.

II. METHOD

A. General approach: LDA potential and LCAO

The calculations discussed below are nonrelativistic. They are performed at zero temperature. The only effect of temperature that is considered is that obtained by using the applicable lattice parameters. Our calculations utilized an expanded version of the electronic structure calculation program package from the Ames Laboratory of DOE in Iowa.[9–14] Details of the computational method are available in several previous publications.[9–13,2] We employed the Ceperley-Alder type[15] of local-density potentials as parametrized by Vosko, Wilk, and Nusair.[16] The above referenced publications describe the general features of our method, i.e., the LDA potential and the standard implementation of the LCAO. We discuss below our distinctive implementation of the LCGO or LCAO method in a fashion that circumvents the basis set and variational effect noted above.

B. The BZW procedure

In a typical *ab initio*, self-consistent calculation that employs the LCAO method, electronic eigenfunctions are expanded using basis sets derived from atomic calculations.[17,18] Charge densities and potentials are constructed. The Hamiltonian matrix is generated and diagonalized. Key output quantities are energy levels or bands and related wave functions. The resulting output wave functions—for the occupied states—are employed to generate a new charge density and the computations are repeated. The process of using the output of iteration (n)—for occupied states—to construct the input for iteration ($n+1$) continues until self-consistency is reached. Various measures are utilized to define self-consistency, i.e., when basic quantities, including charge densities, potentials, eigenenergies, etc. are, respectively, unchanged from one iteration to the next.

The trial basis sets are found by various authors by augmenting the atomic orbitals with polarization and diffuse orbitals[17,18] whose numbers, until the work of Bagayoko, Zhao, and Williams[1] and Bagayoko *et al.*,[2] had no particular limit. In fact, from a completeness standpoint, the larger these numbers the better, provided no "catastrophic sinking of energy levels" or negative Millican population numbers occur for occupied states.[17]

The BZW procedure suggests a minimum of three self-consistent calculations that utilize basis sets of different sizes. It generally begins with the minimum basis set, i.e., the basis set needed to account for all the electrons of the atomic or ionic species that are present in a molecule, a cluster, or a solid. In the case of GaN, we chose these species to be Ga^{1+} and N^{1-}. Completely self-consistent calculations are carried out. For the second calculation, the minimal basis set is augmented with one or more atomic orbitals that belong to the next and lowest-lying energy levels in the atomic or ionic species. The self-consistent bands from calculations I and II are compared, graphically and numerically. In general, there will be qualitative (shape and branching) and quantitative (numerical values) differences between the occupied bands from calculations I and II. A third calculation is performed, using the basis set for calculation II as augmented with orbitals representing the next lowest-lying atomic energy levels. This process is continued until the comparison of the occupied energy levels leads to no qualitative or quantitative difference. When the results from calculation N and those from calculation ($N+1$) agree within the computational error, then the optimum basis set is that of calculation N. This selection rests on the fact that a lowering of unoccupied levels, as in calculation ($N+1$), after the occupied levels converged with respect to the size of the basis set, as in calculation N, could be a mathematical artifact. Such a lowering may not be the manifestation of any fundamental interaction, but rather the expression of the basis set and variational effect identified above. This assertion is partly verified by computational experiments reported in Sec. III A. In multispecies systems like GaN, two or more orbitals may be added at a time if the affected atomic levels are close in energy. While we utilized the occupied energy bands for the determination of convergence with respect to the size of the basis set, we suspect that other parameters could be employed. They may include the charge density for occupied states and particularly the potential.

C. Computational details

The wurtzite GaN belongs to the C_{6v}^4 group. We considered two sets of lattice parameters for GaN. The low-temperature values we selected are $a=3.16$ Å, $c=5.125$ Å, and $u=0.377$,[3] where u is the distance between the Ga plane and its nearest-neighbor N plane in the unit of c. Even though our calculations are for zero temperature, we also performed calculations for experimentally measured lattice constants for room temperature, where $a=3.1878$ Å, $c=5.1850$ Å, and $u=0.375$.[19] In the C_{6v}^4 group, the Ga and N atoms are in ($2b$) positions as follows: Ga, (0, 0, 0), (1/3, 2/3, 1/2); N, (0, 0, u), (1/3, 2/3, 1/2+u).

The atomic wave functions of the ionic states of Ga^{1+} and N^{1-} were constructed from the self-consistent, *ab initio* atomic calculations. The radial parts of the atomic wave functions were expanded in terms of Gaussian functions. A set of even tempered Gaussian exponents was employed with a minimum of 0.166 and a maximum of 0.5585×10^5 in atomic unit. We used 19 Gaussian functions for the s and p states and 16 for the d states. A mesh of 24 k points, with proper weights in the irreducible Brillouin zone, was used in the self-consistent iteration calculations. The computational error for the valence charge was about 0.000 22 for 52 electrons. The self-consistent potentials converged to a difference around 10^{-5} after about 35 iterations. The total number of iterations varies with the input potentials.

In the self-consistent LCAO calculations for Si in the diamond structure, we used the experimental lattice constant of $a=5.43$ Å in the calculations. The atomic wave functions were constructed from results of self-consistent, *ab initio* atomic calculations. The radial parts of the atomic wave functions were expanded in terms of Gaussian functions. A set of even-tempered Gaussian exponents was employed with a minimum exponent of 0.099 and a maximum of

TABLE I. The atomic orbitals used in calculations I to V for RuO_2. Superscript zeros indicate added orbitals representing unoccupied atomic levels.

Basis set 0: core-state orbitals in calculations I to V
Ru($1s,2s,3s,2p,3p$), O($1s$)
Basis set I: Set 0 plus Ru($4s,5s,4p,3d,4d$), O($2s,2p$)
Basis set II: Set I plus Ru($5p^0$), O($3s^0,3p^0$)
Basis set III: Set II plus Ru($6s^0$)
Basis set IV: Set III plus Ru($6p^0$)
Basis Set V: Set IV plus O($4s^0$)

0.65×10^6 in atomic units. We included 19 Gaussian orbitals in the basis set for the expansion of the atomic wave functions of Si. For the extra atomic wave function of Si($3d^0$), we used 15 Gaussian orbitals. In the self-consistent calculations, we included 60 general k points in the irreducible Brillouin zone with proper weights. The computational error for the valence charge was about 0.000 95 for 24 electrons. The self-consistent potential converged to about 10^{-5}.

Diamond (C) has a lattice constant of $a=3.567$ Å. The bond length of the C-C nearest neighbor is 1.545 Å, which is much shorter than the Si-Si bond length of 2.351 Å. The Gaussian functions we used to expand the carbon atomic wave functions have a minimum exponent of 0.12 and a maximum of 0.1×10^6. Sixty k points were used in the self-consistent electronic structure calculations.

Ruthenium dioxide (RuO_2) is a member of the transition-metal oxide family. RuO_2 has a rutile structure and exhibits metallic conductivity. Tetragonal RuO_2 has the symmetry of the $P4_2/mnm(D_{2h}^{14})$ space group.[20] RuO_2 has six atoms per unit cell, two ruthenium and four oxygen. The ruthenium atoms are located at the Wycoff $2(a)$ sites: (0,0,0) and $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$. The oxygen atoms occupy the Wycoff $4(f)$ sites: $\pm(u+\frac{1}{2},\frac{1}{2}-u,\frac{1}{2})$ and $\pm(u,u,0)$. The lattice constants of ruthenium dioxide are $a=4.492$ Å, $c=3.106$ Å, and $u=0.306$.[21] The basis sets for each of the five self-consistent calculations used in the BZW procedure are indicated in Table I. The optimal basis set for the RuO_2 calculation is basis set II in Table I. A total of 25–37 iterations were necessary for convergence. The convergence of the potentials was up to 10^{-5}. We considered 60 k points in the irreducible wedge of the Brillouin zone.

III. RESULTS

A. Electronic energy bands of wurtzite GaN

We have calculated the electronic properties of wurtzite GaN (α-GaN) using the recently introduced procedure.[1,2] Succinctly stated, the implementation of this calculation procedure first consisted of carrying out completely self-consistent calculations for GaN using a minimal LCAO basis set. Namely, the initial charge density for α-GaN was calculated using the atomic orbitals of Ga($1s2s3s4s$, $2p3p4p$, $3d$) and N($1s2s$, $2p$).

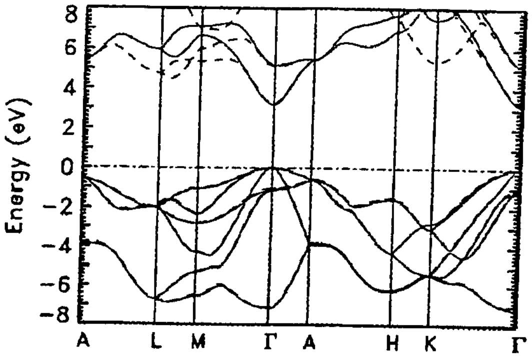

FIG. 1. The calculated, electronic band structure of GaN. The solid lines represent the results of calculation I; the dashed lines show the bands of calculation II. The lattice constants are $a=3.16$ Å, $c=5.125$ Å, and $u=0.377$.

We then repeated the self-consistent calculation using the above basis set as augmented by the orbitals describing the first excited state (i.e., the lowest in energy) of Ga. Hence, Ga($4d^0$) orbitals were added to the basis set. The superscript index of zero indicates that these states are unoccupied in the free atoms (ions). We then plotted the energy bands obtained from these two distinct self-consistent calculations. In Fig. 1 the solid and dashed lines represent the calculated results from the first and second calculations, respectively. Figure 1 shows that the occupied bands from the two calculations differ slightly. In particular, the difference is not a rigid shift of one set of bands with respect to the other. Hence, as noted above, the larger basis set, for the second self-consistent calculation, is preferred to that for the first. This preference is based on physical considerations, i.e., actual, physical interactions are responsible for the difference between the two sets of bands. Completeness requirements, partly to describe the redistribution of the electronic cloud in the solid environment, dictate this preference. The next natural step was to repeat our procedure, for a third time, with a new basis set that includes a N($3s^0$) orbital. The results of this third calculation (dashed lines) and of the second calculation (solid lines) are shown in Fig. 2. Unlike in the case of Fig. 1, the calculated bands for occupied states are fully converged. In particular, the changes in occupied energies, from calculation II to III, are in the range of computational errors that are due to other factors, including rounding errors and possible limitations of LDA. In contrast to the unchanged nature of the occupied states, the lowest unoccupied states at the Γ and A symmetry points are shifted downward by approximately 0.8 eV.

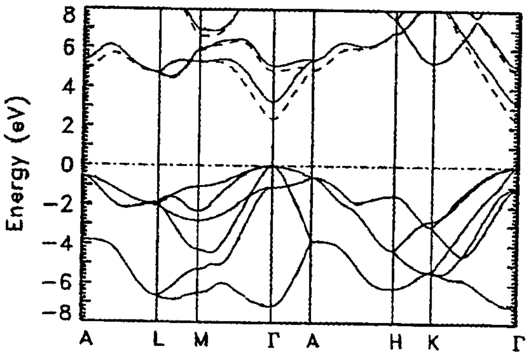

FIG. 2. Comparison of the results of calculation II and III. The solid lines represent the GaN electron bands from calculation II; the dashed lines show the bands from calculation III. The lattice constants are $a=3.16$ Å, $c=5.125$ Å, and $u=0.377$.

TABLE II. The calculated electronic energy levels (in eV) for wurtzite GaN using two sets of lattice constants. Calculation A (LDA A): $a=3.160$ Å, $c=5.125$ Å, and $u=0.377$. Calculation B (LDA B): $a=3.1878$ Å, $c=5.1850$ Å, and $u=0.375$. The lattice constants in the *GW* calculations of Rubio *et al.* are those for calculation A. The minimum band gaps are the energies at Γ_{1c}. See our theoretical DOS for the calculated, low-temperature, "practical" band gap of 3.4 eV.

GaN	LDA A	LDA B	Rubio LDA	Rubio *GW*		LDA A	LDA B	Rubio LDA	Rubio *GW*
Γ_{3v}	−7.1	−7.0	−7.4	−8.0	M_{1v}	−6.5	−6.3	−6.8	−7.4
Γ_{5v}	−1.1	−1.0	−1.1	−1.2	M_{3v}	−5.3	−5.1	−5.6	−6.1
Γ_{5v}	−1.1	−1.0	−1.1	−1.2	M_{1v}	−4.3	−4.2	−4.4	−4.9
Γ_{1v}	0.0	0.0	0.0	0.0	M_{2v}	−2.8	−2.7	−2.8	−3.1
Γ_{6v}	0.0	0.0	0.0	0.0	M_{3v}	−2.3	−2.2	−2.4	−2.6
Γ_{6v}	0.0	0.0	0.0	0.0	M_{4v}	−1.1	−1.0	−1.0	−1.1
Γ_{1c}	3.2	3.0	2.3	3.5	M_{1c}	5.3	5.3	5.1	6.5
Γ_{3c}	5.1	4.9	4.6	5.9	M_{3c}	5.9	5.8	5.7	7.4
Γ_{6c}	10.2	10.1	10.1	11.9	M_{3c}	7.0	6.7	6.2	8.1
Γ_{1c}	10.3	10.1	9.5	12.1	M_{1c}	9.3	9.1	9.1	11.5
$A_{1,3v}$	−3.8	−3.8	−4.1	−4.6	$L_{1,3v}$	−6.7	−6.5	−7.0	−7.6
$A_{5,6v}$	−0.6	−0.5	−0.5	−0.6	$L_{2,4v}$	−2.0	−1.9	−2.0	−2.2
$A_{5,6v}$	−0.6	−0.5	−0.5	−0.6	$L_{1,3v}$	−1.9	−1.9	−2.0	−2.2
$A_{1,3c}$	5.4	5.2	4.6	6.1	$L_{1.3c}$	4.7	4.6	4.4	6.0
$A_{5,6c}$	9.2	9.0	8.7	10.8	$L_{1,3c}$	8.3	8.1	8.0	9.9
K_{1v}	−5.4	−5.2	−5.6	−6.1	H_{3v}	−6.2	−6.1	−6.4	−7.1
K_{3v}	−5.3	−5.2	−5.5	−6.1	$H_{1,2v}$	−4.3	−4.1	−4.6	−4.9
K_{3v}	−3.1	−3.0	−3.2	−3.5	H_{3v}	−1.5	−1.5	−1.5	−1.6
K_{2v}	−2.8	−2.6	−3.0	−3.2	H_{3c}	6.8	6.7	6.6	8.3
K_{2c}	5.3	5.3	4.9	6.6	$H_{1,2c}$	7.5	7.4	7.4	9.4
K_{3c}	8.6	8.4	8.3	10.6					

In light of the iteration procedure described above, and that only includes the wave functions of occupied states in the reconstruction of the charge density, potential, and Hamiltonian, the preferred basis set is that in calculation II. The drastic changes in the unoccupied states, in going from calculation II to III, are believed to be simple consequences of the variational theorem noted above. Namely, this lowering may not be due to a physical interaction, but rather to a mathematical artifact stemming from the variational theorem. While no other graphs are shown here, we continued to add orbitals of higher and higher excited states to the basis set for calculation four and five. As expected, these calculations did not lead to changes in the occupied states. They led, expectedly, to drastic changes in higher and higher, unoccupied bands.

Our claim relative to the use of the wave functions of the occupied states in the self-consistent procedure as a basis for preferring the optimum basis set to larger ones is verified by the following computational experiments. These computational tests, on GaN, addressed the self-consistency of the potential and the effect of the size of the basis set separately. We diagonalized the Hamiltonian matrix, using the larger basis set of calculation III, while utilizing only the self-consistent potential obtained with the optimum basis set. The bands resulting from this diagonalization—for both the occupied and unoccupied states—are the same as the dashed lines in Fig. 2. We also utilized the self-consistent potential obtained with the optimum basis set and diagonalized the Hamiltonian using the minimum basis set. The bands from this calculation closely follow those of calculation II for the occupied states and those of calculation I for the unoccupied states. These tests verified that the potential obtained with the optimum basis is practically identical to that generated with the larger basis set of calculation III and that it is different from the potential obtained with a basis set smaller than the optimum one. A comparison of the results of the diagonalization tests noted above to the self-consistent bands obtained with the optimum basis set is revealing. It consists of a comparison of the effects of the size of the basis set, given that all three calculations employed the self-consistent potential obtained in calculation II. A plot of the results of the diagonalization, using the basis set of calculation III and the self-consistent potential from calculation II, and of the bands from calculations II practically reproduces Fig. 2. Similarly, Fig. 1 is practically obtained by graphing the results of calculation II and those of the diagonalization using the basis set in calculation I and the self-consistent potential from calculation II. These computational experiments verified our contention that due to the variational theorem and the use of the wave functions of the occupied states only in the iterative procedure, the optimum basis set as defined above should be selected instead smaller or larger basis sets.

The electronic band structure of α-GaN, obtained with the optimum basis set of calculation II, is shown in Fig. 2 in solid lines. The zero of the energy is set at the top of the valence band. In our nonrelativistic calculations, the effect of spin-orbit interaction is not considered.

Table II lists the energy levels at high symmetry points in the Brillouin zone for both sets of lattice constants. It also shows, for the same points, the LDA and *GW* results of Rubio *et al.*[3] Our results in columns two and seven (calculation A) are the ones to compare with the *GW* findings of Rubio *et al.*, as they are obtained with the same low-temperature lattice constants specified in Table II. The LDA results of Rubio *et al.* were obtained at slightly different lattice constants representing their theoretical LDA values ($a=3.126$ Å, $c=5.119$ Å, $u=0.377$). Our results in columns three and eight were obtained for room-temperature values of the lattice parameters (calculation B).

Our LDA results from calculation A are different from the LDA findings of Rubio *et al.*, particularly for the conduction bands. Some of these differences are due to that between the sets of lattice constants. Upon superposing the tops of the valence bands, their LDA bands are systematically lower than or the same as ours in energy, except at M_{4v} and $A_{5,6v}$. Their *GW* results are systematically lower and higher than ours for the occupied and unoccupied states, respectively. In all cases, our calculated conduction bands for low temperature lie between their corresponding LDA and *GW* results. As expected from the band structure in Fig. 2, the differences between their LDA results and ours are the smallest at the *H* and *L* symmetry points. The least lowering of unoccupied levels occurs at these points, when basis sets larger than the optimal one are utilized.

The largest difference between corresponding LDA energies for the occupied states is 0.3 eV. This is also the largest difference between occupied or unoccupied LDA energies at the *H* and *L* points. In contrast to the case of occupied states, some LDA conduction-band energies, from the work of Rubio *et al.*, are up to 0.9 eV (at Γ_{1c}) lower than that of our corresponding values. Except at Γ_{1c} where the difference is just 0.3 eV in magnitude, the *GW* results for the conduction bands are generally 0.7 to 2.2 eV higher in energy than we found in calculation A (LDA with low-temperature lattice constants). For the lowest valence states in Table II, the *GW* results are 0.7 (at K_{1v}) to 1.1 eV (at $L_{1,3v}$) lower than our LDA findings.

The effective mass is a measure of the quality of the calculated bands. Specially, the agreement between calculated and measured effective masses indicates an accurate determination of the shape of the bands. Our calculated effective mass for the *n*-type carriers of α-GaN near the Γ point is $0.22\pm0.03m_0$. This result is in a good agreement with the experimental data of $0.2\pm0.02m_0$.[22,23]

B. Density of states, band gap, and charge distribution for GaN

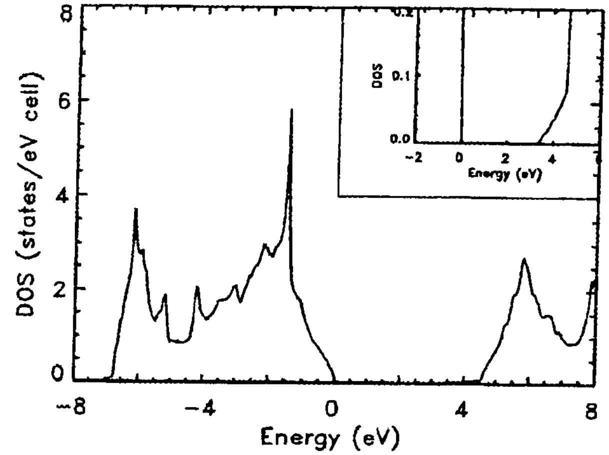

FIG. 3. The calculated density of states for wurtzite GaN, as obtained from the bands in solid lines in Fig. 2. The inset shows that the practically measurable band gap is 3.4 eV.

Figures 3 and 4, respectively, show the total and partial density of states (DOS) for wurtzite GaN, as obtained from calculation A. While much difference is not expected between our DOS and those obtained from previous LDA calculations, for the occupied states, significant discrepancies are obvious for the unoccupied levels. In particular, previous LDA calculations, on account of results in Fig. 2 and Table II, have conduction-band DOS that are shifted toward lower energies as compared to ours. This shift, as per Fig. 2, is not rigid. On the other hand, the *GW* results of Rubio *et al.*, for the conduction bands, are shifted toward much higher energies as compared to ours.

The band gap, until now, has been generally calculated as the difference between the energies for the minimum of the conduction band and the maximum of the valence band. We refer to this band gap, calculated in this fashion, as the theoretical, "minimum" band gap. Our calculation A, with low-temperature lattice parameters, found a minimum gap of 3.2 eV, while the LDA and *GW* works of Rubio *et al.*, respectively, reported 2.3 and 3.5 eV. These minimum band gaps are the energies at Γ_{1c} in Table II. These gaps, as per Table II or Fig. 2, are direct gaps found at the Γ point. Our total DOS curve in Fig. 3, particularly the inset, shows that the calculated, "practical," and measurable band gap for low-temperature GaN is 3.4 eV–in excellent agreement with experiment.[23–26] Indeed, the specially parabolic feature of the bands around Γ_{1c} leads to the very small tail structure that is likely to be difficult to measure. The reported experi-

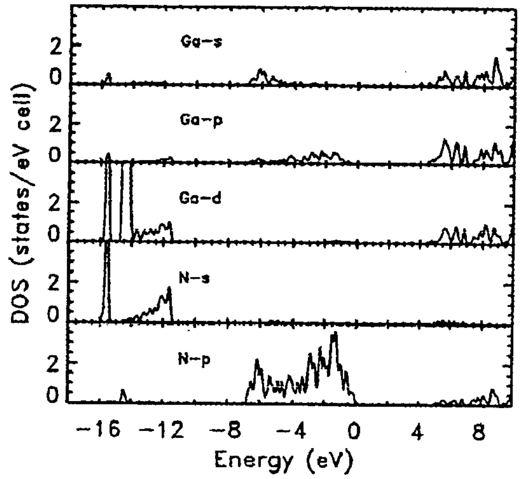

FIG. 4. The PDOS for wurtzite GaN from the contribution of the *s*, *p*, and *d* states of Ga atoms and from the *s* and *p* states of N atoms. These PDOS are derived from the bands (solid lines in Fig. 2) obtained with the BZW optimal basis set.

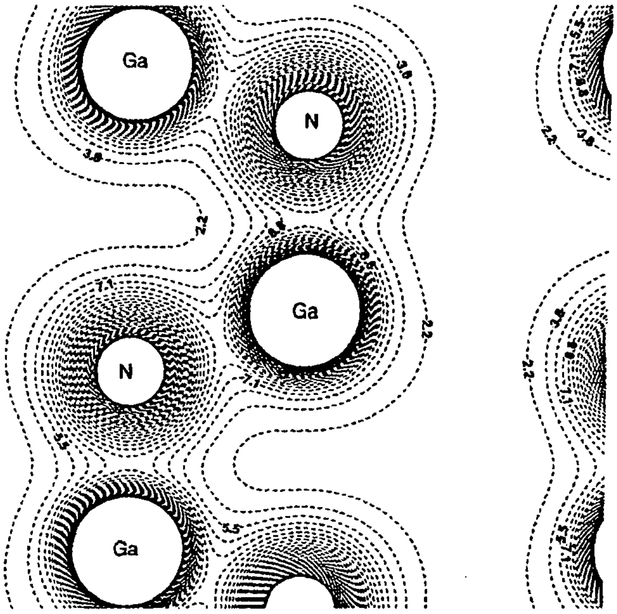

FIG. 5. The charge density distribution on a (010) plane passing through Ga and N atoms. The lattice constants (room temperature) are $a=3.1878$ Å, $c=5.1850$ Å, and $u=0.375$.

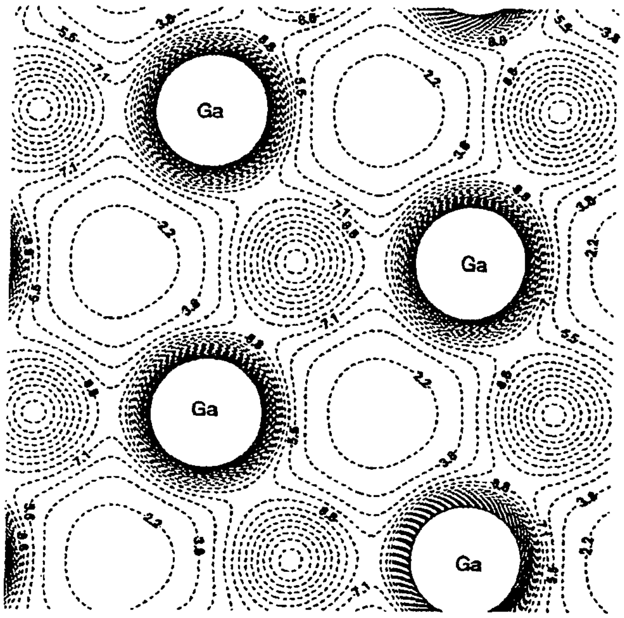

FIG. 6. The charge density distribution on a (001) plane of Ga atoms. The lattice constants (room temperature) are $a=3.1878$ Å, $c=5.1850$ Å, and $u=0.375$.

mental optical-absorption spectrum[25] actually shows the need to define a "practical" band gap, distinct from the minimum band gap. The GW minimum gap of 3.5 eV is therefore expected to lead to a measurable band gap of approximately 3.7 eV or higher, assuming that the *GW* bands preserved the parabolic structure around Γ_{1c}. Our calculation B, with room-temperature lattice constants specified in Table II, found a minimum band gap of 3.0 eV and a practical band gap of 3.2 eV, in excellent agreement with room-temperature experiment.[23,26]

We also calculated the effective charge and charge transfer for wurtzite GaN using the obtained electron wave functions. The calculated charge transfer led to an effective ionic formula of $\mathrm{Ga}^{1.5+}\mathrm{N}^{1.5-}$ for wurtzite gallium nitride.

Figures 5 and 6 show the contour plots of the charge distribution, for room-temperature lattice constants (calculation B), in different symmetry planes, i.e., a (010) plane containing Ga and N atoms, and a (001) plane containing Ga atoms. The unit of the labeled charge density values is 10^{-2} electrons/a_0^3, where $a_0=0.529\,177$ Å. The high charge-density region around the nuclear sites has been cut off in these diagrams at a value of 0.5 electrons/a_0^3, leaving hollow spheres to represent the atomic cores. There are some portions of empty space in the wurtzite structure of GaN, as seen from the charge distribution in Figs. 5 and 6. The empty tubes are distributed in a hexagonal structure along the *c* direction. The calculated electron charge distribution of Fig. 5 indicates that there is a quite strong covalent character of the Ga-N bonds. This can be seen from the noticeable charge distribution at the middle of the Ga-N bond. The size of the nitrogen ions appears larger than that of gallium ions in Fig. 5. The radii of the Ga and N ions in wurtzite GaN are estimated as $r(\mathrm{Ga})=0.92$ Å and $r(\mathrm{N})=1.01$ Å.

C. Electronic properties and optical transitions in silicon

Silicon is probably the best known semiconductor. It has been studied for more than 40 years. We found that the *optimum basis set* for the LCAO calculation consists of the atomic orbitals of Si($1s2s3s4s\,2p3p\,3d$). Here, the Si($4s\,3d$) are empty shells and are used to augment the basis set to account for charge redistributions in the solid environment. The electron band structure of Si, calculated with the optimum basis set, is shown in Fig. 7 without spin-orbit interaction. Figure 7 shows that the top of the valence band is at the Γ point. The minimum of the conduction band is at a general point between Γ and *X*. The calculated indirect band gap is about 1.02 eV, which is very close to the experimental value of about 1.14–1.17 eV.[27,28] The calculated conduction band minima are at $(2\pi/a)(0.79,0,0)$ and at the equivalent points, one along each cube edge. The effective mass of the *n*-type carriers at the conduction-band minimum is very anisotropic. The calculated transverse and longitudinal effective masses are, from the band dispersions in Fig. 7, $m_{nt}=0.20\pm0.03m_0$ and $m_{nl}=0.93\pm0.03m_0$, respectively.

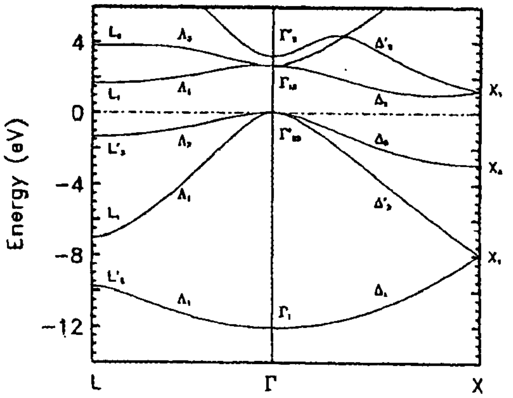

FIG. 7. The calculated electron band structure of Si along the symmetry directions Λ and Δ, as obtained with the optimal basis set of the BZW procedure.

TABLE III. Comparison of the calculated interband-transition energies (in eV) for silicon (Si) with experimental results.

Si	This calculation	Measurements
E_g	1.02	1.14,[a] 1.17[b]
$\Gamma_{1v}\rightarrow\Gamma'_{25v}$	12.1	12.5±0.6[b]
$\Gamma'_{25v}\rightarrow\Gamma_{15c}$	2.68	3.0,[c] 3.4[d]
$\Gamma'_{25v}\rightarrow\Gamma'_{2c}$	3.19	
$X_{4v}\rightarrow\Gamma'_{25v}$	2.93	2.9,[e] 3.3±0.2[f]
$\Gamma'_{25v}\rightarrow X_{1c}$	1.26	1.3[b]
$L'_{2v}\rightarrow\Gamma'_{25v}$	9.80	9.3±0.4[b]
$L_{1v}\rightarrow\Gamma'_{25v}$	7.04	6.8±0.2[b]
$L'_{3v}\rightarrow\Gamma'_{25v}$	1.36	1.2±0.2[b]
$\Gamma'_{25v}\rightarrow L_{1c}$	1.66	1.65,[g] 2.1[h]
$\Gamma'_{25v}\rightarrow L_{3c}$	3.78	3.9±0.1,[b] 4.15±0.01[i]
$L'_{3v}\rightarrow L_{1c}$	3.0	3.2±0.2,[b] 3.45[d]
$L'_{3v}\rightarrow L_{3c}$	5.14	5.1±0.2,[b] 5.5[d]

[a] Reference 27.
[b] Reference 28.
[c] Reference 29.
[d] Reference 30.
[e] Reference 31.
[f] Reference 32.
[g] Reference 33.
[h] Reference 34.
[i] Reference 35.

These calculated effective masses are very close to the experimental values of $m_{nt}=0.19m_0$ and $m_{nl}=0.98m_0$.[28] The good agreements between the calculated effective mass and the band gap, with corresponding experimental results, indicate that the lowest conduction band in Fig. 7 is reasonably reliable.

Table III shows the calculated interband-transition energies, along with experimental results, at selected critical points in the optical spectrum. In this table the indices v and c refer to the valence and conduction bands, respectively. The calculated optical transitions agree well with experimental results. This agreement is particularly significant in light of difficulties in analyzing experimental data, including the effect of lifetime corrections. These corrections are expected to be significant for larger transition energies. In the experimental optical spectrum, each of the structures includes all possible optical transitions. The assignment of one structure to a particular transition from the experimentally measured optical spectrum has been a difficult problem in solid-state spectroscopy.[36] The reported experimental $\Gamma'_{25v}\rightarrow\Gamma'_{2c}$ transition energy of 4.2 eV from the low-field electron-reflectance measurement,[36] disagree with the calculated value of 3.19 eV. Our calculated data suggest that the 4.2 eV transition is rather the $X_{4v}\rightarrow X_{1c}$ transition energy. This conjecture is based on the following reasons. (1) The small phase-space volume around the Γ'_{2c} point only contribute a tail-like structure to the density of states and to the optical spectrum. (2) The Δ_5 and Δ_1 bands are nearly parallel for a substantial portion of the phase-space volume, increasing the possibility for mistaken assignment of structures, and the calculated transition energies from X_{4v} to X_{1c} states are about 4.2 eV. (3) The doubly degenerate Δ_5 bands have a spin-orbit splitting from the Γ'_{25} to the X_4 points, consistent with the experimental observations of the peak structures.

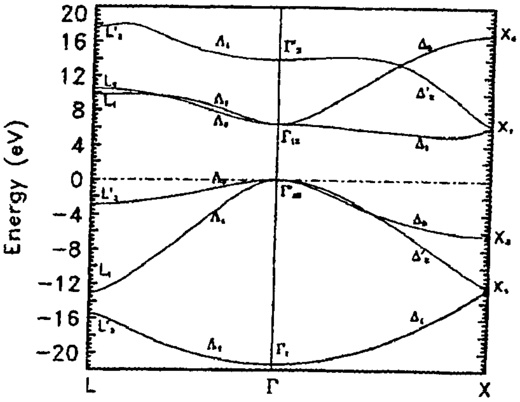

FIG. 8. The calculated electron band structure of diamond (C) along the symmetry directions Λ and Δ, as obtained with the optimal basis set of the BZW procedure.

The $\Gamma_{1v}\rightarrow\Gamma'_{25v}$ transition is a measure of the valence-band width. Our calculated valence-band width of 12.1 eV is in an excellent agreement with the experimentally measured value of 12.5±0.6 eV.

D. Electronic properties and optical transitions of diamond

The BZW procedure leads to an optimum basis set of C($1s2s3s\,2p$) for the LCAO calculation for diamond. Here, the C($3s$) orbital is empty. The calculated electronic band structure of diamond is shown in Fig. 8. The top of the valence band (band edge) is at the Γ point. The bottom of the conduction band is near $(2\pi/a)(0.81,0,0)$. The calculated indirect band gap (E_g) is about 5.05 eV, which is close to the experimental value of about 5.3–5.48 eV.[27,28] There are some experimental complications in determining the exact band gap, including the tails of the optical spectra that can extend to several tenths of an eV.[37,38] The calculated effective masses for the n-type carriers around the conduction-band edge are $m_{n\parallel}=1.1\pm0.2m_0$ and $m_{n\perp}=0.30\pm0.03m_0$. Here, the notations ∥ and ⊥ refer to the directions parallel and perpendicular to the Δ_1 band, respectively. Our calculated effective masses are very close to the reported experimental results of $m_{n\parallel}=1.4m_0$ and $m_{n\perp}=0.36m_0$.[28] There is a strong nonparabolic dispersion of the Δ_1 band around the conduction-band minimum. This leads to a relatively larger uncertainty in obtaining the effective mass and is also part of the reason for the differences in calculations of the effective masses for $m_{n\parallel}$, using different methods.

We listed in Table IV some calculated interband-transition energies at selected critical points. The calculated valence-band width of 21.35 eV is in an excellent agreement with the experimental value of 21±1 eV. The calculated transition energies agree very well with experimental results.

E. Electronic properties of RuO$_2$: Negligible BZW corrections for metals

Our results for the calculated electronic band and related wave functions are characterized by the following two major points: (a) our calculations II through V gave exactly the same results for the valence and low-lying conduction bands

TABLE IV. The calculated interband-transition energies (in eV) for diamond (C).

Diamond	This calculation	Measurements
E_g	5.05	5.3,[a] 5.48[b]
$\Gamma_{1v}\rightarrow\Gamma'_{25v}$	21.35	21 ± 1,[c] 24.2 ± 1[d]
$\Gamma'_{25v}\rightarrow\Gamma_{15c}$	6.36	6.0 ± 0.2,[b] 7.3[e]
$\Gamma'_{25v}\rightarrow\Gamma'_{2c}$	13.87	15.3 ± 0.5[f]
$L'_{2v}\rightarrow\Gamma'_{25v}$	15.49	15.2 ± 0.3[f]
$L_{1v}\rightarrow\Gamma'_{25v}$	13.18	12.8 ± 0.3[f]

[a] Reference 27.
[b] Reference 28.
[c] Reference 37.
[d] Reference 39.
[e] Reference 38.
[f] Reference 37.

in Fig. 9, and (b) these results almost perfectly reproduce those of Ref. 40. The significance of these points stems from the fact that they clearly indicate that corrections expected from the application of the BZW procedure are negligible for metallic RuO_2, unlike in the case of semiconductors. Consequently, our calculated total density of states (DOS) in Fig. 10 are the same as those of Glassford and Chelikowsky[40]—in qualitative and quantitative terms. These authors did not provide the partial density of states (PDOS) we show in Fig. 11. These PDOS qualitatively agree with some results of Schwarz.[41] Our PDOS are different from those obtained by Schwarz for energies between −5 and −10 eV. The differences are both qualitative and quantitative. For instance, our calculated PDOS for Ru 4*d* and O 2*p* clearly show a double-peak structure not discernible from the augmented spherical wave (ASW) results of Schwarz. The magnitudes of the peaks in Fig. 11, between −5 and −10 eV, are more than double the corresponding ones as obtained by Schwarz. We ascribe these discrepancies to differences between our *ab initio* calculations and the ASW method.

The negligible nature of the BZW corrections for metallic RuO_2, as illustrated above, pertains only to descriptive calculations. Namely, computations of properties of a material known to be a metal at a given stoichiometric composition and under specified conditions of temperature and pressure.

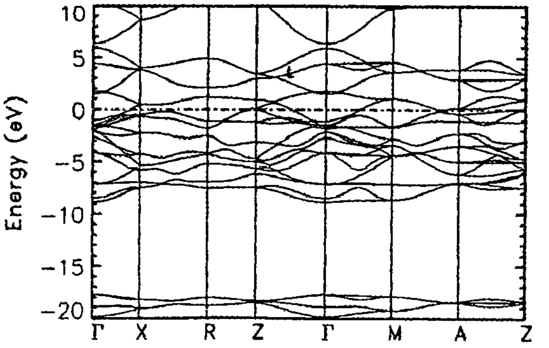

FIG. 9. The electronic band structure of RuO_2 obtained with the BZW optimal basis set. All results here were obtained with basis set II. The shown bands are the same for calculations III–V.

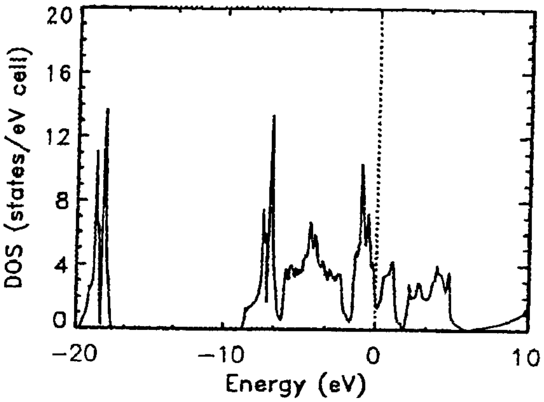

FIG. 10. The DOS for RuO_2.

The BZW procedure is expected to be necessary for predictive calculations, i.e., those for materials whose metallic state is not known or for which elemental composition and related concentrations, pressure, or temperature are changed. While no discrepancies were found between our calculations II to V, for the valence and low-energy conduction bands, the variational theorem necessarily leads to differences for the highest conduction bands. For instance, the fundamental theorem of algebra dictates that the number of calculated eigenenergies increase as the size of the Hamiltonian increases.

IV. DISCUSSION

A. Choices of basis sets and of lattice parameters

It is important to note that the optimal size of the basis set for a given calculation varies with the nature and quality of the trial orbitals. Two computations for the same material, using Gaussian orbitals, are expected to lead to different sizes of the optimal basis set if the Gaussian exponents in the two calculations are different. The essential point is that both calculations must properly implement the procedure to arrive at the optimal size that applies, given the input orbitals. Fur-

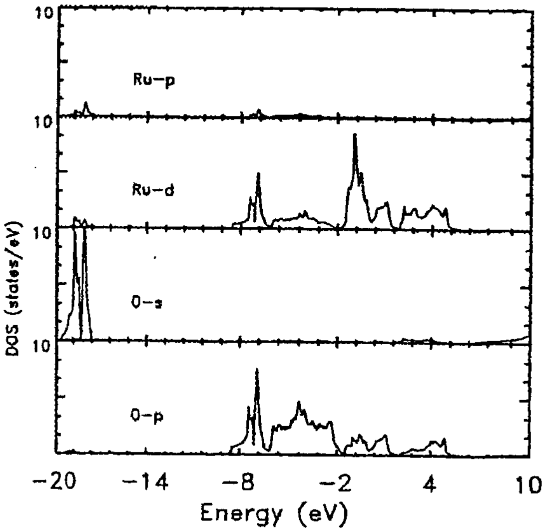

FIG. 11. The PDOS for RuO_2.

ther, Bagayoko showed[18] that the use of contraction of orbitals leads to a rigid shift of the bands. This rigid shift does not affect the physics of the problem. It is a simple manifestation of the referenced variational theorem. The bands obtained with contracted orbitals are shifted upwards as compared to those obtained with uncontracted orbitals—where the dimension of the matrices in the eigenvalue problem is larger.

The above points apply irrespective of the nature of the trial orbitals, i.e., Gaussian, exponential, or others, provided the increases in the size of the basis set progressively account for higher and higher energy orbitals of the input species (atoms or ions). In the case of plane waves, and in light of the relatively large number of orbitals, the implementation of the BZW procedure is expected to be more time consuming if plane waves are added or subtracted one at a time. Additionally, complications arise if higher and higher exponent plane waves are added, as done in some plane-wave calculations, as opposed to beginning with the highest exponents (representing lower, occupied states). The difficulties could be reduced by using augmented plane waves. The adequacy of the trial basis set directly affects the number of additions or subtractions of orbitals for the purpose of determining the optimal basis set for molecules, clusters, or solids. As in the case of Gaussian orbitals, a set of the trial functions describing the ground states of the affected atomic or ionic species is expected to be a good start.

Our choices for the lattice constants were dictated by two considerations. The first one stems from the fact that our program package does not yet include accurate codes for the calculation of the total energy. The search for equilibrium lattice parameters requires high accuracy. The second consideration, equally important, actually dictates that we utilize experimental lattice constants for some comparisons with measurements to be meaningful. Specifically, in the case of GaN, we considered two sets of lattice parameters to enable general comparison with experimental findings and specific comparison with the low-temperature results of Rubio *et al.* In the case of silicon and diamond, matters are complicated further by the fact that some experiments reported slightly different lattice constants. While the use of experimental lattice parameters, as opposed to those for the minimum of the total energy curve versus the lattice parameter, is tantamount to applying pressure to a solid, the results discussed here are best fit for comparison with actual measurements.

B. LDA prediction of properties of semiconductors

The comparison of our results for GaN with those of the *GW* work of Rubio *et al.*[3] should be placed in context. Namely, their *GW* results were obtained by utilizing the valence state eigenfunctions of their LDA calculations. Specifically, their Eq. (3) (Ref. 3) is $E_{n\mathbf{k}}=\epsilon_{nk}^{LDA}+\langle n\mathbf{k}|\Sigma(E_{n\mathbf{k}})-V_{xc}^{LDA}|n\mathbf{k}\rangle$, where $E_{n\mathbf{k}}$ is the *GW* quasiparticle energy, ϵ_{nk}^{LDA} is the corresponding LDA eigenvalue, and $\Sigma(E_{n\mathbf{k}})$ is the energy-dependent self-energy. V_{xc}^{LDA} is the LDA exchange-correlation potential, and $|n\mathbf{k}\rangle$ is the LDA wave function at **k** for band n. In the above equation, ϵ_{nk}^{LDA} is increased or decreased by the many-body correction. The differences between our results and the non-ground-state, quasiparticle eigenenergies from the *GW* calculations are due not only to the difference between the states of the system under considerations, but also to the difference between our LDA results and those of Rubio *et al.*[3] The *GW* eigenenergies are not for the ground state of GaN, as in the case for LDA. They rather belong to a GaN many-body system to or from which an electron is added or removed,[42] respectively. We conjecture that the above corrections could be small if LDA results do not include the basis set and variational effect for some unoccupied bands.

Our results, as presented above, clearly established that some limitations previously ascribed to local-density approximation are not necessarily due to LDA. In particular, and as far as GaN is concerned, a basis set and variational effect was confounded with limitations, if any, of LDA. Bagayoko *et al.* showed the above assertion to hold for their LDA description of $BaTiO_3$.[2]

The possible overestimate of the band gap by quasiparticle calculations is not unique for GaN. The results of Hybertsen and Louie[42] for Si and those of Rohlfing, Krüger, and Pollmann[43] for Si and C are consistently above the experimental numbers. Schöne and Eguiluz[44] recently performed self-consistent *GW* calculations for silicon. They reported a minimum (or absolute) self-consistent band gap of 1.91 eV for silicon. The non-self-consistent gap was 1.34 eV. These authors assert that the self-consistent *GW* overestimates the band gap by as much as "previous" LDA underestimated it. The point of our work, we hope, is to show that the BZW procedure, by avoiding the basis set and variational effect noted above, clearly predict the low, unoccupied energy levels or bands and the band gap—within a local-density approximation.

These results raise questions about other disagreements between LDA and experimental findings. Specifically, the universality of the basis set and variational effect indicates that the BZW procedure should give improved LDA results for molecules, clusters, semiconductors, and insulators. The work of Williams[6] suggests that in the case of metals, the basis set and variational effect should generally be very small. This situation is intuitively understandable in light of the crossing of the Fermi level by some bands. The occupied bands and several low-lying conduction bands converge, simultaneously, with respect to the size of the basis set. This situation partly explains the relative success of previous LDA calculations in describing metals[45] as compared to semiconductors or insulators.

This work and related ones[2,6] noted above established the predictive capability of LDA—provided the BZW procedure is utilized. This procedure avoids the basis set and variational effect on unoccupied eigenstate energies in molecules, clusters, semiconductors, and insulators, while ensuring adequate completeness of the basis set as measured by the convergence of the physical quantities with respect to the size of the basis set. Future calculations with the BZW procedure, we contend, are expected to show a similar predictive capability for other computations based on density-functional theory,[46,47] including investigations using fully relativistic,[48] nonlocal,[49] or temperature-dependent[48] potentials. The applications of the procedure are not limited to density-functional calculations. The BZW procedure is expected to be needed in many self-consistent calculations that utilize basis sets and reconstruct intermediate quantities (i.e., charge density), using only some attributes (i.e., wave functions) of the occupied states.

V. CONCLUSION

Our calculated LDA valence-band structures of GaN, Si, and diamond (C) generally agree with those from previous first-principle calculations. Moreover, our calculated, low-energy conduction bands, band gaps, and effective masses of n-type carriers also agree well with experimental results. This work and the related ones noted above established a predictive capability for the local-density approximation in describing properties of materials. Further, the BZW procedure is expected to be needed by most self-consistent calculations utilizing basis sets in a variational method of th Rayleigh-Ritz type—as long as intermediate steps utilize th wave functions of the occupied states only.

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NAFEO KEYNOTE MESSAGE

DIOLA BAGAYOKO, PH.D.
Director, Timbutu Academy
Southern University System Distinguished Professor of
Physics and Chancellor's Fellow
Director of Campus Coordination, Louis Stokes Louisiana
Alliance for Minority Participation

THE LAW OF PERFORMANCE AND EXCELLENCE IN RESEARCH

A COMPREHENSIVE, PRECISE, DYNAMIC, AND QUINTESSENTIAL GUIDE TO SUCCESSFUL CAREERS IN SCIENCE, MATHEMATICS, ENGINEERING, AND TECHNOLOGY (SMET) FIELDS AND OTHERS

"Luck is what happens when preparation meets or makes, recognizes, and acts on opportunity."

This paper first identifies essential attributes (knowledge, skills, experience, behavioral traits) that undergird successful careers in SMET and other fields. It then presents the Power Law of Performance and the Law of Performance that assert that any individual not suffering from a severe physiological or mental impairment can excel in any discipline of study, including SMET fields, and can secure successful and rewarding research-based careers. *Devoting adequate time to learning and to the practice of research, according to the Law of Performance or of Practice (LP), is the a condition that applies to every individual—irrespective of "perceived" notions of "innate" abilities.* Using meta thinking, we attempt to warn the reader about common errors and misconceptions related to careers, in general, and the ones in SMET, in particular. Specifically, the dynamic or ever-changing nature of work, market, and related environments is a fundamental reason for acquiring the versatility bestowed by research performance and skills. In the context of changes that are becoming faster, due to developments in SMET, research proficiency is both a warranty for continued employment, by virtue of its versatility, and of happiness, due to its many reward$ that include money and very much more. *Hence, beginning immediately and continuing to prepare oneself is the key to excellence.*

INTRODUCTION

While we have no need or intention to sound pretentious, we are compelled to warn the reader that no less than total concentration and the harnessing of most intellectual attributes are needed to appreciate fully what follows. Given the complexity of the issues, we had to utilize universal and powerful principles to address the topic in a comprehensive fashion. We did so by avoiding minutia that change with time and by focusing on overarching principles, trends, and patterns that are germane to the dynamics of human activities—from antiquity to the present and beyond. The size of this paper dictates that the reader be referred to current and future sources that delve into the details of careers in many professions. A second reason for this referral stems from the fact that these details change continually. The "smart" approach, in such instances, is to get the permanent sources of information as opposed to a specific piece of information that may be obsolete in a year or less [1]. The rest of this article follows the order intimated in the abstract.

THE "IMPERATIVES" FOR A SUCCESSFUL CAREER (IN RESEARCH IN SMET)

Language and Communication Skills

A detailed analysis of the tasks a person performs at most jobs reveals the following: (a) the need to read and to understand information from a variety of sources, including written and oral sources, diagrams, videos, etc.; (b) the need to transmit information to others in a flawless fashion—this perfect transmission requires that the information possess the following qualities: *accuracy, precision, completeness, coherence, and clarity (i.e., APC^3)*; the volume of information to transmit and the need for continuity often dictate that a flawless transmission include *written materials*; (c) the fact that learning is cumulative and that the more one knows about a subject or task, the better and faster one can learn additional, related materials, topics, processes, or instruments; and (d) the fact that thinking, after all, is done in a language.

In the case of a research careers in competitive sectors (public or private), having enough knowledge and experience to read and understand the literature and being able to write articles that pass peer or departmental reviews are simply non-negotiable. Further, the continual changes noted above require, to avoid obsolescence, that one follow new developments in *a regular fashion*—through professional magazines (i.e., science, nature), journals, web sites, books, and conferences. To do so, however, demands competitive language and communication skills (i.e., reading, writing, listening, and speaking). These skills, that are acquired and enhanced through practice, constitute the first "imperative" for a successful career. The implication of this everlasting reality is that there is no substitute for the mastery of the applicable language and of the utilization of the key qualities of information (i.e., APC^3). This mastery has to include that of the grammar, vocabulary, syntax, etc. in that language—as verified by standardized tests as opposed to self-misleading perceptions of mastery [see American College Test (ACT), the Graduate Record Examination (GRE), and other tests]. *Consequently, from pre-K to the Ph.D. and beyond, very well-informed individuals regularly and consistently work to hone their language and communication skills. (Well, parents have to ensure the regular and consistent learning up to middle school, in many cases.)*

Homework: As all good professors, the only way we can verify that learning occurred is to close the feedback loop. So, the homework to be done for the above chapter on "competitive language and communication skills" is the following. Conduct three or more interviews of *successful* researchers and professionals (government, academia, or in industry). Design and ask ten (10) or more questions aimed a determining the extent to which language and communication skills play a role in their work. Hint: Do they get information from others? Do they transmit information to others? Do they write proposals? Do they have to follow guidelines or procedure manuals? Do they write strategic or other plans? Do they write reports or any kind? Do they conduct reviews (that require extensive reading)? Do they publish? Do they receive or send letters, memoranda, or electronic mails? Without APC^3, how do they avoid misunderstandings of all kinds—particularly when vital or critical issues are at $take? To what extent have their communication skills (i.e., language and APC^3) contributed to their advancement or promotion? How could they function successfully *without* the communication tasks noted above? Please note, in these web and e-mail days, that many of these interviews could be conducted at a distance!

Mathematics (the language of Science and Technology)

Numbers and mathematics, believe it or not, have been inextricably woven into the fabric of human activities from the dawn of humanity to present. Further, scientific and technological developments that partly rest on mathematics are rendering the master of some mathematics an inescapable condition for successfully fitting into current and particularly future societies. This assertion could be substantiated, at an elementary level, by looking around oneself. What do you see, hear, or feel that can be totally characterized without using mass (numbers), shape (numbers and geometry), volume (numbers and geometry), or intensity (as of light or of sound, numbers)? At the intermediate level, motions of all kinds require numbers and mathematics for a complete description. It will require more than one book to describe the mathematics that went into the design and production of tools of all genres [i.e., kitchen appliances, pieces of equipment in hospitals, cars, airplanes, computers, sophisticated software products performing formidable operations, etc.]. **The ubiquity of mathematics is the reason it is the second "imperative" for a successful career (and for simply fitting functionally into present and future societies).**

The direct and obvious consequence of the above status of mathematics is that from pre-K to the Ph.D. and beyond, well-informed individuals work regularly and persistently to acquire, maintain, and enhance their mastery of mathematics. This mastery, as in the case of language and communication skills, is to be determined by objective measures and not delusional perceptions or ideas of mastery. Be kind and inform your younger relatives and your descendants that a solid mathematics course (or more) should be taken every year of high school—up to calculus, at a minimum. Inform parents you know that Algebra I should be taken in the 8th grade, at the latest. In college, the calculus series is a necessity, from calculus I to III. (Pre-calculus courses may need to be taken, before the first college calculus, if the high school mathematics was not adequate; before this paper, it is presumed that many people, unfortunately, did not know the utter seriousness with which mathematics has to be taken at all grade levels.) SMET undergraduate students should generally take, in addition to the calculus series, differential equation. Physics majors should add complex variables, vector calculus, and college level linear algebra. We provide below the general way of determining the needed mathematics courses for any major.

Mathematics is the language of science and technology, period, understanding it or not. Unfortunately, one has to know a great deal of science and technology to know appropriately the extent to which this assertion is true. So, a student is generally at a loss as to what mathematics courses to take and in what sequence—given that she/he does not know enough to know. The simple solution to this conundrum is to consult seriously (not in passing) with successful faculty members, researchers, engineers, technologists, medical doctors, etc. while one if far away from their level. (We advise doing it in the freshman or sophomore years if possible.) A synthesis of the responses from these professionals as to what mathematics courses to take and in what order will provide a clear road map. The reason this is critical rests in part on the fact that knowledge is often sequential or taxonomic in mathematics, i.e., Algebra I is needed before Algebra II, irrespective of one's "innate" abilities. *(Remember that no "innate abilities" guarantee championship titles in the Olympics, the National Basket Ball Association (NBA), the National Football Association (NFL), tennis, golf, etc., without extensive and sustained practice over time. Similarly, it takes studying, reviews, practice to excel in intellectual endeavors—so says the law of performance discussed below!).* Oh, some people do not understand that most difficulties in a mathematics class, *for someone who is studying appropriately*, are due to an inadequate background and not to any lack of innate "smartness" as explained below with the law of performance.

Fundamentals of Probability and Statistics

Our third "imperative" is "fundamentals of probability and statistics," a part of mathematics. While space limitation does not allow us to provide details on this affirmation, its importance is the reason it is addressed here by itself. This importance includes system failure issues in engineering, the plethora of probability and statistical systems in physics, and the inescapable presence of probability and statistics in dealing with large numbers of anything (people, electrons, atoms and molecules, nuclei and their decay processes, the parts in a complex system, etc.). Understanding that statistical correlations have nothing to do with causation, in general, may save one from falling under the spell of false claims by ill-informed sources. The complexity of issues in science, technology, and in society makes it patently necessary that a leader, lawyer, scientist, engineer, well-meaning politician, etc., understand the fundamentals of probability and statistics in order to avoid doing the opposite of what she/he meant! The June 15 issue of *Science* reads in part, on page 1971 [2], *"statistics have become indispensable to scientists in almost every discipline."*

If you find the little book entitled "How to use and misuse statistics," or a similar one, you will have illustrations of the above point. The overall need for "probability and statistics" and the *need for it in most graduate programs in SMET demand that one take at least an introductory course in "probability and statistics" before completing the Bachelor's degree program.* In some SMET departments, the above introduction is provided in some courses (i.e., statistics and thermodynamics, in the case of some physics departments). The online textbook by David Lane of Rice University [2] is an ideal self-help tool for an introduction to the basics of statistics. The online, interactive demonstrations of key concepts are noted by *Science* as a distinction of this new resource that was developed in part with funding from the National Science Foundation (NSF).

RESEARCH PROFICIENCY: ULTIMATE VERSATILITY, LIFE-LONG EMPLOYMENT WARRANTY, ETC.

The process of creating new knowledge, i.e., research, is a very complex one. To begin with, it generally demands "competitive language and communication skills" that partly enable life long learning. In SMET, it also demands the mastery of some fundamental mathematics: the scope and depth of the needed mathematics vary with SMET fields, the experimental or theoretical nature of the work, and other factors. Please recall that without some serious mathematics, one cannot even read many publications in SMET let alone add to them.

Research proficiency or expertise includes knowledge, comprehension, application, analysis, synthesis, and evaluation. These six intellectual attributes are known as categories of the Bloom taxonomy of the cognitive domain. As noted above, research proficiency demands "competitive language and communication skills" and "adequate knowledge and skills in some areas of mathematics"—particularly in the case of SMET fields. The performance of research in SMET often follows *the scientific method* that can be written in a variety of ways. Our succinct rendition follows: (1) observations and note taking in accord with APC^3; (2) search for explanations in the scientific literature and note taking according to APC^3; (3) design of experiment or construction of a theory—accompanied with written notes that follow APC^3; (4) conduct of experiments or applications of a new theory—with detailed notes obeying APC^3; (5) analysis of findings (from experiment or theory) and comparison with observations and established, theoretical or experimental knowledge—documented in writing that obeys APC^3; (6) writing report and publishing findings—while paying special attention to accuracy, precision, completeness, coherence, and clarity (APC^3) for every proposition or statement; (7) in case of problems in a step (or if the comparison in step 5 does not lead to agreements), then go back to (1), (2), (3), or (4) to (a) look for possible oversights or errors or (b) formulate a new hypothesis, design a new experiment, or to construct a new theory. It must be clearly understood that while high school and other discussions of the scientific method do not generally include the extensive, detailed, and complete writing according to APC^3, this writing is the hallmark of an understanding of the actual scientific process or method. Laboratory journals or research journals or notes, the latter for theoreticians, are indispensable in the actual practice of research. (Let the hypocentral need for *accurate, precise, complete, coherent, and clear notes* be another reminder of the indispensable role of "language and communication skills" in SMET and in most intellectual endeavors.)

Once the research questions are posed, most research can be thought of a "problem-solving"! Indeed, the only difference may be that some research problems may require months or years to solve completely while some mundane or classroom problems can be solved rapidly. Essentially, however, research is just a form of problem-solving. Some of the researchers we admire the most, besides the ones in SMET, include law enforcement and forensic professionals. For the latter groups, *the critically of paying attention to every detail and of recording every detail cannot be overemphasized.* Indeed, in this area, some data or information can be lost forever—making a solution to the problem extremely difficult if not impossible. For training oneself in problem-solving, i.e., some aspects of research, the reader is urged to consult "A Problem-Solving Paradigm (PSP)" by Bagayoko, Kelley, and Hasan [3], in *College Teaching.* For the first time to our knowledge, there is finally a comprehensive way for teaching or learning problem-solving. The mental attributes or dispositions involved in problem-solving are often the same ones for research—even though the specific, *technical knowledge and skills* for research in different fields could be vastly different.

We assert that research proficiency through the process described above is applicable to most human activities! In particular, the actual practice of research in SMET fields and in others follows our seven steps rigorously. Hence, research proficiency acquired in a discipline, except for some specific technical knowledge and skills, is transferable to research processes in many others. This transferability (i.e., versatility) is a key reason that research proficiency is our fourth "imperative" for a successful career in SMET and other fields. When a division in a major corporation is closed, for any reasons, professionals with research proficiency will generally be transferred to other divisions or will easily find other research-based jobs in the private or public sectors. There lies the reason that research proficiency is life-long employment warranty.

In the event the reader does not know, we should underscore the loss of employment by individuals with no research experiences or skills, upon the closure of their divisions, and the great difficulties they have in finding comparable positions that pay adequately. The increasingly rapid developments in science, mathematics, engineering, and technology are fueling the changes in the job markets. *[Unfortunately, some are not still getting it that good salaries without research skills are very often traps; if and when robots, new technologies, or new knowledge render their positions irrelevant, they will find themselves in debt (house, car, and other notes) and without a meaningful prospect for employment or self-employment.]*

The above point is very difficult to understand. The difficulties stem in part from the fact that some parents or acquaintances without research experiences seem to have done or to be doing rather well! *A reason* for that situation is that when they entered the workforce, the rate of changes was very slow compared to the picture today: there were not cellular phones, Internet, genome maps, sophisticated transportation means, nano-materials, global warming, or space tourism, etc. It is therefore critical *"not to move forward to the past." A second reason* that can lead to grave errors is explained by statistics. The "impressions about some doing very well without research expertise" are very often ill-informed. *Yes, exceptions are not rules. Let the rules guide you.* Indeed, with some basic knowledge of statistics, one can see that anecdotal cases, however glittering or numerous they may be, are never to be taken as central tendencies (a statistical concept) without a full knowledge of the total picture of the groups or systems under study. In other words, the relative success of a few high school or college dropouts, for the cautious thinkers, must not overshadow the dead-ends faced by the great majority of them! *Always remember and be guided by these two reasons.*

Another illustration of the *exception and rule* scenario for you and your peers or relatives follows. Knowing a few NBA or NFL draftees who did very well, financially and otherwise, is one thing; choosing basket ball or football as your profession is another. While the expanding nature of the job market in SMET and related fields can accommodate SMET graduates, particularly the ones with research skills, the NFL or NBA teams, in fixed numbers, cannot employ all college graduates who are good basket ball or football players! To understand this further, just calculate the total numbers of players on the NBA and NFL teams and compare them to the total numbers of college seniors on college teams! Do not stop there, remember also that most teams already have a full roster and only take a few draftees in a given year!

THE LAW OF PERFORMANCE:
Adequate practice begets excellence in school, college and in research—the same way it does in sport!

THE LAW OF PERFORMANCE:

Adequate practice begets excellence in school, college and in research—the same way it does in sport!

The Power Law of Human Performance or of Practice (PLP) states that the time (T) it takes an individual to perform a given task decreases as the number of times (N) the individual practiced the task increases. In mathematical terminology, the law is [4]:

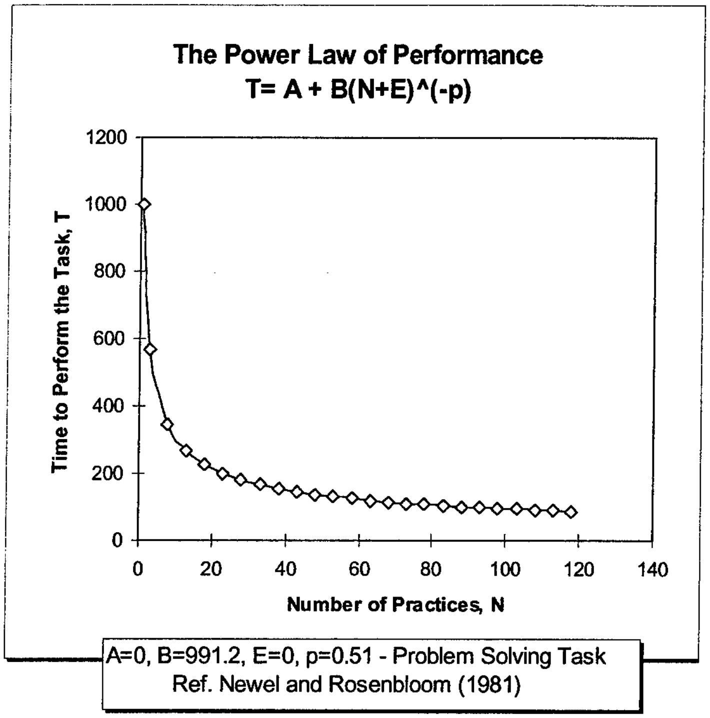
$$T = A + B\,(N + E)^{-p} \quad \text{or} \quad T = A + B/(N + E)^{p}$$

where A, B, E and p are constants that vary **(a)** with the task at hand and **(b)** with the individual performing the task. A represents a physiological limit. B and E partly denote prior experiences before the beginning of the practice sessions, and p is the learning rate. In other words, the law states that *"practice renders perfect."* This law applies to the performance of *sensory-motor (or athletic), creative (or artistic), and cognitive (or intellectual) tasks.* The shorter the time T to perform the task - *completely and correctly* - the higher the level of proficiency. *Hence, as the number of practices increases, so does the proficiency of the individual.* The figure below graphically shows the plot of the above expression for a problem-solving task.

The dramatic impact of this law becomes apparent when one considers its application to several tasks over several days, months, and years. Then, it becomes clear that *genius is mostly the result of sustained, competitive practice.* The same way adequate practice, at an adequate scope and depth, is needed for the making of Olympic, National Basketball Association, National Football Association, and Major League Soccer champions and for the making of musicians and artists, the same way it is needed for the making of science, engineering, and mathematics scholars and researchers in any discipline.

Further, this law is implacable. It applies whether one likes it or not! It applies to the refinement or the enhancement of the *teaching,* mentoring, research, and writing skills of a teacher or faculty member! The law implicitly addresses the need to strive for quality! Indeed, practicing bad grammar, incorrect mathematics, etc. renders one very good at them! So, even though the power law and the law of performance do not explicitly factor in the issue of quality, they do so indirectly.

The compound law of human performance, or simply the *law of performance* (Education, Vol. 115, No. 1, pp. 31-39, 1994), is the convolution of the power law of performance as simultaneously applied to several tasks over a long period of time. The main difference between the *power law* and the *law* is that the former follows a simple equation that involves an exponent or power (i.e., p) while the mathematical form of the latter is yet to be determined. *The quintessential point here, however, stems from the fact that according to the law of human performance, the abilities, skills, and attributes (of individuals) that are meaningfully engaged and challenged in and outside the classroom (as by lessons, assignments, research)—from pre-K through graduate school and beyond — are the ones that will develop!* The law of human performance provides the scientific basis for high expectations for all students! Professional mentoring, as defined elsewhere by Bagayoko (http://www.phys.subr.edu/timbuktu.htm), provides an almost fail-safe strategy for promoting the academic excellence of all students (female or male, minority or nonminority, young or mature). Student retention, on-time graduation, and their success in graduate school are partly by-product of the quest for proficiency and excellence— through competitive teaching, learning, and research. *It is critical to note that the same way the LP applies to the cognitive domain, the same way it applies to non-cognitive (i.e., behavioral) variables: Character and study habits are also molded through practice!*



Newel, A. and P. S. Rosenbloom (1981)."Mechanisms of Skill Acquisition," Edited by Anderson, J. R. Hillsdale, N. J.: Erlbaum

DIRECT APPLICATIONS: the need to plan and to execute (i.e., practice)

By linking prior experiences or practice to the speed with which one learns or discover new knowledge, the law of performance states that our levels of achievements in the classroom, in athletic events, artistic endeavors, and in research are determined for the most part by us—given that **we decide every day on the time we devote to various tasks!** Further, the law of performance is a great liberator that says that there is nothing wrong in not being an expert in a subject or a task at once—no one is! Hence, consulting experts, getting the appropriate materials, doing adequate practice is all that is needed.

Each and every one of the *imperative proficiencies* described above (*i.e., in language and communication, mathematics, probability and statistics, and research)* is acquired through practice! And no one should forget, in light of the meaning of B and E, that difficulties in mathematics, science, engineering, and technology courses are very often caused by an inadequacy of background, practice, prior experiences, or of studying. In fact, for individuals not suffering from a severe physiological or mental impairment, that is the case.

In particular, research expertise often requires many years of practice. Hence, the sooner one starts performing research, the better it will be. *If you missed the opportunity in high school, make certain that you start as soon as possible in college.* (And if your institution or department does not understand this point, then find one that does and that has good faculty research-mentors.) Of course, the law of performance says to remember, at the beginning of new learning experiences, that the feeling or impression of being lost is a sign that one started learning new things! (Oh, yes, I know, many students erroneously take it to mean that they are not "smart" enough. Please explain the facts to them.) At conferences, the best experts do not know or understand everything—including the ones making the presentations! So, you are not alone. And, these experts know that research questions can be found, in a quasi–infinite number, in the professional and technical literature (magazine, journals, books, etc., on paper or in electronic media) and not by looking at the sky or ground. *The experts keep on learning; according to the law of practice, that is how they built and continue to enhance their expertise!*

We explained above the need to consult several faculty members, peers, experts, etc. in order to determine the background that is needed for career options one is contemplating. The same is true for courses one has to take in college or in graduate school. Hence, there is a critical need to plan professionally, in writing. Only through such a planning can one determine indispensable background or experiences and take the needed steps to acquire them — through regular and persistent efforts. *"A college portfolio"* should be prepared by 10th or 11th grade students; *"a graduate school portfolio"* should be prepared by college sophomores or juniors; and *"a research career portfolio"* should be prepared by every graduate student. The preparation of these portfolios, first and foremost, brings to light needed credentials, background, experiences, etc. when there is still time to acquire them. See Reference [1] for an example of a "college portfolio" that can be easily adapted to design other portfolios noted above.

CONCLUSION

At the beginning of this presentation, I noted that it had already been delivered by Dr. Norman Y. Mineta, the honorable U.S. Secretary of Transportation. It has also been reiterated by Dr. Henry Ponder, the President of NAFEO. Indeed, these officials just addressed you and underscored the fact that the opportunities in science, mathematics, engineering, and technology are almost limitless. Paraphrasing Dr. Mineta's statement, we see that the sky is the limit in transportation alone. (And, if you ask NASA, even the sky or ocean floor may not be limits!) We added that many interdisciplinary areas offer more opportunities than can hold on a single list. Some of these areas include Earth Science, Energy and Environmental Science, Global Climate Change Research (with possible application to other planets), Materials Science, Engineering, and Technology (MSET), Genomics and the nascent Proteomics, Agriculture Science and Technology, Biomedical Research, and many others. Honorable Dr. Mineta and Dr. Ponder acknowledged your present accomplishments, including the research you already performed and the technical presentations many of you will make in the following session.

In light of the foregoing, it is my deepest hope that you will fully utilize the content of this provocative address not only to take your accomplishments and preparedness to new heights, but also to inform many other people, including your peers, young relatives, and your descendants. *"Luck is what happens when PREPARATION (through effort or practice as per the LP) meets or makes, recognizes, and acts on opportunity."* We are counting on you.

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[1] http://www.phys.subr.edu/timbuktu/careers.htm This site provides a listed of hot links to extensive information on careers in science, mathematics, engineering, and technology. Sources include the American Institute of Physics, the American Physical Society, the American Chemical Society, the American Mathematical Society, the American Psychological Association, etc. Available information include: how to prepare for a career, interview tips, resume preparation, free posting of a resume, etc. (Also visit the site of the American Association for the Advancement of Science: http://www.aaas.org/)

[2] Science, Vol. 292, No. 5524, Page 1971, June 15, 2001. See *"Scoop on Stats"* in the Section on Netwatch. The web site on a recently developed online statistics textbook, by David Lane at Rice University, is provided (http://www.ruf.rice.edu/~lane/rvls.html).

[3] *"A Problem Solving Paradigm,"* D. Bagayoko, Ella L. Kelley, and Saleem Hasan. College Teaching, Vol. 48, No. 1, pp. 24-27, 2000. Understanding, knowing, and paying attention to the five (5) categories involved in problem-solving is a prerequisite for properly teaching or learning it, by design. These categories are *knowledge, skills, resource, strategy/experience, and behavioral bases* of problem solving proficiency or expertise.

[4] *"The Dynamics of Student Retention: A Review and a Prescription,"* D. Bagayoko and Ella L. Kelley. Education, Vol. 115, No. 1, Pages 31-39, 1994. This paper elaborates extensively on the Power Law of Performance and it introduces the compound law (or simply the Law) of Performance. The article utilizes the law of performance to explain the creation of educational, research, and professional value-added (high academic achievements and expertise).

[5] Jaime Escalante, in our view, rigorously applied the law of performance when he worked with his Hispanic American students to make calculus geniuses out of them. Please think about his equation that says the following: **"determination + discipline + hard work = success."** Anyone who understands and heeds this equation will be following the law of practice by devoting significantly large amounts of time to learning and research tasks at hand, and that over months and years.

[6] "*Writing for Success: A User-Friendly Manual for Effective Communication,*" By Professor Ora Plummer and Dr. Diola Bagayoko. Publisher: McGraw Hill. ISBN: 0-07-154196-9 (1998). A copy of this book was provided to student participants of this 2001 NAFEO High Tech Expo with the hope that it will be *persistently* used for "continuous improvements" of language and communication skills. Please refer to the first "imperative" discussed above. [Note: Dr. Bagayoko does not make any money from sales of this book; he donated his share of the royalties to the Southern University Foundation for the purpose of establishing and endowment for the Timbuktu Academy.]

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LE MONTAGE OU DEVELOPPEMENT DE PROJETS SPONSORISES
(Ecrire ou ne pas écrire, ça c'est la question!)

Par

Diola Bagayoko, Ph.D
(bagayoko@aol.com)
Professeur Distingué de Physique
Southern University and A&M College
Baton Rouge, Louisiane 70813, USA
et
Mohamed Diarra, Ph.D.
Mission au Mali, US Agency for International Development
Bamako, Mali

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SOMMAIRE

Notre ambition, dans ce précis sur le développement ou montage de projets sponsorisés, est de provoquer des interêts vis à vis de ce sujet. Un seul livre, aussi volumineux qu'il soit, ne peut pas couvrir le développement des projets dans toute sa diversité, importance, et subtilité. C'est pourquoi nous avons choisi d'adresser les points essentiels ou les lignes générales -- de telle façon que le lecteur peut les utiliser opérationnellement—sans pour autant attenter un traitement détaillé. Les détails vont suivre pour tous ceux qui vont se mettre à la tâche importante de monter des projets pour améliorer l'instruction, l'encadrement des étudiants, ou la recherche (scientifique et technique ou autre).

I. QUELS SONT LES « GRANTS,» CONTRATS, ET AUTRES PROJETS SPONSORISES?

Les termes de **projets** et **programmes sponsorisés** sont généralement employés pour indiquer des activités proposées et effectuées par une entité (une école, une université, etc..) et pour lesquelles le support financier est fourni par une autre entité (une agence fédérale, une agence d'Etat, une fondation, une société, etc..)

Une variété de mécanismes est utilisée pour "proposer" un projet à des sources de financement. En général, les sources de financement publient les directives ou les sollicitations qui doivent être suivies par les individus ou organisations cherchant leur support. Ces directives ont quelques spécificités qui dépendent du cadre juridique applicable pour les sources concernées. En particulier, les «grants» (subventions) et les contrats sont deux formes fondamentalement différentes de support financier, du moins aux USA. Pour l'éducation, la forme de financement est généralement à travers des grants. Les contrats sont les formes premières de financement quand les destinataires sont des organisations à caractère lucratif (sociétés, firmes, etc.).

Les contrats ont généralement de très rigoureuses stipulations légales qui doivent être suivies à la lettre. Les contrats ont des conditions d'enregistrement étendues. En general, des rapports trimestriels, et parfois mensuels, sont exigés par les contrats. *Les grants offrent beaucoup plus de flexibilité et exigent moins de rapports que les contrats.* Les rapports annuels et semi-annuels sont souvent le cas pour les grants. Les accords coopératifs sont d'autres formes de financement où l'agence ou la source de financement est "activement" impliquée dans l'exécution des projets.

La règle d'or dans "le montage de projet" est qu'il n'existe aucune stratégie singulière pour monter un projet sensible (*i.e, qui adresse strictement les stipilations des sollicications*) et concurrentiel (*qui démontre une chance de succès aussi grande ou meilleure que les autres*). Il y a autant de stratégies de montage ou de développement de projets qu'il y'a de directives ou sollicitations qui doivent être suivies à la lettre. ***Si on veut une règle d'or, elle est de suivre les directives ou sollicitations pertinentes à la lettre.***

II. L'AMPLEUR OU L'ETENDUE DES FINANCEMENTS DE PROJETS

Aux USA, il existe des livres entiers sur le nombre quasi-infini des opportunités de financement des projets et programmes dans l'enseignement primaire, secondaire, et superieur. Les sources majeures de financement, aux USA, comprennent les agences fédérales, les agences d'Etat, les fondations philanthropiques, les programmes de financement des corporations et d'individus. *La raison pour laquelle cet atélier est important est que il y'a également de nombreuses sources de financement internationales qui attendent des projets sensibles et concurrentiels de tous ceux qui peuvent et veulent écrire (développer ou monter) des projets.*

Les agences fédérales déboursent plusieurs MILLIARDS de dollars par an pour des projets d'instruction et de recherches dans les établissements d'éducation. Comme illustration, nous notons que, vers 1990, cinq agences fédérales américaines ont dépensé $11 milliards de dollars dans des projets de recherches dans des établissements d'éducation superieure! Les principales agences fédérales qui supportent des projets dans les établissements éducatifs incluent les suivantes:

Les agences Fédérales	**Niveaux D'Enseignement Supportés**
Le Ministère de L'Education (US-ED)	Tous les niveaux
L'Institut Nationale De La Santé (NIH)	Ecoles de Médecine et autres niveaux
La Fondation Nationale de la Science (NSF) et technologie	Recherche (Sci. et Tech.), instruction (Sci. et Tech.)
Le Ministère de l'Energie (DOE) (US-DOE)	Recherche(par les universités, Labs,et dans le secteur privé
Le Bureau de la Recherche Navale (ONR)	Recherche dans les universités et ailleurs
Le Ministère de l'Agriculture (US-DA)	Recherche et Services par les universités
La Dotation Nationale Des Humanités (US-NEH)	Recherche et Services par les universités
La NASA (National Aeronautics & Space Administration)	Recherche et Services par les universités,...

De nombreuses agences des états américains dépensent des millions de dollars chaque année pour des projets dédiés à l'éducation et à la recherche. Cela est vrai pour tous les états. Il convient de noter que plusieurs agences fédérales fournissent des fonds de programmes à travers diverses agences des états!

Il y a plus de 22.000 fondations aux USA qui distribuent plusieurs milliards de dollars par an à ceux qui répondent à leurs sollicitations (ou conditions d'acceptabilité) et qui soumettent des projets competitifs. Il y a des fondations locales, regionales, nationales, et internationales. **Des centaines de fondations internationales financent des projets dans des pays autres que ceux dans lesquels elles résident légalement.**

Les sociétés, grandes et moyennes, financent par an plus de projets que nous ne pouvont énumérer dans un seul livre!

III. LES SOURCES D'INFORMATION SUR LES POSSIBILITES DE PROJETS

Les sources d'information sur les programmes de financement sont les agences de financement elles mêmes, y compris les organismes et agences identifiés ci-dessus. **En particulier, tout individu peut avoir toute les informations nécessaires à travers l'Internet !** Cela est vrai depuis 1995. D'ailleurs, plusieurs sources locales ou internationales de financement ont commencé à publier leurs sollicitations UNIQUEMENT à leur site Internet ! (Economie de fonds et dissemination illlimitée sont des raisons simples pour cette approche.) Nous avons pourvu, à la fin de ce document, des adresses Internet pour quelques sources internationales et américaines de financement de projets. **La méthode générale pour trouver l'information est d'utiliser les engins de cherche sur l'Internet.** En effet, les cherches simples (taper le nom de la source ou le sujet d'un projet entre des guillemets) et raffinées donnent les informations nécessaires.

IV. COMMENT ECRIRE UN PROJET SENSIBLE ET CONCURRENTIEL (Competitif)?

La réponse à cette question est fondamentalement fournie dans le dernier paragraphe dans la section I. En effet, **le secret d'un bon montage de projet réside dans une adhérence stricte aux directives ou sollicitations applicables**, y compris les apostilles (notes au bas de de la page)! L'affirmation ci-dessus est en partie corroborée par les différences suivantes entre les projets soumis à quelques agences fédérales, des sociétés, et fondations philanthropiques.

Un dossier (proposal an Anglais) d'un projet typique de recherche soumis à la Fondation Nationale des Sciences (NSF) aux USA a environ quinze (15) pages de récit, ne comptant pas les formulaires et les appendices. Nous appelons récit ou narratif la substance du dossier (proposal an Anglais) typique, exclusive du budget, des lettres de support, et d'autres attachements et formulaires à remplir. Il y'a des cas spéciaux où le dossier d'un projet soumis à la Fondation Nationale des Sciences peut être de quatre (4) ou cinq (5) pages! *Une fois de plus, la clé est de suivre les sollicitations qui s'appliquent.*

Un dossier typique de projet soumis à une fondation philanthropique ne compte générallement pas plus de quatre (4) à dix (10) pages de récit. Veuillez bien noter le terme "typique." Il y'a des cas où le dossier d'un projet soumis à une fondation philanthropique peut contenir cinquante (ou plus de) pages ! *La clé est, encore, d'adhérer aux sollicitations.*

Une lecture et une mise en valeur minitieuse de quelques points clés dans les directives ou solliciations est une première étape nécéssaire pour le développement d'un projet. Cette lecture doit être **suivie de séances de réflexion (cogitation) sérieuse**, de préférence avec des collègues, pour produire un sommaire (les grande lignes) du projet. **Notez bien que la lecture regulière de rapports annuaux (des facultés, des départements, des ministères, d'organisations nationales ou internationales, d'associations professionelles, ... sont des sources inépuisables d'idées de projet et d'information quantifiées** tres utiles! (Ne donner pas ce secret à tout le monde!)

Tandis que les sections spécifiques, dans un projet, peuvent changer d'un programme à l'autre, un dispositif est commun à tous les projets: **ils sont des documents de vente développés pour**

convaincre les agences de financement que votre projet est le meilleur investissement qu'elles peuvent probablement faire. Ce point doit toujours être à l'esprit pour le développement de bons projets (bons signifiant sensibles et concurrentiels).

Pour les projets avec plusieurs pages (10 ou plus), une **table des matières** est critique. Une table des matières bien faite et approfondie est le guide aux sections et documents raffinés de support dans le dossier du projet.

La substance d'un projet, comme noté ci-dessus, est désignée souvent sous le nom du "récit du projet," de narratif, ou de "la description du projet" ; le plus souvent, cette substance nécéssite les sections suivantes (brièvement décrites). En faisant face à ces sections, on doit toujours se rappeler que les quantités (nombres), toutes les fois que cela s'applique, sont préférées. *Les nombres permettent de juger l'impact, les accomplissements, et la qualité d'un projet.* Une belle prose, sans nombres, ne suffit générallement pas. ***Trois choses sont critiques pour élaborer*** *(développer) un dossier précis et concis d'un projet sensible et concurrentiel.* ***Elles sont les nombres, les nombres, et plus de nombres.*** La simple raison de cette importance des nombres provient du fait que les agences ou organisations ne financent pas des projets sans pouvoir autant mesurer le succès, l'impact, et la qualité de ces projets.

Veuillez au fait que le nombre, la teneur, et l'ordre, ... des sections suivantes d'un projet changent avec la nature (recherche, formation ou service) des projets proposés aussi bien qu'avec les sources de financement (voir les sollicitations qui s'appliquent).

Veuillez noter que les dossiers de projet, une fois financés par la plupart des agences ou organisations aux USA, deviennent des documents publiques! Par conséquent, l'examen d'un dossier d'un projet financé est fortement recommandé avant de se lancer dans le développement ou la redaction. (Ceci, naturellement, n'est pas nécessaire dans tous les cas.) Pour avoir une copie du dossier d'un projet récemment financé, il suffit *d'écrire à la source de financement en question. (Un message électronique ou e-mail suffit!)*

V. SECTIONS TYPIQUES DU RECIT (OU NARRATIF) D'UN PROJET (Ne comptant pas la page de couverture, la table des matières, les formulaires, et appendices)

Introduction: Une introduction doit preparer le terrain pour la teneur du projet. Indiquez qui vous êtes (votre établissement et votre départment/faculté). De façon convaincante, identifier, dans ses grande lignes, le problème que vous voulez adresser (*résoudre).* Ce qui précède est pour des projets qui ne sont pas de recherche. Pour les projets de recherche, adressez cette section en fournissant une revue technique de la littérature comtemporaine (sur le sujet pertinent). Cette revue doit guider au problème que le projet se propose de résoudre.

Buts et objectifs du projet: Cette section doit présenter, d'une façon précise et concise, les buts ou objectifs que l'on veut atteindre avec le projet. *(Naturellement, il est espéré que ce but sera la solution (totale ou partielle) du problème posé dans l'introduction !)* Des mots clés dans cette section comprennent les objectifs, les résultats prévus (escomptés), les buts, et les groupes ou entités qui seront affectés. **Les objectifs et buts doivent être exprimés en des termes QUANTITATIFS (nombres) autant que possible.**

Veuillez noter ici que les objectifs (résultats finaux à obtenir) ne doivent pas être confondus avec les stratégies de mise en place, d'exécution, ou les activités du projet. *Ne pas confondre l'objectif avec ce qu'on fait pour l'atteindre.*

Stratégies de mise en œuvre, d'exécution (ou méthode pour les projets de recherche): Cette section est appelée « Méthode » pour les projets de recherche. La mise en œuvre ou exécution sont les mots préférés pour des projets qui ne sont pas de recherche. **Cette section spécifie comment est-ce qu'on va atteindre les objectifs décrits ci-dessus.** Notez bien que les projets á grande échelle, avec plusieurs issues logistiques, doivent avoir un plan solide de bonne mise en œuvre. Certains auteurs présentent une sous-section pour « la procédures de gestion »; d'autres adressent telles issues dans la prochaine section. **L'échelle de temps** pour l'exécution du projet doit être clairement fournie dans cette section ou dans la section précédente. PRIERE DE NOTER QUE CETTE SECTION EST GENERALEMENT LA PLUS LONGUE. Elle doit repondre à toutes les questions possible (de logistiques, sur activités, et autres)

Personnel et Autres Resources: Ne faites pas l'erreur, concernant le personnel, de simplement dire aux lecteurs (évaluateurs) de lire les (curriculum vitae) résumés dans les appendices. Il faut donner une description décente mais concise de la formation, des experiences, des travaux passés, et des qualifications du personnel—*avec accent sur ce qui a trait au succès du projet.* Les évaluateurs des dossiers de projets ne sont pas toujours obligés de lire les appendices ! Quant aux **autres resources**, tout dépend du projet. La règle est de ne pas manquer de noter les salles, les équipements ou laboratoires entiers, et d'autres resources auxquelles on a accès et qui peuvent aider dans l'exécution du projet.

Evaluation du projet/Plan de continuation: Des évaluations internes et externes sont exigées pour la plupart des projets á grande échelle ou envergure. Cette section n'est parfois pas nécéssaire pour plusieurs projets de recherche; les publications et les présentations sont utilisées par plusieurs agences de financement comme les meilleures mesures pour le succès d'un projet de recherche. Les projets sont généralement renforcés par la fourniture d'un plan de continuation. Fondamentalement, un tel plan consiste d'une description de la façon dont on a l'intention de possiblement préserver et mettre en valeur les gains du projets au delà de la période de financement. Une mannière fréquente d'adresser la continuation consiste à institutionaliser les parties (activités et autres) du projet qui tombent dans le cadre normal de l'opération de l'organisme auquel l'enquêteur principal (ou le directeur du projet) appartient. En une période d'un an ou plus, on a le temps de plannifier et d'exécuter graduellement une telle institutionalisation qui est aimée par la plupart des sources de financement.

Sommaire du projet: il est exigé, par la plupart des sollicitations de la Fondation Nationale des Sciences (NSF) aux USA, que cette section soit composée de 200 mots ou moins ou limitée à une page—dépendant du projet. *C'est la première partie des dossiers des projets pour NSF, suivant la table des matières.* Pour les agences qui n'ont pas un format spécifique de projet, comme est le cas pour la plupart des fondations philanthropiques, *le sommaire est souvent la* *dernière section* du narratif (la dernière impréssion!). Inutile d'ajouter qu'un sommaire doit mentionner tous les dispositifs exceptionnels ou de base (identification de l'organisation, objectifs, activités ou méthodes, résultats anticipés, ...) du projet. Les agences de financement éditent souvent les sommaires des projets, avec l'intention d'informer le public (et parfois des concurrents) des "excellents" projets qu'elles supportent ! Des centaines de sommaires de projets se trouvent au site Internet de la Fondation Nationale Des Sciences aux USA (http://www.nsf.gov/).

VI. BUDGET

Le budget d'un projet est mieux compris après avoir vu des exemples. Selon la règle d'or, le budget doit suivre les points énoncés dans la sollicitation pertinente. Le budget doit passer ce qu'on appelle l'examen PJR (permissible, justifiable, et raisonable). PJR est JAR en Anglais (justifable, allowable, and reasonable). Le lecteur est prié de se référer aux exemples de budgets fournis aux organisateurs de cet symposimum inaugural et à la direction du Projet TOKTEN (Transfer of Knowledge Through Expatriated Nationals)—un projet de l'Univesrsité du Mali-financé par des organisations internationales et autres. En général, le budget d'un projet adresse le personnel, les bénéfices associés avec l'emploi (retraite et autres), les coûts indirects, l'acquisition d'équipement et de materials, le support des participants, et les frais d'opération (frais de communication) parmi d'autres.

VII. LES APPENDICES ET FORMULAIRES

Prière de suivre la règle d'or. Les sollicitations générallement dictent l'ordre dans lequel les differentes parties d'un dossier de projet, y compris les lettres de support, doivent apparaître. Il y'a des formulaires qui sont avant et d'autres qui sont après le narratif. Le numbre et la nature des documents dans les appendices sont générallement indiqués par les sollicitations !

VIII. COMMENTAIRES POUR LES INSTITUTIONS

Un Bureau de développement de Projets existe dans la majeure partie des universités américaines. De 1987 à 1989, l'un de nous (Bagayoko) a dirigé un tel bureau pour son université. (Pendant cette periode, nous avons augmenté par un facteur de quatre le nombre de nos projets financés par la Fondation Nationale des Sciences. En Janvier 1989 nous avions quatre fois plus de projets qu'en Janvier 1988.) Ces bureaux de développement sont censés aider serieusement les professeurs, départements, facultés, et autres dans leurs efforts de développement de projets. **En fait, le directeur d'un tel bureau doit signer la plupart des dossiers de projets avant qu'ils ne soient envoyés aux differentes agences externes.** Une raison pour l'établissement et le propre fonctionnement d'un tel bureau est que *les sources de financement estiment que l'existence du bureau est un signe de maturité, de sophistication, et de progrès continu!* Mais oui, ces bureaux servent également à aider les directeurs de projet et enquêteurs dans l'exécution des projets—*avec un accent particulier sur les aspects administratifs et financiers de la mise en œuvre des projets.* (Notez, cependant, que quelques fonctionnaires du système scolaire ou universitaire, dans un tel bureau, peuvent reduire leur rôle à "autoriser" ou à "ne pas autoriser," "approuver ou ne pas approuver," au lieu d'informer, de supporter, et d'encourager ceux qui fournissent des efforts dans ce domaine crucial de montage de projets. Une évaluation annuelle et quantitative de tels bureaux, tenant en compte le progrès en terme du nombre et de la qualité des projets et du montant total des financements est une formule infaillible pour éviter ces problèmes potentiels du rôle changé ou pas rempli.) Pour les dix dernières années, Bagayoko a tenu ce language à de nombreuses universités où il a servi comme consultant. Si votre universite n'a pas un tel bureau, alors allez voir le président (or Chancellor, ou Recteur dans le cas du Mali) pour l'établissement d'un bureau. Oh, plus il y'a de professeurs qui développent des projets, plus le besoin pour ce bureau sera ardent!

SITES INTERNET DE QUELQUES SOURCES DE FINANCEMENT ET DE SOUTHERN UNIVERSITY AND A&M COLLEGE

The United Nations: http://www.un.org/
The World Bank: http://www.worldbank.net/

African Development Foundation: http://www.adf.gov/

The United State Agency for International Development (US-AID): http://www.usaid.org/
National Aeronautics and Space Administration (NASA): http://www.nasa.gov/
National Science Foundation (NSF): http://www.nsf.gov/

The Foundation Center (from which one can reach most international foundations in the US) http://fdncenter.org/

Web site of Southern University and A&M College in Baton Rouge (SUBR): http://www.subr.edu/

Web site of **the Timbuktu Academy** at SUBR, funded by the Department of the Navy, Office of Naval Research (ONR), and directed by D. Bagayoko: http://www.phys.subr.edu/timbuktu.htm

Web site of **the Program to Increase the Pursuit of Education and Learning in Engineering and Science (PIPELINES)**, funded by the NASA and directed by Dr. Diola Bagayoko. http://www.phys.subr.edu/pipelines/

Le site Internet de Diola Bagayoko, Ph.D., SUBR (avec les versions courte (5 pages) et longue de son résumé (ou palmarès) et au moins une photo): http://www.phys.subr.edu/faculty/Bagayoko/

Problem-Solving Paradigm

Diola Bagayoko, Ella L. Kelley, and Saleem Hasan

The complexity of problem solving partly explains professors' continuing efforts to develop students' problem-solving expertise (Woods 1994, 1993a, 1993b, 1987). (We use the unusual order of citation because the sequence of the author's arguments is best understood in reverse chronological order.)[1] Advances in understanding the creation of educational value added offer a comprehensive explanation of the development of problem-solving proficiency (Moore and Bagayoko 1994, Bagayoko and Kelley 1994a). Our aim is to present the resulting problem-solving paradigm (PSP), also known as the problem-solving pentagon (see figure 1).

A Problem-Solving Paradigm (PSP)

A comprehensive discussion of problem-solving scenarios might require a book. For simplicity, we will focus on academic problem solving, even though the pentagon described below is valid for real-life problems as well. One essential difference between the two, despite their overlap, is that the academic problems are generally well defined. In solving actual problems, problem definition, delineation, and redefinition pervade the entire process.

To develop the problem-solving expertise of students, we recommend that teachers make concentrated and sustained efforts to develop the following five categories. (The order of the categories is not one of decreasing or increasing importance.)

1. *Knowledge base.* Cognitively condensed and meaningfully organized knowledge is very different from a set of disjointed pieces of information. We will discuss an often neglected part of the knowledge base—the applicable language or information transmission modes (Adamczyk and Wilson 1996).

One cannot consistently and correctly apply that which one does not know critically. Cognitively condensed knowledge is organized or structured in a meaningful fashion, using causal, functional, and logical relationships (Bagayoko and Kelley 1994b). This organizing, bunching, and clustering of knowledge is a central tool for the implementation of "less is more" (AAAS 1989; NSTA 1990) through teaching and learning processes.

In chemistry and physics classes, for example, the last, cognitively condensed form of the ideal gas law that a teacher should leave with students is $PV = nRT$. Respectively, P, V, n, R, and T are the pressure, the volume, the number of moles, the ideal gas constant, and the temperature. It is only our suggestion to use this form in introducing the concept of ideal gas. The essential point is that, with $PV = nRT$, students should be able to recover any of three laws that apply when P and n, V and n, or T and n are respectively held constant. In addition, concept mapping (AAAS 1989) is one of the best ways of condensing and integrating new knowledge into an existing knowledge base.

2. *Skill base.* Cognitively condensed procedural knowledge has some overlap with the organized knowledge of category 1, even though it is distinct. This distinction is apparent in problem-solving situations that require physical dexterity. The idea that the time rate of change of distance is speed may belong to Category 1, but carrying out the differentiations, given several mathematical expressions for the distance, requires the know-how or skills in Category 2.

Procedural knowledge can be cognitively condensed or structured as discussed above. Algebra provides one of the best means of illustrating this category. Indeed, knowing how to solve a given equation is one thing, and solving it correctly is another. For the latter, one has to properly execute basic operations and the rules of exponentiation. Teaching through classroom examples and graded assignments promotes the mastery of these skills through practice.

3. *Resource base.* The nature of this base may vary drastically depending on the problem. Both human and material

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Diola Bagayoko is a professor in the Department of Physics and director of the Timbuktu Academy, **Ella L. Kelley** is an associate professor of chemistry, and **Saleem Hasan** is a research assistant in the Department of Physics at Southern University and A & M College, Baton Rouge, Louisiana.

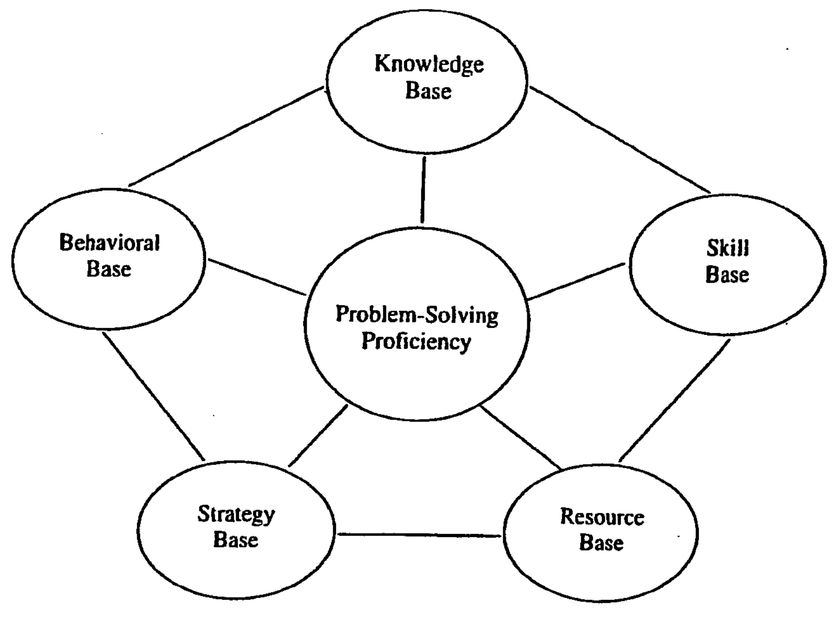

Figure 1. A Problem-Solving Paradigm (PSP)

resources are necessary. For ordinary academic problem solving, calculator, protractors, computers and applicable software products, reference books, and journals are typical material resources. In addition, for creative thinking the resource base should not be limited because new ideas may require new tools.

4. *Strategy-Experience base.* Strategy and experience may be specific to certain kinds of problems, or they may be transferable. We know that practice enhances proficiency, as dictated by the power law of performance (Bagayoko and Kelley 1994a). Strategy or method, in this category, should not be confused with the skill base in Category 2. A useful analogy is that Category 2 represents individual musicians, skilled at playing various instruments, and Category 4 refers to the conductor of the orchestra. (Room is provided for improvisation by the conductor, as problem-solving strategies do not always follow, at all stages, an algorithmic approach.)

One's strategy-experience base, Category 4, essentially grows over time. Its growth is generally concomitant with those of Categories 1, 2, and 5. Category 4 could also be called "effort," to place emphasis on the role of practice in the development of problem-solving proficiency. Teaching, then, should include judiciously selected graded assignments that will expose students to key strategies for solving problems on the topics at hand.

5. *Behavioral base.* The affective domain has a bearing on the outcome of problem-solving attempts. In particular, this category is distinguished from Category 4 in that the knowledge of, or experience with, a strategy or method is not sufficient for guaranteeing the self-discipline that is sometimes needed to adhere to it. Individual reactions to various constraints in problem solving (e.g., panic attack as opposed to strong focus), although partly determined by the other categories, strongly hinge on one's emotional and behavioral traits, partly molded through practice.

As in the other categories, students can change their behavior through training and/or practice. Failure to know adequately some basic subject content (Category 1) or to develop some key skills (Category 2) often prompts students to panic. Most professors can recount several such cases, when students *guess and hope* instead of *think and reason.* That can have a profound negative impact, including destroying self-confidence (Bagayoko and Kelley 1994a).

Unfortunately, the compound power law of performance dictates that students who frequently repeat such behavior patterns virtually make lack of confidence their second nature! Conversely, adequate preparation (Categories 1-4) reinforces self-confidence and behavioral patterns that are favorable for expert problem solving.

Application and Implications

A first implication of the above paradigm stems from its conflict with current descriptions of problem solving. Indeed, expressions such as *problem-solving skills* or *problem-solving abilities* may be construed to mean that the skills, in the sense of procedural knowledge or some innate ability, are the answers to problem solving. The problem-solving pentagon leads to the conclusion that the word *skills,* in its common sense, represents at best one-fifth of what is required for problem-solving expertise. We therefore suggest that *problem-solving pentagon* or *problem-solving expertise* replace the potentially misleading term *problem-solving skills.*

The problem-solving pentagon (PSP) shows that the failure of some old approaches to teaching problem solving stems not so much from flaws in the approaches as from a neglect of the other sides of the pentagon. One of these methods consists of having the instructor solve sample problems while the students watch. That approach is very valuable, if properly implemented. We will discuss an effective use of this approach, along with others.

Every fall and spring semester, the physics department enrolls 140-170 students in other sciences and engineering in General Physics, a calculus-based, introductory mechanics course. These students attend two-hour sessions of problem solving every week, in addition to the lecture and laboratory sessions. There generally are six to eight sections of problem solving. Over the four years 1986–1990, students in the two sections where the problem-solving paradigm was rigorously applied have clearly outperformed the others in two ways. Their averages on the common lecture class exams have consistently been above those of the students in the other problem–solving classes, and 91 percent of the time, one of the students in the PSP group has made the highest score on the common exams. We attribute the differences to the implementation of the problem-solving paradigm.

"Slow" and Guided Solving

In particular, one experience that the students in other sections did not have was the "slow and PSP-guided example problem-solving." In the selected sections, very few problems, different in nature and complexity, were solved in class. In general, only one example problem was collectively solved per week. In keeping with the paradigm, the problem was solved interactively using Socratic dialogue. The students did the thinking while the teacher mostly guided, wrote on the board, and commented extensively. The problems involved a combination of fundamental principles or definitions, key laws, and several skills to obtain peripheral facts from the core or central theme around which the rest is condensed.

Exposure to and practice of the needed knowledge, skills, strategies, and behavioral traits lead, over time, to building the students' problem-solving proficiency.

The key to the success of this approach, we think, resides in

1. the Socratic dialogues that engage the students,
2. extensive comments at every step, to note the category or categories of the pentagon that made the successful step possible, and
3. the relatively slow pace (due in part to the dialogues) that helps students remember not only the concepts and skills but also some strategies and related behavioral patterns.

It is important that the instructor help the students to understand the relevance of every category of the pentagon. The need to read carefully and to study a problem (Categories 5 and 4) and the indispensable role of adequate knowledge (Category 1) and skills (Category 2) must become obvious to the students.

To further reinforce adherence to the paradigm, we gave weekly quizzes of ten to fifteen minutes. The quizzes did not stress the speedy recall of a plethora of minutiae, but rather they reinforced the mastery of cores of cognitively condensed knowledge and skills. We assigned weekly homework problem sets, collected them the following week, and graded and returned them the next. As per the power law of performance, there *is no substitute for actual practice*. The students in the selected sections wasted much less time attempting to guess or to apply a key principle, law, or skill that they did not know.

Discussion

Contrary to the belief of some practitioners that doing several homework problems does not develop problem-solving skill, we assert that practice does enhance problem-solving proficiency by virtue of the compound law of performance. The mathematical formulation of the power law of performance has been discussed by Bagayoko and Kelley (1994a). Qualitatively, the law states that the time it takes a person to perform a sensory-motor or a cognitive task decreases as the number of times that the person practices the task or related ones increases. The composition of the power law—for which no single mathematical formulation is yet available—follows from compounding the results from the power law for a series of tasks over relatively long periods.

It is critical to note that the development of problem-solving proficiency is clearly explained, for the most part, by the compound or integrated law of human performance. Namely, adequate exposure to and practice of the applicable knowledge, skill, strategies, and behavioral traits leads, over time, to building the students' problem-solving proficiency. Thus, the problem solver grasps the importance of harnessing the needed resources for the problems at hand. To this end, we underscore the pivotal role of teaching and the related feedback in developing the problem-solving proficiency of students. Good teaching develops students' proficiency through (*a*) modeling of the use of the categories identified above, (*b*) graded assignments, and (*c*) testing. The testing must emphasize and require thinking as opposed to the recall of disjointed facts.

Students' evaluation of the problem-solving courses that employed this paradigm averaged a rating between 4 and 5, out of 5, each semester, on a twelve-item instrument. Perhaps the most rewarding aspect of our experience has been several anecdotal accounts from our students that they have learned to think and that they employed their training in the course to problem solving in other courses (mostly chemistry and engineering).

That good evaluation notwithstanding, at the beginning of the course, students always showed some resistance to this approach. In particular, they had to be "forced" to follow our unfailing demand that they thoroughly read and study a problem (Category 5) before attempting to solve it and that they demonstrate mastery of a certain few fundamental concepts and laws (Category 1) before trying to apply them.

From our experience, this paradigm permits a clear dissection of students' problem-solving difficulties. Early in the courses, we identified student deficiencies in mathematics knowledge (Category 1) and skill (Category 2), as in algebraic and calculus operations. The deficiencies were remedied by having students read pertinent book chapters and handouts and then giving them physics homework assignments, quizzes, and tests on the contents of assignments.

We found that the paradigm works very well only when it is fully implemented, that is, when every category receives explicit attention. This conclusion is

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strongly suggested by the National Science Education Standards (NRC, 1996) and in teaching videos produced by the Third International Mathematics and Science Study in 1996.[2] When every category is included, practice over time indeed enhances problem-solving proficiency.

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NOTES

1. See the following articles by D. R. Woods: "New Approaches for Developing PS Skills: What's New in Problem-Solving?" *Journal of College Science Teaching* 23(3) (1994): 157–8. "Problem-Solving—What Doesn't Seem to Work, *Journal of College Science Teaching* 22(1) (1993a): 57–8; "PS—Where Are We Now?" *Journal of College Science Teaching* 22(5)(1993b): 312–14; and "How Might I Teach Problem-Solving?" in *Developing Critical Thinking and Problem-Solving Abilities,* ed. J. E. Stice. (San Francisco: Jossey-Bass, 1987).

2. VHS (or CD-ROM) video examples from the Eighth-Grade Mathematics Lessons: U.S., Japan, and Germany. Available from: Superintendent of Documents, P.O. Box 37954, Pittsburgh, Pennsylvania 15250-7954, USA. The reference number for the VHS Video Examples is GPO #065-00-01025-9.

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Misconceptions and the Certainty of Response Index (CRI)

Saleem Hasan†, Diola Bagayoko‡ and Ella L Kelley‡
† *Department of Science and Mathematics Education, Southern University and A&M College, Baton Rouge, LA 70813, USA*
‡ *The Timbuktu Academy, Southern University and A&M College, Baton Rouge, LA 70813, USA*

We describe a simple and novel method for identifying misconceptions. This approach utilizes the Certainty of Response Index (CRI) in conjunction with answers to multiple choice questions.

We define misconceptions [1] as strongly held cognitive structures that are different from the accepted understanding in a field and that are presumed to interfere with the acquisition of new knowledge. While a lack of concept or knowledge can be remedied with instruction and subsequent learning, misconceptions are believed to hamper, unwittingly, the proper acceptance and integration of new knowledge or skills. Before the correct concept can be taught, it is essential for the student to 'unlearn' the misconception. For the purpose of this work, 'preconceptions' and 'alternative concepts' are synonyms of misconceptions, inasmuch as they are different from the established concepts as accepted in a field. The importance of finding a means of distinguishing a lack of knowledge from a misconception cannot be overemphasized. Although both are relevant to the understanding and the assimilation of a subject matter, the instructional methods for eliminating misconceptions and for remedying a lack of knowledge can differ considerably.

Identification of misconceptions and distinguishing them from a lack of knowledge is a fertile area in education research. However, the tests developed during such research, although refined, are cumbersome and not easily amenable to application in the classroom. The purpose of this study was to develop a simple and effective method for distinguishing a lack of knowledge from misconceptions. The simplicity of the method is expected to lead to a routine utilization of it by schoolteachers and college professors. The method is universally applicable in science, mathematics, engineering and other fields, from middle to graduate school. It is centred on associating a Certainty of Response Index (CRI) with each answer on diagnostic and other tests.

Certainty of Response Index (CRI)

The CRI is frequently used in social sciences [2], particularly in surveys, where a respondent is requested to provide the degree of certainty he has in his own ability to select and utilize well-established knowledge, concepts or laws to arrive at the answer. The CRI is usually based on some scale. For example, the six-point scale (0–5) in which 0 implies no knowledge (total guess) of methods or laws required for answering a particular question while 5 indicates complete confidence in the knowledge of the principles and laws required to arrive at the selected answer. Similarly, when a student is asked to provide a CRI along with each answer, we are in effect requesting him to provide his own assessment of the certainty he has in his selection of the laws and methods utilized to get the answer.

If the degree of certainty is low (CRI of 0–2) then it suggests that guesswork played a significant part in the determination of the answer.

Irrespective of whether the answer was correct or wrong, a low CRI value indicates guessing, which, in turn, implies a lack of knowledge. If the CRI is high (CRI of 3–5), then the respondent has a high degree of confidence in his choice of the laws and methods used to arrive at the answer. In this situation (CRI of 3–5), if the student arrived at the correct answer, it would indicate that the high degree of certainty was justified. However, if the answer was wrong, the high certainty would indicate a misplaced confidence in his knowledge of the subject matter. This misplaced certainty in the applicability of certain laws and methods to a specific question is an indicator of the existence of misconceptions. The results of this study demonstrate that the requested CRI, when used in conjunction with the answer to a question, enables us to differentiate between a lack of knowledge and a misconception.

The method

We first describe the test, as it is available in the literature [3]. We then explain how the Certainty of Response Index was added to the test. We utilized a diagnostic test, developed by Halloun and Hestenes [3], for the Classical Mechanics (college freshman level) course. The test contains 36 questions divided into 11 groups. Each group contains questions related to specific concepts and laws of classical mechanics. These topics include relative speeds, generalities on motion, including free fall, forces and Newton's Laws, energy and its conservation, and combinations of these fundamentals. It is essential to note that the test, by design, is to elucidate the understanding, or lack thereof, of fundamentals. As such, it does not entail long or complicated operations or calculations. Each of the 11 groups contains closely related questions based on a few major principles or laws. The closely related questions in a specific category permit the probing of the depth of comprehension of the students. For instance, a thorough understanding of the work–energy theorem will lead to its proper application to seemingly unrelated problems involving an inclined plane, a pendulum or a roller-coaster. The questions require minimal computation but always involve the application of fundamentals such as basic vector operation (i.e. addition), Newton's laws of motion, and the conservation of the total mechanical energy.

Summary of topics on the diagnostic test (classical mechanics)

I (1)	Relative speeds of moving particles.
II (2–5)	Free fall. Relationship between kinetic energy, speed and potential energy.
III (6, 7)	Frictional force and its relationship to the normal force.
IV (8, 9)	Projectile motion. Free fall.
V (10–12)	Newton's First Law and Newton's Third Law.
VI (13–20)	Projectile motion and its relationship with the kinetic and potential energy of the moving object. Independence of horizontal and vertical motions.
VII (21–23)	Impulse and its application to a moving particle.
VIII (24, 25)	Application of several forces and their effect on the motion of an object.
IX (26–29)	Forces and uniform motions ($\boldsymbol{a} = 0$ or $\boldsymbol{a}_t = 0$)
X (30–32)	Conservation of the total mechanical energy. Dependence of the gravitational potential energy on height.
XI (33–36)	Conservation of the total mechanical energy. Motion under the influence of gravity.

The new feature of our method consists of requesting a Certainty of Response Index (CRI) for each answer in the test described above. The Certainty of Response Index (CRI) provides a measure of the degree of certainty with which a student answers each question. This index is generally captured on a Lickert type scale. Specifically, for each question in the multiple-choice test, a student was requested to:

(a) select a preferred answer from the available choices and

(b) provide a CRI, between 0 and 5, for that answer. A CRI of 0 was requested for a total guess of the 'preferred answer', while a CRI of 5 was requested if the answer was derived from solidly anchored knowledge and skills, as believed by the respondent.

Table 1 shows the four possible combinations

Table 1. Decision matrix for an individual student and for a given question. Based on combinations of correct or wrong answer and of low or high CRI.

	Low CRI (< 2.5)	High CRI (> 2.5)
Correct answer	Correct answer and low CRI (CL) Lack of knowledge (lucky guess)	Correct answer and high CRI (CH) Knowledge of correct concepts
Wrong answer	Wrong answer and low CRI (WL) Lack of knowledge	Wrong answer and high CRI (WH) **Misconceptions**

Table 2. Decision matrix for a group of students (a class) and for a given question. Based on combinations of correct or wrong answer and of low or high *average* CRI.

	Low CRI (< 2.5)	High CRI (> 2.5)
Correct answer	Correct answer and low *average* CRI (CL) Lack of knowledge (lucky guess)	Correct answer and high *average* CRI (CH) Knowledge of correct concepts
Wrong answer	Wrong answer and low *average* CRI (WL) Lack of knowledge	Wrong answer and high *average* CRI (WH) **Misconceptions**

of the answer (Correct or Wrong) and the CRI (High or Low) on the part of an individual student. For a student and for a given question, a correct answer with a low CRI (CL) indicates a lack of knowledge and a correct answer and a high CRI (CH) points to knowledge of correct concepts. A wrong answer with a low CRI (WL) suggests a lack of knowledge, while a wrong answer with a high CRI (WH) indicates the presence of misconceptions.

The identification of misconceptions for a group of students (a class) proceeds in the same manner as described above for a student except that average values of the CRI are utilized. In the case of a class, there are generally some correct and some wrong answers for a given question, unlike in the case of an individual student. Table 2 is utilized for identifying misconceptions in a group of students.

Illustrative application

The test was administered to three sections of the Classical Mechanics (college freshman level) course, enrolling a total of 106 students. The students were given 45 minutes to complete the test. All questions were multiple choice. Each answer was assigned a mark of 1 if correct or 0 if wrong. The results were tabulated in such a way that, for every student, each question had a mark (0 or 1) and a corresponding CRI (from 0 to 5). The total number of students who answered a question correctly was obtained by adding the marks. Dividing this sum by the total number of students (106) gave the number of correct answers as a fraction of the total number of students. For a given question, the total of CRI for wrong answers was obtained by adding the CRI of all students who had given a wrong answer for the question. The average CRI for wrong answers, for a given question, was obtained by dividing the above sum by the number of students who gave the wrong answer for that question. We similarly computed, for each question, an average CRI for correct answers.

We discuss below our analysis of the results and the prospective use of the outcomes to guide classroom instruction and related assignments. While classroom activities are based on the average CRI values, perhaps the best utility of this work resides in the use of the individual CRI values for a student. Of course, this is best done on a one-to-one basis, where the student explores the identified misconceptions with the assistance of a teacher or a tutor (i.e., in a Socratic dialogue) with a solid grasp of the topics.

Figures 1 and 2 show the average CRI values for correct and wrong answers for each question, along with the fraction or proportion of answers that are correct. For the purpose of deciding whether a CRI is low or high, we adopted a threshold value of 2.5. A CRI above or below 2.5 is considered to be high or low respectively.

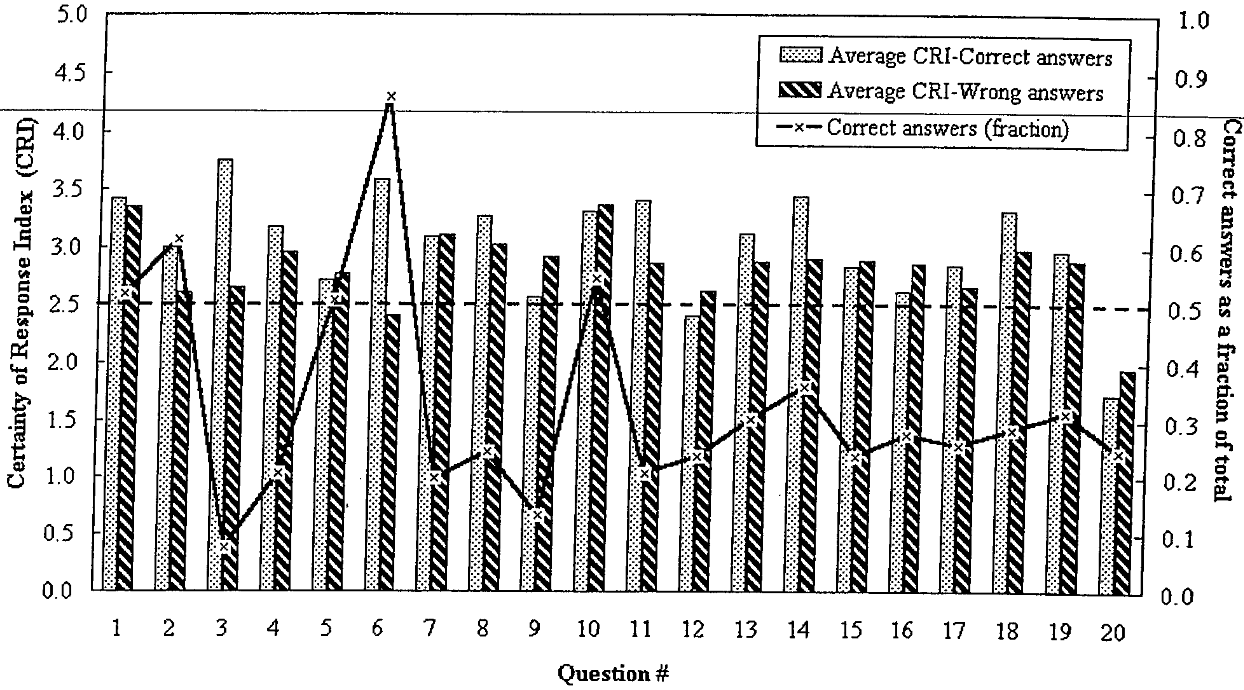

Figure 1. Chart based on the results of 106 students who took the Pre-Spring 1997 Diagnostic Test. The bar graph shows the values of the average CRI for correct and wrong answers, for each question. Question numbers are shown on the horizontal axis.

Other choices are possible for the threshold, including the one where values between 2 and 3 are considered to be in a zone of undetermination.

Given below are the directions for completing the answer sheet.

Directions

For each answer you select, provide in the square below one of the following numbers indicating whether you answered using KNOWLEDGE LEARNED IN CLASSES/ BOOKS (RATING 1 to 5) OR NOT (rating of 0 for a total guess).

0	Totally guessed answer
1	Almost a guess
2	Not sure
3	Sure
4	Almost certain
5	Certain

Given below are two sample questions, #6 and #7 (group III) that deal with a frictional force and its relationship with the normal force. These questions are provided by Halloun and Hestenes [3], except for the CRI. For each question, the student is requested to circle the selected answer from the given choices and write a CRI in the square provided below the answers.

III Figure 3 shows a block that is released from the top A of an incline of given length AB and slope angle θ.

Q6 What variable(s) affect the *speed* that the block reaches at the bottom of the incline?
(a) Shape of the block.
(b) Surface of the incline.
(c) Air density.
(d) Shape of the block and air density.
(e) Shape of the block, surface of the incline and air density.

☐ Enter a CRI value, from 0 to 5.

Q7 Suppose we *ignore air resistance*, and the incline is *frictionless*. What variable(s) affect the *speed* that the block reaches at the bottom B of the incline?
(a) Shape of the block.
(b) Mass of the block.
(c) Shape and mass of the block.

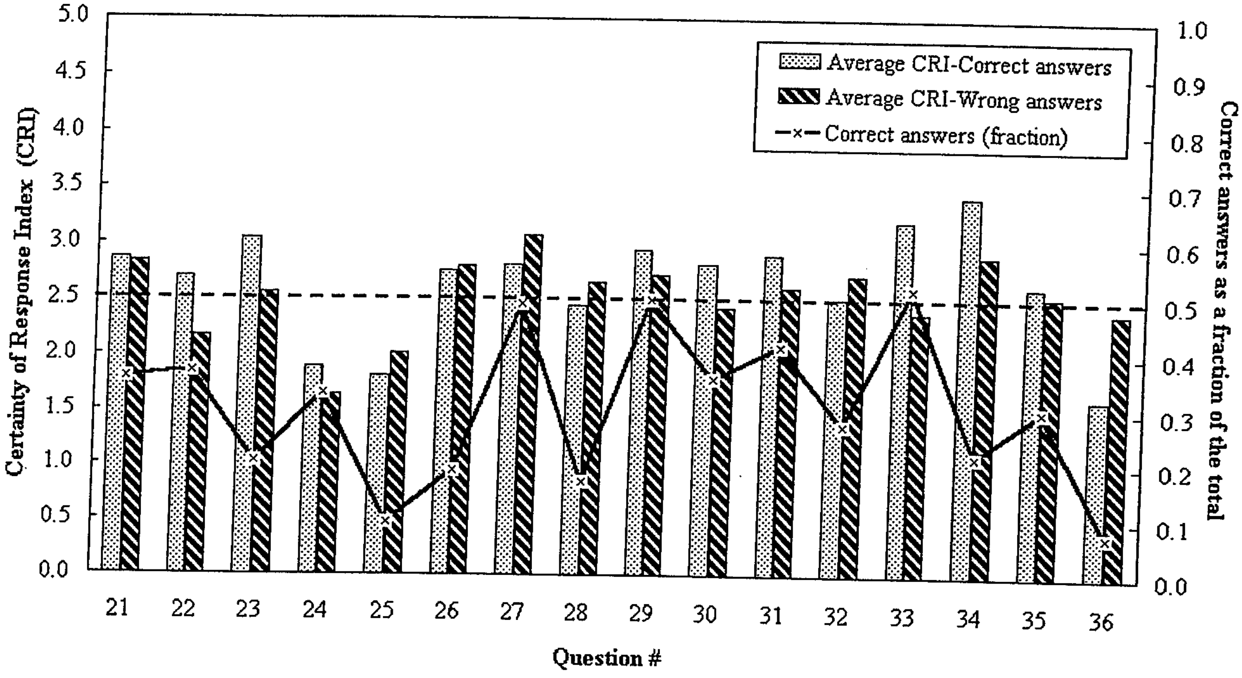

Figure 2. Chart based on the results of 106 students who took the Pre-Spring 1997 Diagnostic Test. The bar graph shows the values of the average CRI for correct and wrong answers, for each question. Question numbers are shown on the horizontal axis.

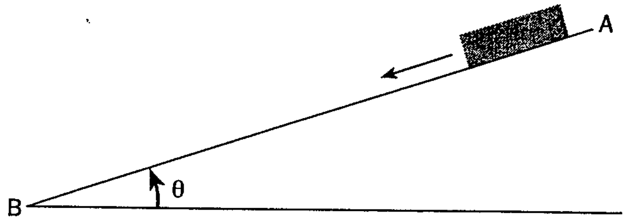

Figure 3. Drawing for sample questions #6 and #7 (group III). The block is released from the top of an incline of length AB and slope angle θ.

(d) Density of the block.
(e) None of the above.

☐ Enter a CRI value, from 0 to 5.

From figure 1 and for question #6, the average CRI for correct answers is 3.6, that for wrong answers is 2.4, and the correct answers as a fraction of the total are 0.88. Based on the threshold of 2.5 and using table 2 (WL), the data suggest a lack of knowledge as opposed to misconceptions. This conclusion is further strengthened by the high percentage of answers that are correct (i.e. 88%). This percentage indicates that only a small number of students had difficulty answering this question. Their difficulties were probably due to a lack of knowledge. The relatively low (2.4) average CRI for wrong answers supports this contention.

For question #7, the average CRI for correct answers is 3.2, that for wrong answers is 3.2 and the correct answers as a fraction of the total are 0.2. Based on the threshold of 2.5, the data suggest the presence of misconceptions. As shown in table 2, wrong answers and a high average CRI (WH) indicate the presence of misconceptions. This conclusion is further strengthened by the small percentage (20%) of correct answers.

Using the above definitions, questions #1, 3, 4, 7, 8, 9, 10, 11, 13, 14, 15, 16, 18, 19, 21, 26, 27 and 34 have high average CRI values for wrong answers (WH). For these questions, close to 50% of the students felt reasonably certain about their knowledge and skills and yet selected a wrong answer. In table 2, this corresponds to wrong answer and high average CRI (WH). At varying degrees that depend on the average CRI values, we suspect the presence of misconceptions associated with the students' 'perceived' grasp of the topics in these 18 questions.

A low average CRI for wrong answers is associated with questions #2, 5, 6, 12, 17, 20, 22, 23, 24, 25, 28, 29, 30, 31, 32, 33, 35 and 36. Hence, as per table 2, these low average CRI values indicate a lack of knowledge. The lack of certainty in the ability to select and utilize the required principles and laws, as indicated by the low average CRI for wrong answers (WL), denotes a lack of knowledge as opposed to the presence of a misconception.

In cases where the average CRI was very close to 2.5, the fraction of correct answers was utilized to decide whether the average CRI value should be considered high or low. The average CRI for wrong answers for questions #3 and #28, around 2.5, were considered to be high due to the large proportion of students who answered the questions incorrectly. Indeed, this large proportion and the average CRI around 2.5 suggest that significant number of students might have given a high CRI value for their wrong answers. Even though these average CRI values are not much higher than 2.5, prudence suggests that the instructor address these topics as if the students had some misconceptions. The average CRI values for wrong answers for questions #5, 12, 23, 28 and 32 were also very close to 2.5, but they were classified as low average CRI because the number of students selecting the correct answer was relatively high. In this case, no special action is suggested for the entire class, given the probably small number of students with misconceptions.

A trend in the average CRI values for correct answers provides additional evidence that the CRI is a useful indicator of the certainty with which the students answer questions. Each group contains several questions that are designed to probe the depth of students' comprehension of that specific topic. In figures 1 and 2, the average CRI for correct answers in several groups is higher for the first one or two questions and then decreases as the questions increasingly probe the depth of knowledge of the specific concepts or skills.

Conclusions

This work can be easily utilized by high school teachers and college instructors to differentiate misconceptions from a lack of knowledge. If the answers and related CRI values indicate the presence of misconceptions, then instructional deliveries should be modified accordingly, with the explicit intent of removing the misconceptions. Classroom examples, homework assignments and quizzes should be designed to ascertain the grasp of the correct concepts. The information obtained by utilizing this method can also be used to address other areas of instruction. In particular, it could be used:

(a) as a means of assessing the suitability of the emphasis placed on different sections of a course;
(b) as a diagnostic tool, enabling the teacher to modify the delivery;
(c) as a tool for assessing progress or teaching effectiveness when both pre- and post-tests are administered; and
(d) as a tool for comparing the effectiveness of different delivery methods, including technology-integrated or reform-imbued approaches, in promoting understanding and problem-solving proficiency.

Acknowledgments

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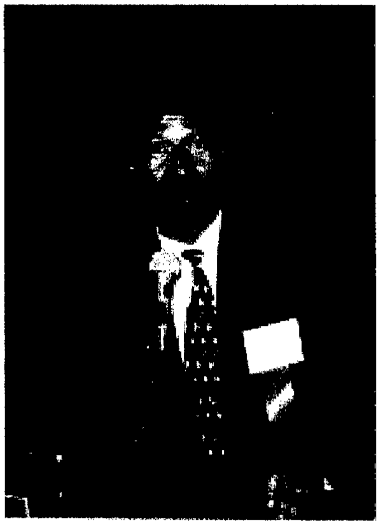
* Excerpt from the *Fifth Annual DoE EPSCoR and LS-LAMP Research Conference Proceedings 2001* (ISBN 0-9704609-4-5), pages 52-54.

SESSION PRESENTATIONS

Traveling as far away as New York City, the students also participated in conference discussions on the use of LabWorks technology, financing graduate education, and succeeding in graduate school. Sessions like "Reinvigorating your Research Program through Collaborations," "Undergraduate Research as a Vehicle for Success for Underrepresented Students in Science and Engineering," and the "Role of Undergraduate Research in the Recruitment/Retention of Students" provided information and resources on improving undergraduate research in two-year and four-year colleges and universities. The following pages are presentations made during the conference as submitted by the speaker for these proceedings.

Avoiding (or Closing) Academic Achievement Gaps

Diola Bagayoko, Ph.D.
SU System Distinguished Professor of Physics
Director, Timbuktu Academy and PIPELINES
Co-Investigator, Louis Stokes Louisiana Alliance for Minority Participation



The Power Law and the Law of Performance:
A Rosetta Stone for Deciphering the Process of Education

Recent articles in the Baton Rouge *Advocate* (http://www.theadvocate.com) addressed the achievement levels of students on the American College Test (ACT) and other standardized examinations. Please see "Test score gap offers challenge" (the Advocate, 10/02/00, page 1A), "Suburban parishes ACT scores mixed" (*Advocate*, 8/29/00, page 1B), "Reading, science scores static in national tests: gap grows between black, white students" (*Advocate*, 8/25/00, page 1A), and "1999 ACT scores of area schools" (*Advocate*, 2/29/00).

In light of the enduring interest reflected in these articles and many others, we presume that the public is interested in a complete explanation of "what determines achievement levels on tests." Specifically, two publications explained, using the power law of human performance also known as the power law of practice, how achievement levels are reached [See *Education*, Vol. 115, No. 1, pp. 31-39, 1994 and pp. 11-18].

The first of these publications provides an extension of the power law known as the compound law or simply the law of practice (CLP or LP). This law clearly, unambiguously, and implacably shows that the achievement level of a student on a standardized test is directly determined, first and foremost, by (a) the exposure of that student to appropriate subject contents and skills, (b) the adequacy of the scope and depth of this exposure, and (c) the actual amount of time the student spends learning, applying, and practicing said contents and skills—*in and outside the classroom. "Appropriate" and "adequate" are objectively defined by competitive standards and not some parochial or self-serving norms or criteria set by some individuals.*

According to the law, socioeconomic status, ethnicity, and gender, among others, are not intrinsic factors that determine the achievement levels of students! *Their effects are indirect. Academic achievement levels depend first and foremost upon access to and utilization of competitively engaging, standard-based education and in-*

directly upon socioeconomic and cultural conditions. Negative, indirect effects of socioeconomic, ethnic, and gender factors on academic achievements, if any, can be avoided by ensuring items (a) through (c) as noted above.

The power law of practice (or of performance) and its explanation of the achievement levels of students are presented in detail in a video tape, *Genesis of Genius,* available from the Louis Stokes Louisiana Alliance for Minority Participation (LS-LAMP) at Southern University and A&M College, Baton Rouge [http://www.ls-lamp.org, telephone: (225) 771-2777.

Interestingly, most individuals are familiar with the necessity for items (a) through (c) in sports and the arts. It is the same for intellectual endeavors! We hope that interested parents, teachers, students, and others will take advantage of this video tape that also explains how achievement gaps between various groups of students, on standardized tests, are formed. *These gaps, according to the LP, can be avoided or closed by the application of items (a) through (c) listed above.* The Timbuktu Academy has been doing so since 1990 (http://www.phys.subr.edu/timbuktu.htm)! The rigorous application of the above law allows the Academy to register quantum leaps in the ACT scores of its pre-college, summer students every year. Details on these leaps are available at the web site of the Academy and upon request. In each of 2000 and 2001, 10 of these pre-college scholars of the Academy were among the National Achievement and National Merit semifinalists!

Explaining American College Test (ACT) Scores of U.S. High School Graduating Class of 1999 (Similar results are found from 1996 to 1999, with slightly changing gaps)

The law of performance (LP) explains academic achievement gaps. Note the smaller mathematics gap (mathematics) that widens with course taking! The key (i.e., Rosetta Stone) to the puzzle is that the scores, as per the LP, are determined (causally so) by the actual learning (practice)—mediated in part by (a) course taking, (b) the topics, their scope, and depth in every course, (c) the actual practice by the students as mediated (or induced) by graded homework assignments, tests, and others. *All algebra courses are not equal or equivalent; and, all students taking given courses do not devote equivalent times to these courses; the needed time for a course, incidentally, depends on the background of a given student!* Therein lies the quintessential source of differences between the achievement levels of students who took similar courses. Course taking alone, as shown in the table below, accounts for most of the rest of differences between the achievement levels of students. Genes, intelligence quotient (IQ), ethnicity, and gender do not enter into this explanation or equation.

Note the large gap, in English, for those taking less than four years of English. It is partly at the root of the large gaps, of similar sizes, in reading and in science reasoning! See exposure (at home, school, etc.) to Standard English and a rich vocabulary environment, from birth to the test date, to explain the gap in English—as per the law of performance or of practice.

Noting how the English gap contributes to the gaps in others, the Timbuktu Academy doubled the time devoted to English by its summer pre-college students in 1996-97. Following this change, ACT score improvements, over a six-week period, jumped from an average of two to an average of four or five. The strong and positive correlation between the SAT and the GRE scores in the verbal and quantitative sections, respectively, gave the Timbuktu Academy an added incentive to close the English gap. As expected, the gaps in reading and science reasoning narrowed significantly. After all, languages are the vehicles of thought. See Table I.

For the Creation of Educational Value-Added (i.e., High Academic Achievements)

(1) *The law of performance says that all students can learn—at a competitive level.* It is the scientific basis for high expectations for all students! It also says that exposure to competitive curricula, over the years, and adequate learning and practice are necessary for high academic achievements by most students.

(2) *The law of performance also says that exposure to substandard curricula, over the years, will ineluctably result in low achievements, irrespective of intellectual quotient, genes, ethnicity, gender, etc.* Whatever the reasons, tracking a student in "low ability" groups guarantees that said student will underachieve.

(3) There is no substitute for standard-based subject matter and skills content of each and every course, from pre-K to graduate school and beyond.

(4) There is no substitute for the adequacy of the battery of courses taken at every grade level. A national, reference curriculum, from K through college, will inform parents and students of prevailing competitive norms or standards.

(5) There is no way to circumvent the *internal rigidity* (i.e., sequential nature of aspects of knowledge). Consequently, the knowledge and skills base of the learner has a great influence on the "acquired ability" to learn. Particular difficulties in many courses are often due to utterly inadequate background as opposed to a lack of "smartness." Writing follows reading. Calculus follows arithmetic, algebra, and basic geometry and trigonometry.

(6) There is no substitute for the devotion of "adequate" time to learning tasks! So says the law of performance (LP). "Adequate" is to be determined using competitiveness criteria and national norms and standards. In the absence of a reference curriculum, those with the least intellectual, material, and financial means are likely to have the most difficulty in the determination of a competitive curriculum and of the "adequacy" of the time on learning tasks. This holds for parents, teachers, and students.

(7) There is no substitute for quality teaching, with its inherently closed feedback loop. Such a teaching commands a significant portion of the out-of-class time through graded assignments. These assignments simulate the actual way in which knowledge is applied and research is conducted. They do so better than any test, however comprehensive it may be. Further, they mold study habits over time; these habits are critical aspects of the unwritten curriculum.

(8) There is no substitute for parents or guardians in ensuring that adequate time is spent on learning tasks during the academic year and in the summer (i.e., reading and report writing). Consequently, they have to limit TV viewing, video playing, and listening to music. These activities and similar ones are privileges that should be earned by young students after doing school work.

(9) There is no substitute for familiarity with the format and subject/skill content of applicable tests. This tautology applies to all standardized tests, whether they are norm- or criterion-referenced, from kindergarten through the doctoral degree.

(10) There is no substitute for efforts and practice in acquiring and enhancing proficiency in a complex process, from reading to writing, research, and problem-solving, sports, and the arts. So says the law of performance, regardless of claims of "innate" abilities.

TABLE I

A comparison of the ACT scores of African American/Black and of Caucasian/White students for the graduating class of 1999. Similar results for the gaps, due to course taking and to the actual time on learning tasks of varying standards, are found for 1996 through 1998, with slightly changing gaps. In the table, E stands for English, A for Algebra, Trig. for Trigonometry, Geom. forGeometry, Hist. for History, Phys. for Physics, Chem. for chemistry.

English Course Pattern	Number of Black Students	ACT English	Number of White Students	ACT English	GAPS
E9, E10, E11, E12, Speech	24,586	**17.0**	250,463	**21.8**	**4.8**
E9, E10, E11, E12	69,780	16.4	422,673	21.3	
Less Than 4 years of English	5,940	**14.8**	38,515	**19.4**	**4.6**
Course Taking Difference (top-bottom)		*2.2*		*2.4*	
Mathematics Course Pattern	Number of Black Students	ACT Math	Number of White Students	ACT Math	GAPS
A 1, A 2, Geom., Trig., Calculus	4,022	**19.7**	46,643	**25.1**	**5.6**
A 1, A 2, Geom., Trig., other Advanced Mathematics	7,085	18.9	75,979	22.6	
Other comb. Of four or more years of Math (i.e., Mathematics)	18,538	19.0	170,873	24.6	
A 1, A 2, Geom., Trig.	10,442	17.3	75,307	21.1	
A 1, A 2, Geom., other Adv. Math	9,518	17.4	83,605	20.9	
Other comb. Of three or 3.5 years of Math	6,181	16.6	37,278	20.5	
A 1, A 2, Geom.	28,288	15.6	144,952	18.2	
Less Than 3 years of math	15,967	**14.8**	75,208	**16.8**	**2.0**
Course Taking Difference (top-bottom)		*4.9*		*8.3*	
Social Science Course Pattern	Number of Black Students	ACT Reading	Number of White Students	ACT Reading	GAPS
US Hist., World Hist., American Government, other History	2,522	**17.8**	21,612	**22.8**	**5.0**
Less than 3 years of Social Science	17,899	**16.2**	104,682	**21.1**	**4.9**
Course Taking difference (top-bottom)		*1.6*		*1.7*	
Natural Science Course Pattern	Number of Black Students	ACT Science Reasoning	Number of White Students	ACT Science Reasoning	GAPS
Gen. Science, Biology, Chem., Phys.	26,733	**18.4**	224,723	**23.2**	**4.8**
Less Than 3 years of Natural Science	24,921	**16.1**	152,562	**19.5**	**3.4**
Course Taking Difference (top-bottom)		*2.3*			*3.7*

SOURCE: *ACT Research Services, P. O. Box 168, Iowa City, Iowa 52243. Telephone: (319) 337-1113; Fax: (319) 339-3020. Courtesy of Merine Farmer and ACT. For the Creation of Educational Value-Added (i.e., High Academic Achievements)*

Diola Bagayoko, Ph.D., is the Southern University System Distinguished Professor of Physics, director of the Timbuktu Academy and PIPELINES, and co-investigator of the Louis Stokes Louisiana Alliance for Minority Participation (LS-LAMP). His email address is Bagayoko@aol.com.

Saleem Hasan, Ph.D., is evaluation coordinator of LS-LAMP. His address is Southern University and A&M College, Baton Rouge, P. O. Box 11776, Baton Rouge, Louisiana 70813.

Robert L. Ford, Ph.D., is professor of chemistry, project director of LS-LAMP, and assistant-associate commissioner for sponsored programs for the Louisiana Board of Regents.

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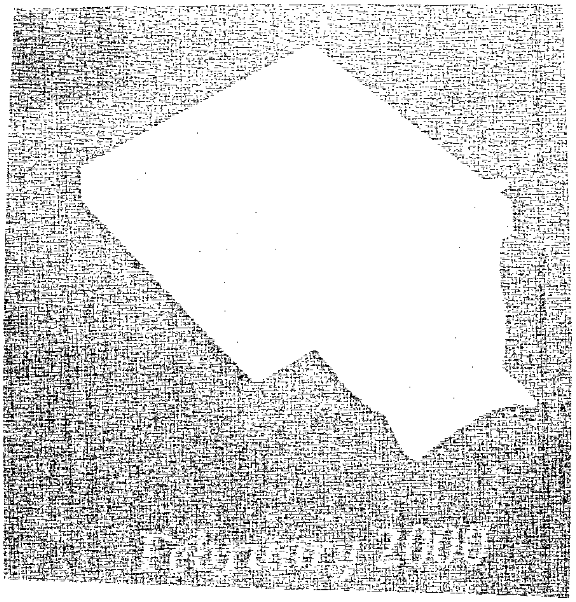
Scholarly Guideposts for Junior Faculty


February 2000

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Fundamentals of Mentoring and Networking

Dr. Diola Bagayoko

Dr. Diola Bagayoko
Southern University System
Distinguished Professor of Physics
and Director, the Timbuktu Academy

Dr. Robert L. Ford
Professor of Chemistry
and Director, LSAMP

Dr. Ella L. Kelley
Associate Professor of Chemistry

Southern University at Baton Rouge
Baton Rouge, Louisiana

Dr. Robert L. Ford

Dr. Ella L. Kelley

Abstract

The aim of this article is to provide an overview of mentoring, in its complexity, and to underscore its importance in the creation of educational, research, and professional value-added. Networking, a prevailing form of peer-mentoring, is directly relevant to attaining, maintaining, and enhancing professional proficiency and competitiveness by junior and senior faculty members as well as other professionals in public and private sectors. The distinction claimed by this work stems from the empirically-established and practice-verified nature of its basic precepts as they relate to mentoring that is viewed as an emerging, interdisciplinary field of scholarly inquiry. The power law of human performance and its extension, the integrated law of performance (ILP), provide a foundation for our approach. It is hoped that the reader will see herein a clear, fail-safe, and comprehensive road-map for the pursuit of competitiveness by students and by faculty members.

Systemic Mentoring includes:

- the weaving of mentoring interests, processes, etc. into the fabric of the department, unit, organization, research center or laboratory and of the whole institution or organization. To do so often requires a mentoring coordinator per department or unit. It also requires, in the long term, an explicit place for mentoring in (a) the definition of the duties and responsibilities of faculty, senior personnel, or managers and (b) the incentive or reward structures.

  On a college campus, the role of a departmental mentoring coordinator includes working with the department chair to see to it that students who need tutoring receive it. Tutoring should be made available at a fixed place, at regular hours, and the tutors should include faculty (one supervisor) and well-trained advanced undergraduates and graduate students. If the actual utilization of technology is taking place, then one expects E-mail communication to be utilized in mentoring and for setting-up some advisement or tutoring meetings, appointments, and more. (For research organization, the coordinator works with the Director of the Center or Laboratory.)

- maintaining a comprehensive data base that captures pertinent information on background, grades, research accomplishments, publication and presentation record, etc. Mentors provide the data on their mentees to the coordinator. Another form of data gathering is needed for the mentoring of junior faculty members or of new employees.

- following-up with the mentees, even after graduation. This entails knowing the graduate school or the employment information of each graduate.

- writing proposals to secure funding from a variety of sources including federal, industrial, and foundation sources, and promoting the inclusion of financial support for mentees in other proposals not necessarily devoted to mentoring activities or projects.

- placing mentees in research projects—on and off campus—and in summer or academic year internship positions (availing opportunities to junior faculty members or new employees).

- interfacing professionally with (a) the Admissions and Recruitment Office, (b) the Junior Division, (c) the Honors College, for matters of recruitment and mentoring, and (d) the Office of Grants and Sponsored Programs for funding opportunities. This list is not exhaustive.

A systemic approach to mentoring has always been, and this is a well kept secret, the engine that maintains the competitive edge of units, departments, research centers, corporations, etc. that implement it! A good understanding of the concept of "distributed responsibilities" and of "shared credits" substitutes cooperative learning/working and synergy to "retrograde competition." Then, positive emulation pervades the stimulated working environment. Individuals discover their real competition: each competes with him/herself to increase his/her contributions—in quantity and quality—to the organization. Continual professional development is understood. The laws discussed below provides the profound reason that mentoring is needed by students, junior faculty, and by others (e.g., networking and peer-mentoring are needed by anyone who is to remain competitive in some endeavors).

The Integrated Law of Human Performance

The power law of human performance (Newel and Rosenbloom, 1981) and its extension, the integrated or compound law of human performance (Bagayoko and Kelley, 1994) provide a rigorous, scientific rationale or reason for holistic and systemic mentoring. It is highly empowering as it shows that efforts and practices—preferably with the assistance of experts—will lead anyone to competitiveness in any endeavor!

We have learned not to be stressed, ashamed, or apologetic for not being experts in different areas. We have learned to recall the integrated law of human performance and to begin learning earnestly whatever we have to learn. We know that, with time and adequate efforts, we shall reach any level of expertise, proficiency, or competitiveness!

The Power Law of Performance or of Practice (PLP) states that the time (T) it takes an individual to perform a given task decreases as the number of times (N) the individual practiced the task increases. In mathematical terminology, the law is (Newel and Rosenbloom, 1981):

$$T = A + B\,(N + E)^{-p} \quad \text{or} \quad T = A + B/(N + E)^{p}$$

where A, B, E and p are constants that vary (a) with the task at hand and (b) with the individual performing the task. A represents a physiological limit. B and E partly denote prior experiences before the beginning of the practice sessions, and p is the learning rate. In other words, the law states that 'practice renders perfect.' This law applies to the performance of sensory-motor (or athletic), creative (or artistic), and cognitive (or intellectual) tasks.

The following figure graphically shows the plot of the above mathematical expression of the power law of human performance for a problem-solving task. The time to perform the task is shown on the vertical axis while the number of times the individual practiced the task (N) is on the horizontal axis. The reader should note the greater rate increase in proficiency (i.e., the decrease in the time) for the first practices. Naturally, for very large numbers of practices, the increase in proficiency per unit practice gets smaller.

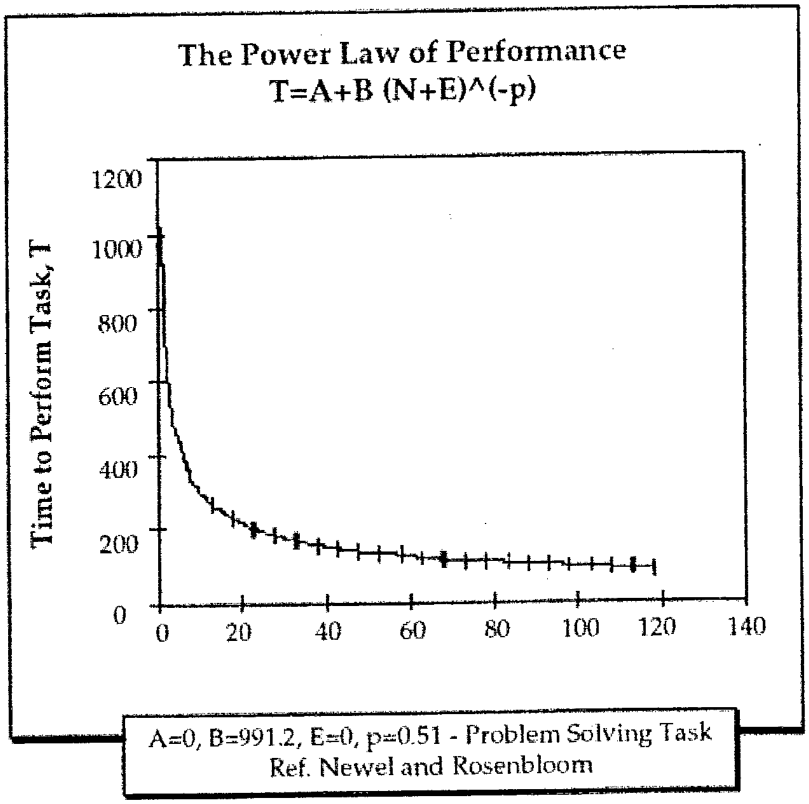

Figure 1. The Power Law of Human Performance. The shorter the time T to perform the task, *completely and correctly*, the higher the level of proficiency. *Hence, as the number of practices increases so does the proficiency of the individual.*

The dramatic impact of this law becomes apparent when one considers its application over several tasks and several days, months, and years. Then it becomes clear that genius is mostly the result of sustained practice. The same way adequate practice, at an adequate scope and depth, is needed for the making of Olympic, National Basketball Association, National Football League, and Major League Soccer champions and for the making of musicians and artists, the same way it is needed for the making of science, engineering, and mathematics scholars, including scholars in the social and behavioral sciences.

Further, this law is implacable. It applies whether one likes it or not! It applies to the refinement of the enhancement of the teaching, mentoring, research, and writing skills of a faculty member or of a mentee! These points are discussed further by Bagayoko and Kelley (1994) and Moore and Bagayoko (1994) in connection with the explanation of the creation of educational value added from K through graduate school and beyond.

The integrated or compound law of human performance (Bagayoko and Kelley, 1994), is the convolution of the power law of performance as simultaneously applied to several tasks over a long period of time. The main difference between the power law and the integrated law is that the former follows a simple equation that involves an exponent (i.e., p) while the mathematical form of the latter is yet to be determined. The quintessential point here, however, stems from the fact that according to the integrated law of human performance, the abilities, skills, and attributes of students (or mentees) that are meaningfully engaged and challenged in and outside (as by mentoring activities) the classroom from K through graduate school and beyond are the ones that will develop!

The integrated law of human performance provides the scientific basis for high expectations for all students! This point is rigorously established by Bagayoko and Kelley (1994). Professional mentoring, as defined above, provides an almost fail-safe strategy for promoting the academic excellence of all students and the professional growth of all faculty members, beginning with the junior faculty! In general, the integrated law of human performance is the tool for increasing proficiency or expertise in teaching, mentoring, learning, networking, developing proposals, conducting research, publishing, etc.

This integrated or compound law of human performance is the "Rosetta Stone" of education and of the development of professional competency or competitiveness. This assertion is obvious in sports and in artistic endeavors. As per this law, the optimum acquisition of expertise in complex processes (e.g., learning, proposal development, research, teaching, and related technology integration) requires mentoring (guidance and support), networking, and practice.

Epilogue

Complex processes generally involve several individuals playing their respective role. This situation led the Timbuktu Academy to introduce the concept of distributed responsibilities and of shared credits. This concept is rooted in that of ultimate value. Various parts of the functionally necessary core of a system could have vastly different prices even though the ultimate value of each one of them is that of the properly operating system. Cars and computers provide common examples. While the engine has a value (i.e., price) much higher than that of the tube bringing the fuel to the engine, these two items have the same ultimate value in the sense that the car will get nowhere without either one of them working properly! In a situation of distributed responsibilities and of shared credits, a problem is that individuals, groups, organizations, etc. could conveniently blame everything on others without taking stock into what exactly they have done themselves!

For mentoring and networking, the responsibilities are distributed between many individuals (faculty, students, center directors, junior scholars, scientists, engineers, etc.), institutional units (a department, a college, research centers, laboratories, institutes, etc.) and external entities (funding agencies, policy makers, etc.)! Responsibilities are distributed and credits are shared. To understand this concept in a profound fashion is to begin good practices of holistic and systemic mentoring and networking for the training of the next generation of productive citizens, managers, and research scholars, and for continual, professional development. We have learned, through practice, (a) not to be misled again by those 'majoring' in blaming others, (b) consistently, thoroughly, and persistently doing and documenting the role we are supposed to play, and (c) politely, persuasively, and persistently requesting that members of a vast network or web of peers or administrators play their roles, whenever needed! It appears that playing one's role professionally is the best way for getting others to cooperate—without saying one word. Good deeds are louder that words!

The practice of mentoring and networking creates and maintains the needed support system and environment in which individuals develop and grow—professionally and otherwise. It is the human equivalent of the proper ecosystem for a plant. This contention is corroborated by human experience through the ages and through different cultures. Indications of the veracity of this proposition include biographies, implicit learning, and the reader's own experiences. The mode of transmission of "knowledge and skills," before the advent of formal schooling, generally included mentoring (apprenticeship, hands-on, and experiential learning).

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This paper is perhaps the one addressing most of the aspects of mentoring as noted in this presentation.

Bagayoko, D. and Ella L. Kelley. "The Dynamics of Student Retention, a Review and a Prescription." *Education* 115, no. 1 (fall, 1994): 31-39.

This publication explains the process of creating educational value added, from K through graduate school and beyond, using the power law and the compound or integrated law of human performance.

Gates, James. "Information-Age Technology: An Opportunity for Enhanced Faculty Effectiveness." *Scholarly Guideposts for Junior Faculty*

Washington, D.C.: Quality Education for Minorities (QEM) Network (1999.

Moore, William and Diola Bagayoko. "A Paradigm of Education: The Model of the Timbuktu Academy." *Education* 115, no. 1 (1994): 11-18.

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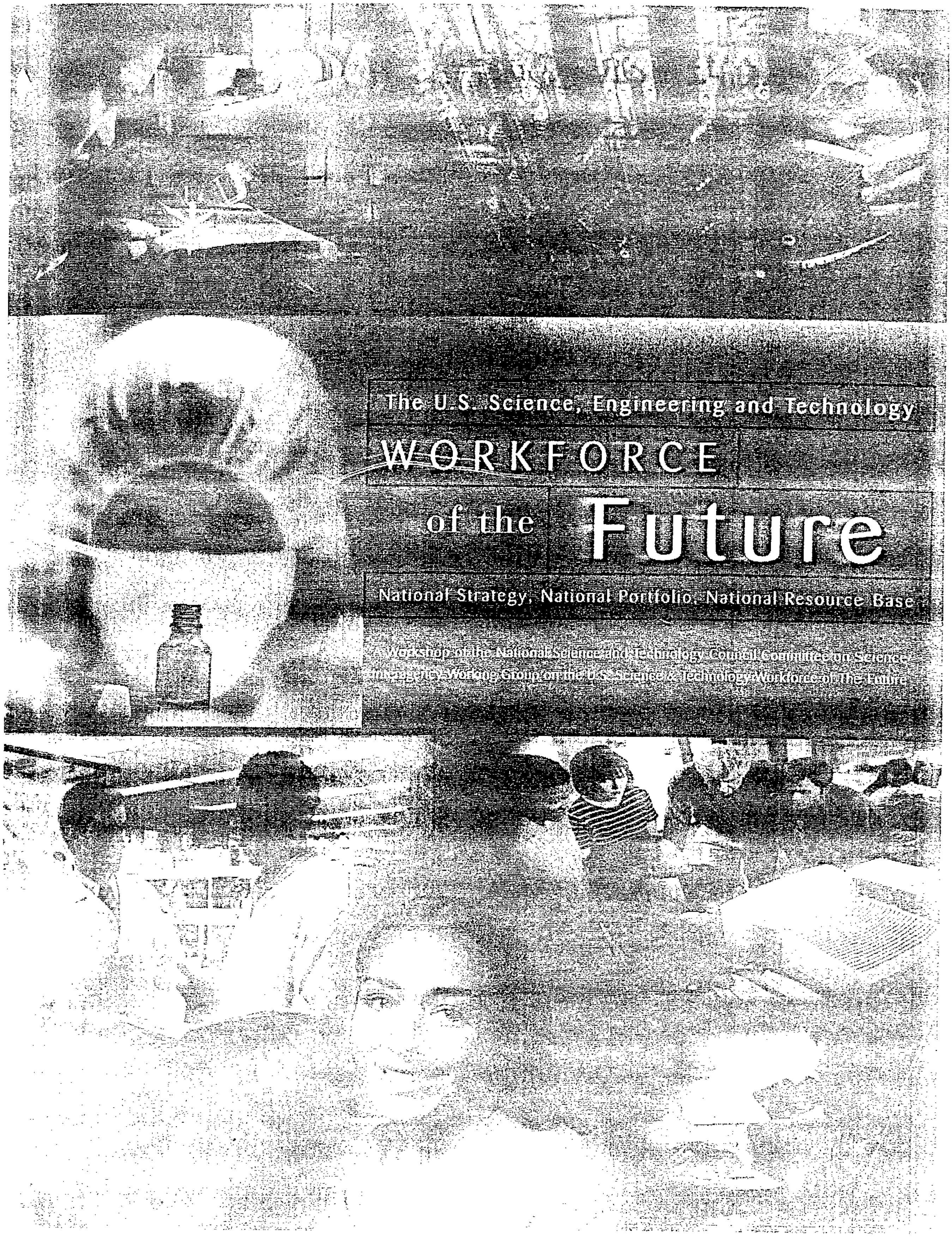

The U.S. Science, Engineering and Technology
WORKFORCE of the Future

National Strategy, National Portfolio, National Resource Base

A Workshop of the National Science and Technology Council Committee on Science
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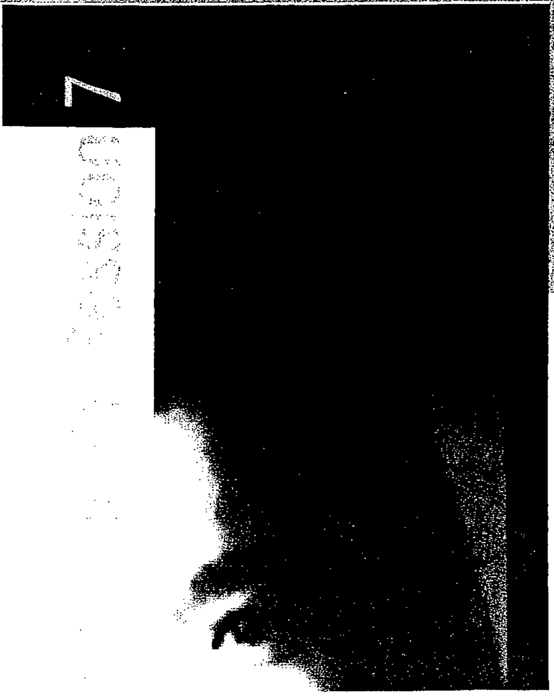
PLENARY SESSION #7

Building Capacity: Developing and Implementing a National HRD Cadre of Presidential Awardees for Excellence in Science, Mathematics, & Engineering Mentoring (PAESMEM)

OVERVIEW

Incentives are not limited to funding. They are found in a family, at school, in a university, and at public and private agencies and organizations. We do what is checked, valued, and rewarded. Southern University-Baton Rouge used this fact to establish formally systemic mentoring in all its science, mathematics and engineering departments in January 1997.



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RESPONDENTS

Ms. Martha Absher
Program Director, NSF Engineering Research Center, Duke University

Ms. Catherine J. Didion
Executive Director, AWIS

DR. HRABOWSKI: Good afternoon. I am Freeman Hrabowski and I am chairing the session focusing on "Building Capacity: Developing and Implementing a National HRD Cadre of Presidential Awardees for Excellence in Science, Mathematics and Engineering Mentoring."

I will present the people in the order in which they will be speaking. The first speaker will be Diola Bagayoko, who is Director of Timbuktu Academy, Southern University and A&M College.

DR. BAGAYOKO: Good afternoon, ladies and gentlemen. I am certainly delighted to be part of this exhilarating experience.

Dr. Bruce Alberts, the President of the National Academy of Science, recently stated that "the world is too complex for a few individuals to make wise decisions about all aspects of public policy."

As one who shares this view, I am pleased to note that we have many participants and that many more have been directly or indirectly consulted in connection with this workshop.

Further, the titles of the plenary sessions denote a "comprehensive approach" to a very complex and critically important matter, namely, educating and training — and competitively so — the science, engineering and technology workforce.

The contribution I wish to make to this workshop is to sing repeatedly, and loudly, the fact that we have embarked on an exhilarating and challenging journey whose moving destination is to be continually reached.

In so doing, I first take stock in some encouraging developments that are expected to be useful during our endless and rewarding journey. These developments include ongoing educational reform efforts and the emerging understanding of the importance of mentoring.

The establishment of the U.S. Presidential Awards for Excellence in Science, Mathematics and Engineering Mentoring Program in 1996 was a salient indication of the emerging recognition for mentoring. This development asserted the relevancy of mentoring and recognized its vital role in promoting quality learning and personal and professional growth. It also recognized the need to engage minority students, along with general students, in a manner that determines success.

The comprehensive approach adopted by these reforms is appropriately emulated by this workshop. The changing road map for this journey includes research efforts and related findings that are guiding the above reforms. The Third International Science and Mathematics Study is a typical example of these research efforts.

In addition to notable research efforts in universities by professional societies, and by the National Research Council, we note the *National Longitudinal Survey, 1988 and Beyond*, and the extensive work of the National Center for Education Statistics and of the NSF Division of Human Resources Studies.

The databases of the Census Bureau and of the U.S. Departments of Labor and Commerce are indispensible tools for the referenced research efforts. The recent solution of the ecological inference problem is expected to be useful.

Guideposts or landmarks on this journey include some very well established principles that I value very much. A few of these guideposts or intrinsic forces include: the perennial role of incentives in promoting and sustaining change in a chosen direction; determinants of the creation of educational, research and professional value added; the continuous nature of generational change; and the need for a system approach, i.e., distributed responsibilities and shared creativities and the related webs of collaborations.

The integrated or compound law of human performance or of practice explains key determinants in the process of creating educational value added from kindergarten through graduate school and beyond.

The importance of time on task, as apparent through the ILHP, is further underscored by the recent unification of behaviorism and cognitivism. Further details are available on these guideposts.

A first recommendation, in light of the above understanding, is that we should develop regular and electronic ways and means to increase the awareness of and access to the current portfolio of successful practices and programs. The presidential awardees could play a significant role in this process, in light of their extensive experiences and successful programs.

For instance, minority 11th graders at the Timbuktu Academy have established, through empirical research and through their work, that the road to excellence is known. Irrespective of innate attributes, the attainment of intellectual and professional excellence includes appropriate exposure to the applicable content and skills, in scope and in depth, and the adequacy of the amount and quality of practice as ascertained by valid, reliable and comprehensive outcome assessments.

Our empirical research found that gaps in standardized test scores of some groups are correlated to certain students receiving correctly sequenced and properly taught courses in subject matters and skill areas that are explicitly keyed to a given test and by the support, encouragement, resources and drive to practice sufficiently in and outside the classroom or laboratory. The increases in the American College Test equivalent scores of the above 11th graders, over a six-week period, have verified this empirical finding every summer, from 1995 to the present.

A second recommendation relates to the need for further understanding and application of distributed responsibilities and shared credits. This understanding enables creative and innovative collaborations for shared success or credits, for individuals as well as organizations.

A third and unavoidable recommendation consists of the needed revisions or updates of incentive structures to promote and sustain change in the right direction. Incentives are not limited to funding. They are found in a family, at school, in a university, and at public and private agencies and organizations. We do what is checked, valued, and rewarded. Southern University-Baton Rouge used this fact to establish formally systemic mentoring in all its science, mathematics and engineering departments in January 1997.

By some chance, some months ago I wrote a publication that seems to respond to much of the talk which happened yesterday, this morning and today at the lunch. This little publication states that earlier guidance pays off.

Having made that point, I would like to remake the statement that we have embarked on a journey. This is an exhilarating and challenging journey whose moving destination is to be reached continually. Hence, do I need to try to say everything here this afternoon? No, this is a journey just beginning.

There are few words more that I will say before I sit down. They have to do with the recommendations.

After we build partnerships for mentoring a single student or for a national program, let's be very careful to always remember to share the credit. Very often the ones who do the work do not create the problem. It is some other who tries to talk about the beautiful job that this organization has done and forget the beautiful contribution this other actor also made.

The word incentive is my last recommendation. If you look at biological processes or evolution, you will see that changes have always been provoked and maintained by incentive structures, whether of a natural, social, or financial measure. For the contributions that we are trying to make, incentives are one item to which we must pay special attention. Thank you very much. end

DR. HRABOWSKI: Next is William Velez, Professor of mathematics, University of Arizona.

DR. VELEZ: Good afternoon. I would like to talk about the role that faculty should be playing in encouraging our children to pursue scientific careers.

I am going to make my comments based on my experience as a mathematician at a research university.

I have been truly fortunate to be part of this community. The mathematics that have been developed over the last 20, 30, 40 years have been phenomenal, and we have made fundamental contributions to science. I am proud to be part of this community.

About these mathematicians who are hard working and deep in thought, I would like to ask you the following question: Do you think these researchers should take time out from their busy schedules of research to actually mentor students? Yes.

When I received the Presidential Award for Mentoring, my department head thought this would be a wonderful excuse to address the faculty on the importance of mentoring, to show them some of the things that I had done in working with minority students. So, we organized a colloquium. We invited our 65 faculty members. Two people showed up.

Do you think that our busy faculty should really take time out from all the things they have to do to mentor our students?

It is not like we are doing so well. As I go around the country, I think it is embarrassing that I have more minority advisees than many departments have total math majors. We graduate more minority bachelor's degrees in mathematics than many departments graduate bachelor's degrees in mathematics.

I think we are in a crisis and we are having some problems, so we are here talking about mentoring and the importance of mentoring. I think that before we design mentoring workshops and programs and brochures and conferences, perhaps we should think a little bit about the culture of being a researcher at a university.

That is what I want to do first of all, and please forgive me for simply talking about myself. I want to emphasize the nature of this culture.

During my second or third year in graduate school, I had a

Density of States, Charge Transfer, and Optical Properties of Magnesium Diboride

D. Bagayoko and G. L. Zhao

Department of Physics, Southern University and A & M College
Baton Rouge, Louisiana 70813 USA

Abstract.

We performed ab-initio, local density functional calculations of the electronic structure, charge transfer, and optical properties of MgB_2, using the LCAO formalism. The Fermi level of MgB_2 cuts through relatively narrow electron bands which have a dominant contribution from B(2p) states. There is a substantial charge transfer from magnesium to boron atoms. We found the ionic formula for this material to be $Mg^{1.68+}B_2^{0.84-}$. A clearly metallic distribution of the electronic charge density in the plane of boron atoms is interwoven with a visibly covalent one in the direction perpendicular to this plane. The calculated optical conductivities from the direct inter-band transitions exhibit a strong anisotropy between $\sigma_{xx}(\omega)$ or $\sigma_{yy}(\omega)$ and $\sigma_{zz}(\omega)$. Due to our application of the BZW procedure, major peaks in the density of states above the Fermi level are at markedly higher energies (1 - 1.5 eV) than the results of previously reported ones. A similar pattern is followed by our findings for optical conductivities.

1. Introduction

The recent discovery of superconductivity in magnesium diboride (MgB_2)[1] with $T_c = 39K$ has attracted much attention around the world.[2, 3, 4, 5, 6] Although hexagonal MgB_2 was identified in the 1950's, its physical properties are not well studied. In 1979, Armstrong and Perkins reported a calculation of the electronic band structure of MgB_2 using an empirical method.[7] Their calculated electron bands of MgB_2 are substantially different from recent ab-initio, density functional calculations that are presented in several electronic-preprints[8, 9, 10] and this work. In this report, we present the calculated electronic band structure, the total density of states and the partial contribution from the s and p states of Mg and B, the calculated charge transfer, and the optical properties of MgB_2.

In the next section, we summarize the computational details. The calculated results are presented in Section III. They are followed by a short conclusion in Section IV.

2. Method

MgB_2 crystallizes in the hexagonal AlB_2-type structure of space group D^1_{6h}. The experimentally measured lattice constants a and c are 3.084 $\mathring{A}$ and 3.522 $\mathring{A}$, respectively.[1, 11] The hexagonal MgB_2 has a relatively simple structure. There are three atoms per unit cell. The atomic positions are: 1 magnesium atom in 1(a) (0, 0, 0), and 2 boron atoms in 2(b) (1/3, 2/3, 1/2) and (2/3, 1/3, 1/2), of the space group D^1_{6h}. There are alternating layers of Mg atoms and graphite like honeycomb layers of B atoms. The B-B bond length is 1.78 $\mathring{A}$, whereas the shortest Mg-B distance is 2.50 $\mathring{A}$.

Our ab-initio calculations utilized the linear combination of atomic orbital (LCAO) method. The self-consistent LCAO calculations included all electrons and full potentials, without shape approximations. Details of the general computational method are available in previous publications.[12, 13, 14, 15, 16] We employed the Ceperley-Alder type[17] of the local density functional potential as parameterized by Vosko, Wilk, and Nusair[18] to describe the many body exchange-correlation interactions of the electron system.

We began the calculation with self-consistent, ab-initio computations for the neutral Mg and B atoms. The radial parts of the atomic wave functions were expanded in terms of Gaussian functions. A set of even tempered Gaussian exponents was employed with a minimum of 0.12 and a maximum of 0.15×10^6, in atomic unit.

We then performed self-consistent calculations for the electronic structure of MgB_2 and obtained an estimate of the charge transfer. These preliminary results suggested that Mg and B in MgB_2 will be close to Mg^{2+} and B^{1-}, respectively, as opposed to neutral species. We subsequently performed self-consistent calculations for free Mg^{2+} and B^{1-} ions to obtain the atomic functions that served as the input for the solid state calculations.

Our solid state calculations employed the Bagayoko, Zhao, and Williams (BZW) method that has been extensively described in our previously publications.[14, 15, 16] Hence, we performed several self-consistent calculations with increasing sizes of the basis set, starting with the minimal basis set. This minimal basis set is just large enough to account for all the electrons in the atomic or ionic species in the system (i. e., Mg^{2+}, B^{1-}). The final results reported here are from the calculation with the optimal basis set, i. e., the smallest basis set for which the occupied energy bands converge vis-a-vis the size of the basis set.[14, 15, 16] Specifically, calculations with basis sets larger than the optimal basis lead to the same occupied bands (in shape, branching, and numerical values) as those obtained with the optimal basis set.

In the self-consistent calculations of the electronic structure of MgB_2, we took Mg(1s) and B(1s) as the core states. Other states such as Mg(2s3s 2p3p) and B(2s3s 2p) are included as valence states in the self-consistent calculations. Here, $Mg(3p^0)$ and $B(3s^0)$

are empty shells in the free atoms (or ions) and are used to augment the basis set to account for charge redistributions in the solid environment. We used 80 k-points with proper weights in the irreducible Brillouin zone in the self-consistent calculations. The computational error for the valence charge was about 0.003 for 16 electrons. The computation for the exchange-correlation potentials was done in real space using a mesh of points around each atom. The numbers of mesh points per atomic site varied from 7028 to 7088, depending on the local structure of the atom. The self-consistent potentials converged to a difference around 10^{-5}.

From the resulting electronic energy levels and wavefunctions, we calculated the optical excitations of direct interband transitions and their contributions to the optical conductivity $\sigma_{\mu\mu}(\omega)$, using the Kubo-Greenwood formula.[19]

$$\begin{aligned}\sigma_{\mu\mu}(\omega) = \frac{2\pi e^2}{m^2\omega\Omega} \sum_{\vec{k}} \sum_{nl} &|< \Psi_{\vec{k}n}(\vec{r})|P_\mu|\Psi_{\vec{k}l}(\vec{r}) >|^2 \\ &f_{\vec{k}l}[1 - f_{\vec{k}n}]\delta(\epsilon_{\vec{k}n} - \epsilon_{\vec{k}l} - \hbar\omega) \qquad (1)\end{aligned}$$

where $\hbar\omega$ is the photon energy; Ω is the volume of the unit cell; $P_\mu = -i\hbar\frac{\partial}{\partial x_\mu}$; $\epsilon_{\vec{k}n}$ is the eigen-energy associated with the eigen-state $|\Psi_{\vec{k}n} >$ at $\vec{k}$-point for band index n.

3. Results

We have calculated the electronic properties of MgB_2 using the newly introduced procedure.[14, 15, 16] Succinctly stated, the implementation of the new calculation procedure first consisted of carrying out completely self-consistent calculations using a minimal LCAO basis set. Namely, the initial charge density for MgB_2 was calculated using the atomic orbitals of Mg(1s2s3s 2p) and B(1s2s 2p).

We then repeated the self-consistent calculation using the above basis set as augmented by the orbitals describing the lowest excited state of Mg. Hence, Mg($3p^0$) orbitals were added to the basis set. We then plotted the energy bands obtained from these two distinct self-consistent calculations. In Fig. 1, the solid and dashed lines represent the calculated results from the first and second calculations, respectively. The Fermi level is set at 0.0 eV. The notations of the high symmetry points in Fig. 1 follows Koster's discussion of space groups.[20] Fig. 1 shows that the occupied bands from the two calculations differ slightly near the H and K points.

The next step was to repeat our procedure, for a third time, with a new basis set that includes B($3s^0$) orbital. The results of this third calculation (dashed lines) and of the second calculation (solid lines) are shown in Fig. 2. The calculated occupied bands as well as the unoccupied bands in Fig. 2 converge to a difference at the order of 1 mRy, that is in the range of computational errors that are due to other factors, including rounding errors and possible limitations of LDA.

Hence, as noted above, the larger basis set, for the third self-consistent calculation, is preferred to that of the minimal basis set calculation. This preference is based on physical considerations, i.e., actual, physical interactions are responsible for the difference between the two sets of bands. Completeness requirements, partly to describe the redistribution of the electronic cloud in the solid environment, dictate this preference.

Furthermore, we added B($3p^0$) orbitals to the basis set of the third calculation. The results of this fourth calculation (dashed lines) and of the third calculation (solid lines) are shown in Fig. 3. Again, the calculated occupied bands and the unoccupied bands in Fig. 3 are fully converged.

However, without the method discussed by Bagayoko, Zhao, and Williams,[14, 15, 16] the test calculations of including more orbitals will continue indefinitely. We presented in Fig. 4 the results of the fourth calculation (solid lines) and the fifth calculation (dashed lines) for which Mg($4s^0$) orbital is added. In contrast to the unchanged nature of the occupied states, some of the low unoccupied states near the Γ and H symmetry points are shifted downward by approximately 1 to 1.6 eV. In light of the discussions presented in our previous publications, the drastic changes in the unoccupied states, in going from calculation IV to V, are believed to be the consequences of the Rayleigh theorem as discused in related mathematical books,[21, 22] since the charge density, potential, and Hamiltonian do not change. While no other graphs are shown here, we continued to add orbitals of higher and higher excited states to the basis set for further calculations. As expected, these calculations did not lead to changes in the occupied states, charge density, and Hamiltonian. They led, expectedly, to drastic changes in unoccupied bands. Consequently, these changes led to a difference in the calculated optical properties, as discussed later. We summarize the atomic orbitals used in Calculation I to VI in Table 1.

Therefore, the electronic band structure of MgB_2, obtained with the optimum basis set of calculation III, is shown as the solid lines of Fig. 3. Our calculated band structure agrees well with other recent ab-initio calculations,[8, 9, 10] but is substantially different from the results reported by Armstrong and Perkins.[7] Our calculated band width for the occupied valence states is 12.3 eV. Armstrong and Perkins reported the band width of the occupied states to be about 28 eV.[7] The electronic energy bands of MgB_2, the solid lines of Fig. 3, show that the Fermi level of MgB_2 cuts through the relatively narrow electron bands which have a dominant contribution of B(2p) states. This shows that boron layers are in a metallic state, with the dominant contribution to the electron-phonon coupling that is reported to be responsible for the superconductivity of MgB_2.[4]

The metallic behavior of boron layers can also be seen from the calculated total and partial density of states (DOS) in Fig. 6. It shows that the occupied valence electron states below the Fermi level (at 0 eV) are mainly attributed to B(2s) and (2p) states. Mg (3s) and (3p) states only contribute about 4% to the total occupied states as shown in Fig. 6, whereas the 2s and 2p states of two B atoms in a unit cell give a contribution up to about 96%. As we discussed in previous publications,[23, 24] the variation of the density of states around the Fermi level, within the range of phonon energy, can have a noticeable effect on the total electron-phonon coupling matrix elements. Fig. 6 shows a noticeable variation of the density of states around E_F. Such effect may lead to an exponent of the boron isotopic effect on T_c, α_B, that is different from 1/2. The experimentally observed boron isotope exponent α_B is about 0.26.[4]

While our density of states are the same as the calculated ones recently reported,[8] for the occupied states, they are markedly different for the unoccupied states. This difference stems from our application of the BZW method as explained elsewhere.[14, 15, 16] In particular, the stiff increase of the density of unoccupied states around 5 eV, as reported by Kortus et al,[8] does not occur in our results until one reaches 6.5 eV. Naturally, this difference will carry over to the description of the contributions of inter-band transitions to the optical conductivity. This result partly modifies our previous suggestion that the BZW[15] procedure may not be needed for materials that are known to be metallic. While this observation holds for occupied states and the unoccupied ones very close to the Fermi level, it does not for relatively high conduction bands. Consequently, the method is still needed for metals as long as excited state energies and related quantities (DOS, optical conductivity, etc) are of interest.

Using the calculated electron wave functions and the LCAO method, we calculated the effective charges and charge transfer in MgB_2. The calculated charge transfers indicate that each Mg atom loses about 1.68 electrons that are gained by two B atoms. The ionic formula for this material can be written as $Mg^{1.68+}B_2^{0.84-}$. The computational error for the charge transfer was estimated at about ±0.2 electrons.

Figs. 7 and 8 show the contour plots of the electron distribution in real space on a boron plane and on a (010) plane that contains Mg and B atoms. The unit of the labeled charge density values is 10^{-2} electrons/a_0^3, where $a_0 = 0.529177$ Å. The high charge density region around the nuclear sites has been cut off at a value of 0.15 electrons/a_0^3, leaving hollow spheres to represent the atomic cores in the figures. The distribution of electrons is strikingly anisotropic. The usual contour map in Figs. 7, in the boron plane, indicates a delocalization of electrons along the ring of the honeycomb. This map denotes the metallic character of the boron plane. In contrast, clearly covalent bonds, between pairs of boron species, characterize the charge distribution in the c direction that is perpendicular to the boron plane (Fig. 8).

We present the calculated optical conductivity from the direct band transitions for MgB_2 in Fig. 9. In the calculation of the optical conductivity using Eq. (1), we employed a much denser mesh of 929 k-points in the irreducible Brillouin. The intraband transitions, which account for the optical conductivity of low excitation energies of less than about 1 eV, can be described by the Drude term. They are not included in this calculation. The solid line in Fig. 9 shows the optical conductivity $\sigma_{||}(\omega) = \sigma_{zz}(\omega)$, for light polarization along the c-direction. The dashed line represents the optical conductivity $\sigma_{\perp}(\omega) = (\sigma_{xx}(\omega) + \sigma_{yy}(\omega))/2$, for polarization perpendicular to the c-direction. The optical conductivities in Fig. 9 show a strong anisotropy. $\sigma_{\perp}(\omega)$ is substantially stronger than $\sigma_{||}(\omega)$ in the excitation energy range of 0.9 eV to 3 eV. This anisotropy of the optical conductivity is attributed to the characteristic of the occupied electronic states near the Fermi level, with a strong contribution from B (p_x, p_y) components of the σ-bands. The sharp structure of $\sigma_{\perp}(\omega)$ near 0.93 eV is attributed to large matrix elements of optical transitions of energy bands around E_F for a very narrow region in k-space near the half way from the symmetry points A to L. This sharp structure can be smeared in experimental measurements, due to thermal effect and other defects in the sample, as we observed when using a broadening method to calculate it. Although, the strong anisotropy of the optical conductivity and other futures are similar to the calculated results of $\epsilon_2(\omega)$ reported by Ravindran, et al,[25] the peak positions in their calculated $\epsilon_2(\omega)$ are shiftied down substantially in comparison with our calculated $\sigma_{\perp}(\omega)$. This difference may partly due to the lowing of their calculated conduction bands as we discussed earlier.

4. Conclusion

We have calculated the electronic structure and the optical properties of MgB_2. We performed the ab-initio, local density functional calculations in the LCAO formalism. The electronic states near the Fermi level are dominated by the B (p_x, p_y) states of the σ-bands. The boron layers are in a metallic state while covalence characterizes the distribution of electrons (around boron) in the c-direction. They give the dominant contribution to the electron-phonon coupling. There is a substantial charge transfer from magnesium to boron atoms. The ionic formula for this material may be written as $Mg^{1.68+}B_2^{0.84-}$. There is a marked difference between $\sigma_{xx}(\omega)$ or $\sigma_{yy}(\omega)$ and $\sigma_{zz}(\omega)$. Our results for the charge transfer and the locations of peaks in the density of states and optical conductivities await experimental findings for comparison.

Acknowledgments

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nority Participation.

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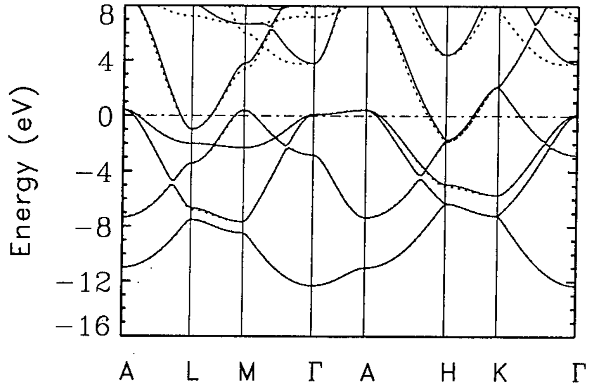

Figure 1. The comparison of the results of Calculation I and II. The solid lines represent the bands of MgB_2 from the minimum basis set calculation (Calculation I); the dashed lines show the bands from Calculation II.

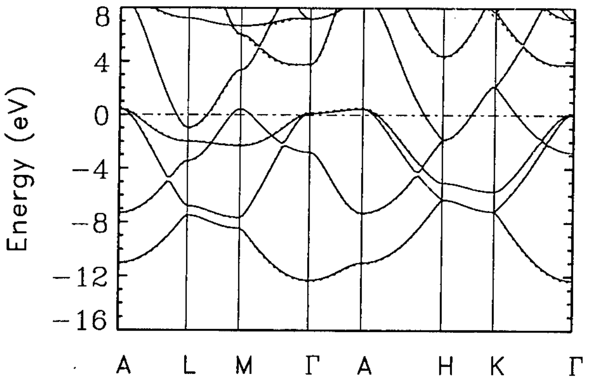

Figure 2. The comparison of the results of Calculation II and III. The solid lines represent the results from Calculation II; the dashed lines show the electron energy bands of MgB_2 from Calculation III.

Table 1. The atomic orbitals used in our self-consistent calculations of the electronic structure of MgB_2 applying the LCAO method.

	Basis Set
Calculation I	Mg(1s2s3s 2p),B(1s2s 2p)
Calculation II	Basis Set I + Mg($3p^0$)
Calculation III	Basis Set II + B($3s^0$)
Calculation IV	Basis Set III + B($3p^0$)
Calculation V	Basis Set IV + Mg($4s^0$)
Calculation VI	Basis Set V + Mg($3d^0$)

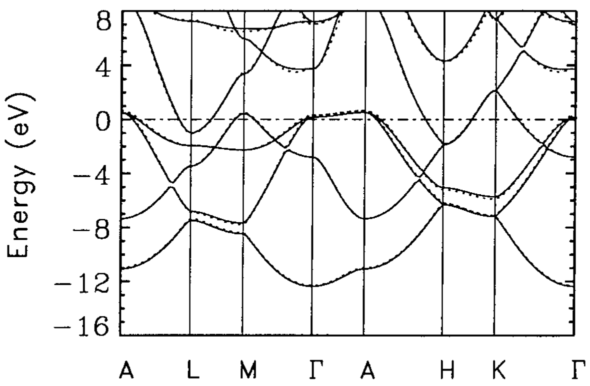

Figure 3. The comparison of the results of Calculation III and IV. The solid lines represent the electron energy bands of MgB_2 from Calculation III; the dashed lines show the bands from Calculation IV.

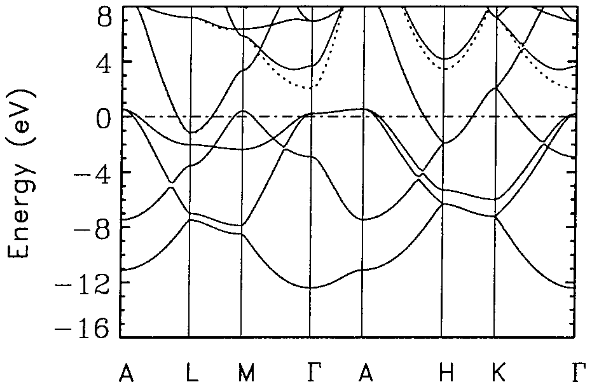

Figure 4. The comparison of the results of Calculation IV and V. The solid lines represent the results from Calculation IV; the dashed lines show the bands from Calculation V.

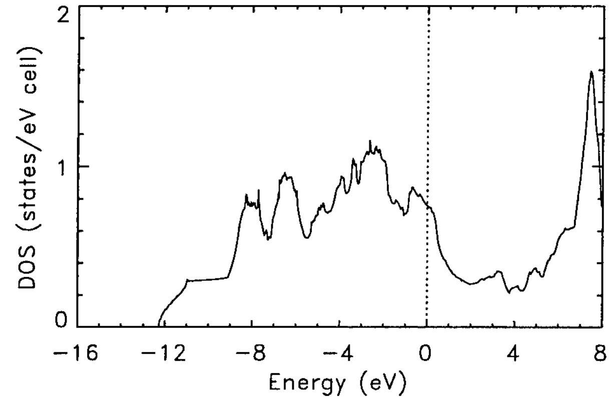

Figure 5. The calculated density of states of MgB_2.

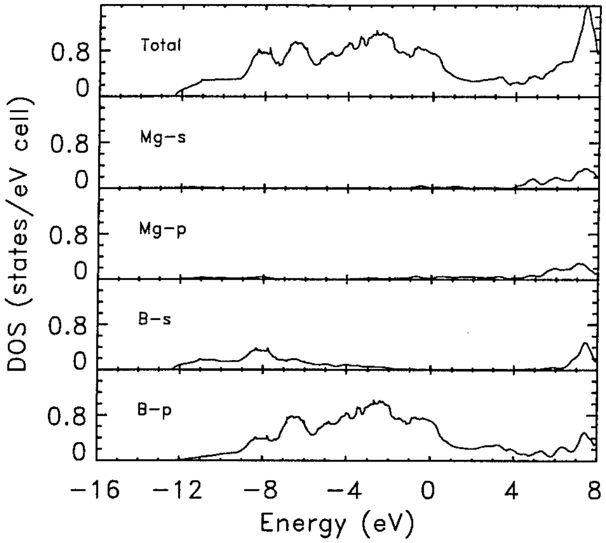

Figure 6. The calculated partial density of states of MgB_2.

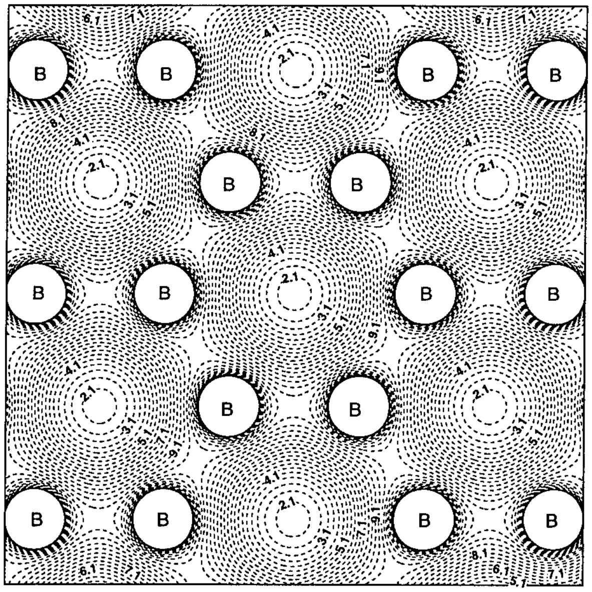

Figure 7. The contour plots of the calculated electron distribution in real space on a boron plane.

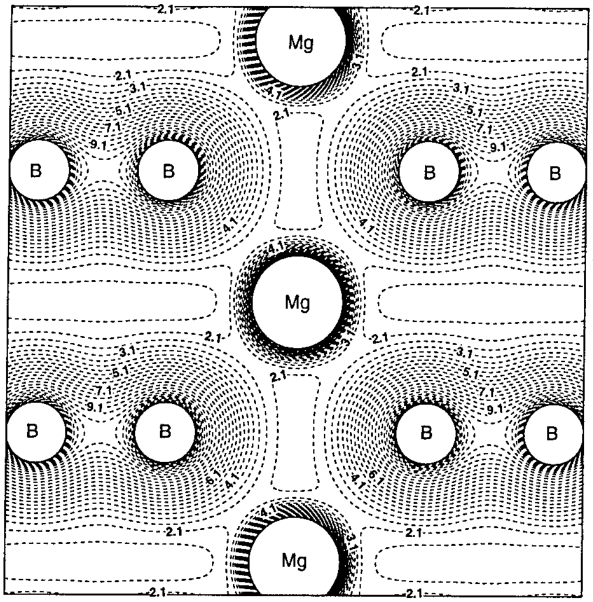

Figure 8. The contour plots of the electron distribution in real space on a (010) plane containing Mg and B atoms.

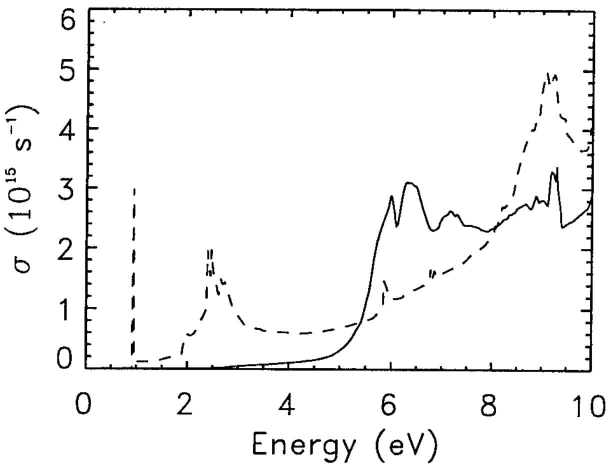

Figure 9. The calculated optical conductivity of MgB_2. The solid line presents $\sigma_{zz}(\omega)$; the dashed line presents $(\sigma_{xx}(\omega) + \sigma_{yy}(\omega))/2$.

Paper for the Tennessee State University (TSU)-AOL Time Warner HBCU Digital Divide Conference at Jackson State University (JSU), Jackson, Mississippi, Fall 2001.

Reverse Digital Divide

A Case Study at the Timbuktu Academy and a Model for the Future

Diola Bagayoko, Ph.D.
(Bagayoko@aol.com)
Southern University System Distinguished Professor of Physics
Director, the Timbuktu Academy and LS-LAMP Campus Coordination
Southern University and A&M College, Baton Rouge, Louisiana

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Introduction

In light of recent interests in the "digital divide," a differential access to and utilization of digital technologies by some socio-economic and ethnic groups as compared to others, a description of the situation in the Department of Physics at Southern University and A&M College seems to be needed. Digital technologies, in what follows, include the computer, computer networks, the Internet, the electronic mail, and others. This contribution begins with recalling the development and adoption of a written plan for "integrating the computer into the physics curriculum." This action was partly prompted by the fact that all our physics majors who conducted summer research at sites around the country had to deal with the computer in their work in 1988! The congruency of their education and training with the realities (a) in graduate schools and (b) in the work place and research laboratories simply demanded this plan. Given that the speaker was the chairman of the Departmental Curriculum Committee that developed the plan, it behooved him to lead our vigorous efforts to acquire needed resources for its effective implementation. The following is the story of how we bridged the digital divide and placed ourselves at the upper end. Our *continuing progress*, for our mostly African American undergraduate Scholars of the Timbuktu Academy (http://www.phys.subr.edu/timbuktu.htm), is tantamount to a "reverse digital divide," i.e., one that is such that we have the upper end. The speaker's personal involvement in the projects identified below facilitated the telling of this story that contains lessons that will remain valid for the foreseeable future.

Closing and Reversing the Digital Divide: Timbuktu Academy, Department of Physics

In 1988, we first acquired five (5) personal computers pursuant to the implementation of a project funded by the Minority Science Improvement Program (MSIP) of the US Department of Education. Naturally, this number was inadequate for us to begin addressing the digital divide. A written proposal was then submitted to the University--for Title III funding (US Department of Education)--to acquire many more computers. As a result, the first instructional computer laboratory was built in 1989, with over 20 computers that were fully networked. We also acquired state-of-the-art equipment for physics laboratory experiments. In 1989-1990, the funding of a second proposal, submitted to a competitive funding program in the State (Louisiana Education Quality Support Fund-LEQSF), provided personal computers for all faculty and staff members. In 1992-93, the funding of another proposal to LEQSF upgraded existing resources and networked the departmental computers to link the resulting network to SUBR's Internet node. Our students are mostly African Americans, a group reported to have much less access to some digital technologies (Computer, Internet, and E-mail) as compared to others. Mr. Carl Grant led the group of students who built our network and our web site, once contractors run the appropriate cabling to all rooms in 1993. (Oh, the contractors were going to bring network connections even to the bathrooms in our building (James Hall), had we not discovered the mistake in time!)

We cannot help it but note that the last LEQSF project above was developed at risks to its director in light of a 1992 written administrative directive from the office of the chancellor forbidding the request or acquisition of computers and related items through sponsored projects! This directive was duly signed by a vice chancellor, in the name of the Chancellor; it was implemented for at least two years. We do not recall it being rescinded, even though it was ignored by others after 1995. Oh, SUBR faculty members built the above referenced node to the Internet with funding from NSF in 1991-92. They had previously built the campus backbone network with LEQSF funding in 1987-89. *Further, that project led to the provision of networking underground conduits throughout the campus in 1988-89, during installation of a new central utility system!* In 1996-97, a high-performance computing laboratory, for research, was established in Physics. It included a SiliconGraphics Origin2000, seven O2 workstations, and several compilers (FORTRAN, C, C++), application programs, and graphics packages (i.e. IDL). In 1999-00, with the funding of yet another project by LEQSF, we built a parallel machine with 32 personal computer processors. Of course, the SGI systems and the Parallel PC Cluster are both linked to the departmental network.

A Next Generation Internet and videoconferencing, caching, and broadcasting (NGI-VCB) facility was established in 1999-2000, in a building close to the Physics Department. The first thesis defense using this facility occurred with the graduate student and her research advisor were at a conference in Hawaii while the rest of the thesis defense committee was at SUBR, in the NGI-VCB facility. This facility has been utilized several times now for conferences, workshops, etc., With the assistance of web-casting facility at North Carolina A&T State

University (Broad band, Internet II facility), our NGI-VCB facility has enabled videoconferencing sessions accompanied with web-casting. For the last two years, the NGI-VCB facility has hosted the international videoconferencing sessions with students from South Africa and several locations in the US, on the occasion of the Day of the African Child. Pre-college summer scholars at SUBR, including some from the Timbuktu Academy described below, partook in these interactive exchange and learning activities.

Beginning in 1997, online subscriptions to pioneer journals and other electronic resources have been in extensive use by research faculty members in the department. From 1993 to present, the integration of the web into the instructional and research activities of the Timbuktu Academy continues to grow. In fact, students other than the Academy scholars have been guided to useful and extensive web resources for studying (the World Lecture Hall at http://www.utexas.edu/world/lecture/), research, mentoring, and other enrichment activities. While some may have images of computers and their mundane use when speaking of the digital divide, the crux of a matter becomes apparent when one conducts a thorough, scientific literature search the old fashion way and repeats that search using e-resources (online journals, magazines, and books and other electronic recourses like the one at Los Alamos National Laboratory http://xxx.lanl.gov/). This exercise is one of the best to appreciate the criticality of having access to and of using competitive electronic or digital resources. The New Journal of Physics (http://www.njp.org/), launched in England 1999-2000, is available only in electronic form! This new and leading journal provides yet another urgent call for closing the digital divide.

From 1988 to present, the integration of the computer into our curriculum and activities has grown significantly. These activities are in instruction (beginning with laboratory reports in 1988-89), research, systemic mentoring, learning, and service activities of the department. We underscore the fact that faculty and staff members and students continue to play critical roles in maintaining the congruency referenced above and that demands *continual progress.* After practically closing the digital divide in 1988-89, with MSIP and Title III funding from the US Department of Education, we established the Timbuktu Academy in 1990. Yes, we were then in position, with computers and other up-to-date laboratory equipment, to promise and to deliver a competitive training to our students--as per the standards in graduate schools and in the job market. It was and still is funded by the National Science Foundation (NSF), the Department of the Navy, Office of Naval Research (ONR), and NASA.

The Timbuktu Academy helped to make the physics enrollment jump from approximately 20 or less in 1990, the year the Academy was established, to 60 in 1996-97. It may take a book to delve into the paradigm, programs, activities and results of the Timbuktu Academy. We urge the reader or listener, for the sake of her or his children or students, to browse its informative web site (http://www.phys.subr.edu/timbuktu.htm). In 1994, the Timbuktu Academy integrated e-mail communication into its 10-step and nationally emulated systemic mentoring model.-- for its college and pre-college students alike. The US Presidential Award for Excellence in Science, Mathematics, and Engineering Mentoring to its director, in 1996, partly supports the Academy's claims to fame. So do the 5, 10, and 10 National Merit and National Achievement Scholars it helped to produce in 1998-99, 1999-00 and in 2000-01, respectively. The 50-100 undergraduate scholars and the 150-200 elementary to high school summer scholars of the Academy are immersed in the utilization of digital technologies-by design.

In 1999-2000, Hewlett Packard funded the Timbuktu Academy in the form of a donation of brand new equipment valued over $35,000. In particular, the more than $10,000 upscale, professional, and color laser printer and the two heavy duty, high speed laser printers have served to draw students from many other units to the Department of Physics. The ONR grant provided extensive funding for supplies, including paper. More reports, theses, etc. have been printed using these unusually reliable Hewlett Packard products than we can list. In these days of flashy Power Point presentations, the above color laser printer may not seem necessary until you ask one of the tens of Timbuktu Academy undergraduate scholars who made poster presentations around the country. While the speaker was personally involved in the development of the proposal to HP, Dr. Rahman Tashakkori, was the instigator and the main author of it.

Dr. Tashakkori also led our efforts to take our "digital advantage (DA)" to new heights by developing one programming (C, C++, etc.) and two computational physics courses that were up to the standards anywhere. From late 1990s to present, the undergraduate physics scholars of the Timbuktu Academy continue to extol the virtues of these new courses--as per their utilization of what they learned at their summer research sites around the country. 40 to 50 physics, engineering, and chemistry scholars of the Academy conduct summer research around the country. [Well, one went to Europe this summer, to the Centre Européen de Recherche Nucléaire (CERN).]

A unique role of the faculty consisted of securing the resources and of creating the climate where computer utilization was inescapable for students. This role also ensures the continued upgrade of resources and their utilization. For the acquisition of the resources, the department chairman (Dr. C. H. Yang) cheered faculty members who were developing proposals. His supportive and encouraging leadership was practically an inspiration and a source of energy for the faculty members. Even though he voluntarily left the chairmanship in early 1999, the momentum has not yet died out, despite a clear decrease. From 1990 to present, external funding to a few dedicated faculty members made possible the acquisition of any software product that was needed--from operating systems, compilers, Oracle's database, instructional programs, and web-development tools to mundane applications programs (word processor, spreadsheet, and graphics packages). A faculty member, staff member, or student names a software product that is needed and we acquire it--with grant funding. Additionally, and in light of the role of our students in building the physical network, our students have had total access to all the noted resources. *(Yes, the issue is not always what is available, but rather the nature, scope, and depth of the access to and use of the resources by a constituent.)* Despite our relatively late start in 1988, the net result of the process has been that our faculty, staff, and students have had more access to state-of-the-art digital resources than their counterparts in most academic departments in this country. There lies the reason of our reference to a *"reverse digital divide."* A point that may be lost easily consists of the fact that the work of our students was made possible by the funding of the Timbuktu Academy. Indeed, these scholars were fully supported to the point that their full time job was "studying and doing research." Not only this funding made it possible for some of them to build, operate, and maintain our network and web site, but also it allowed all other scholars to devote adequate time to their studies and research.

Closing the Digital Divide on Campus: a replication of the Academy model

In 1997, the Faculty Senate adopted systemic mentoring as it top agenda item, after examining the hypocental impact of this significant other in promoting competitive learning, and in coupling research and education. The president of the Senate at the time, the speaker, then developed another Title III project entitled "New Models in Teaching, Mentoring, and Learning

(NTML)." The aim of the project was to enhance the overall computer network infrastructure of the campus and to integrate same into high technology-imbued approaches to teaching, mentoring, and learning. The project established the Campus Network Management office. For the first time there was a systematic, coordinated, and vigorous approach to completing, operating, maintaining, and upgrading the entire network infrastructure of SUBR. Mr. Randy Powe, for whom Mr. Carl Grant is currently working, was and still is the Campus Network Manager. NTML employed two full time technicians and a secretary to support the operation of the Campus Network Management (CNM) Office. NTML has provided extensive and regularly scheduled training sessions for faculty members and students in the area of computer technology. In short, NTML is an attempt to replicate, at the institutional level, the rosy situation in physics relative to digital technology infrastructure and the systemic mentoring of the Timbuktu Academy.

Developments in the State led to the establishment of a student technology fee program on public campuses. A law allowed students to vote and to assess themselves up to approximately $60 per semester for instructional, learning, and related technology infrastructure enhancement purposes. In 1998, this led to the establishment of the Technology and Network Services (TNS) office, led by Mr. Huey Lawson. The establishment of this office, with the merging of CNM into it, was one of the objectives of NTML as far as institutionalization was concerned. With the teamwork of NTML (i.e., CNM) and TNS, SUBR has made significant progress in the last three years.

While the details of this progress may be too long to delve into, a few salient points follow. All buildings, including dormitories, are currently networked internally and linked to the Internet. Five (5), new, multipurpose computer laboratory (with 20 to 45 personal computers) have been established. They added to the 22 laboratories that were built in individual units mostly by their respective faculty members. The 45 PC laboratory in T. T. Allain is open 24 hours a day, seven days a week. The other laboratories have very extended hours; they go for 24 hours should the demand exist. The acquisition of the over 700 courses of Netg, of Blackboard, a web based instructional and mentoring delivery tool, and of numerous site licenses is helping to accelerate digital technology utilization across the campus. This is particular so in light of the regularly scheduled training sessions for students, faculty, and staff. TNS also brought cable TV to the dormitories. It therefore appears that even though SUBR as a whole may not be enjoying the digital advantage of the Timbuktu Academy, it is closing whatever digital divide may currently exists; it is doing so at an increasing rate. We should note that the Timbuktu Academy and the Department of Physics are also taking advantage of the resources of TNS to maintain their digital advantage. So is the SUBR Library that earned a commendation in 2000, during the reaffirmation of the accreditation of SUBR by the Commission on Colleges.

Lessons for the Future: They Apply to most Organizations and Groups

The lessons from this case study can be summarized as follows. *Digital divides, like academic achievement gaps (e-mail Bagayoko for the paper, if interested) are made or created.* And, like the achievement gaps, they can be avoided or closed, provided there is a mechanism to make very many stakeholders responsible for their specific actions or lack thereof. Indeed, the "distributed responsibilities and shared credits (DRSC)" principle of the Timbuktu Academy simply states that parents, students, faculty, staff, school or university administrators at the various levels, policy makers at local and national levels, and funding organizations have their respective roles that can be clearly delineated (distributed). The credits for the accomplishments, however, can generally not be segmented; they are shared. *As explained in the paradigm of the Timbuktu Academy, it is therefore paramount that no individual or group is allowed to blame all ills on others in order to appear cheaply or craftily as the one and only that cares.* Further, when an individual or group does his part verifiably well, then it earns a license to make other account. One can do so by professionally and thoroughly documenting deeds and misdeeds, utilizing normalized and longitudinal data and information in the context of appropriate comparisons with peer units or institutions across the country.

After all, the global market is one, not many; hence, failure to be competitive as per the prevailing standards in that market, irrespective of the size, location, or other attributes of a university, is tantamount to a tragedy. An organizational, group, or institutional **head** who has no *clearly written expectations for faculty, staff, and others relative to digital and other divides*, has no *objective, reliable, and comprehensive evaluation system* that is *honestly and regularly administered*, or has no *provisions to key (or tie) compensations, promotions, raises, etc., to performance*, is at best a misleader; he or she may be so unwittingly; that does not change the devastating impact on the constituents who are falling behind their peers. So say the realities in graduate schools and in the global market, not this speaker. Approximately 60% of the digital and other divides at educational institutions can be traced to what management did or did not do.

On the other hand, the case study above indicated that **faculty members** have no rights or privileges to seat and to wait for funding or digital equipment to fall from the sky; they will not. Many, as illustrated above, have taken their responsibility, even in the face of opposition by the very ones who are supposed to be supporting them (see the directive above). The problem, however, is that in some organizations or units therein, competent and dedicated individuals, after observing others get rewards, promotions, raises, and prizes for not doing even their duties, either leave or go into professional hibernation or retrogression. Competent and productive faculty members should form a Union of Concerned Faculty (UCF) to put their analytic skills to work in conducting annual and thorough review of the state of their units, universities, etc., as compared to their peers and in light of the prevailing trends in graduate schools and the global job market. Such an annual document may actually help immensely in letting some **institutional management or trustees boards** face the realities. Due to a lack of thorough and longitudinal data that are normalized and due to a lack of consideration of unavoidable contexts, many boards think that their institutional are doing well at the very time they are sinking further. Of course, issues of independence, conflict of interests, basic probity, etc., may be other factors influencing the actions of inactions of a board. Nevertheless, *there is no substitute for pertinent accurate and complete data, information, and comparisons (with peers and the trends) in making decisions.* In fact, most of these boards have enough funds to finance such studies on a yearly basis. If concerned faculty members do not have the time or means, they could at least request that the board finance this kind of responsible, annual review.

As for **students**, we noted above that they were (a) the motivation for closing the digital divide in Physics at SUBR and that (b) the undergraduate scholars of the Academy have been the brains behind our digital advantage. Further, please note the impact of the student technology fees at SUBR; students voluntarily voted to assess themselves those fees. It should be added that besides the technicians hired by NTML, most of the many people running the computer laboratories of TNS are undergraduate and graduate students. In fact, it was our plan from the onset to have the network and related technology infrastructure serve as lively and relevant learning laboratories! In this sense, TNS is replicating campus wide what occurred in physics.

On the other hand, it seems that some general **students** do not seem to understand or do not seem to deploy the efforts needed to build their knowledge and skills bases as they relate to the use of digital technologies or to basic training and research. Many of them may not understand that they will indubitably regret this behavior, soon or later, thanks to the realities in graduate schools and in the global market. Some alumni are helping many colleges and universities. Some others are unwittingly helping in the maintenance of archaic, irrelevant, anachronistic practices. A case in point is that of pledges by fraternities and sororities. Why are these pledge conditions and practices not focusing on (a) demonstrating scholarship, (b) promoting values and communication skills germane to flourishing in the global market, and (c) *demonstrating prowess in digital technology utilization (beyond CD and videos) to include programming, web site development, and extensive electronic searches on some useful topics?* Marching across campus, going without sleep, and other sensory-motor oddities would have been appropriate if we were still in Sparta (a militaristic city-state in ancient Greece) or on the verge on some wild physical contests. Intellectual and mental prowess and stamina and attendant knowledge and skills are keenly relevant in graduate schools and in the global market! It is expected that the Timbuktu Academy fraternity, if and when the Academy alumni and others establish one, will have admission criteria and pledging practices that *do not move forward to the past.*

Policy makers and funding agencies have critical roles to play in addressing the digital and other divides. This point cannot be underscored enough, even though it is not meant to provide an excuse for other stakeholders to seat and wait on these agencies. Further, policies and funding pictures can both be influenced or changed with cogent proposals, particularly when they are repeatedly updated and submitted. A sporadic shower of dollars is not going to solve the problem, anyway, at least not in the long run. The utter need for *continual updating and improvements*, to keep pace with developments, is one of the reasons a passing deluge of dollars, alone, will not work. Besides, in a perverse way, large funding without the kind of accountability at all levels as intimated above may actually serve to maintain the status quo while providing added resources for the political patronage of some administrators at various levels. In that sense, perhaps purposeful students, whose very future is what is at stake, may need to empower themselves and demand up-to-standard instructional, research, and service infrastructure and services. Sure, there are some leaders who are keenly aware of the trends and who are meaningfully consulting and engaging all their constituents (faculty, students, staff, alumni, friends, private and public concerns, etc.).

Interestingly enough, the above elements of a solution were implicitly addressed by the **Proceedings of the first TSU-AOL-Time Warner HBCU Digital Divide Conference at Tennessee State University (TSU, http://explorers.tsuniv.edu/tsuaol/default.htm).** The table of contents suffices to corroborate this assertion. The continual process repeated throughout this address clearly leads to the strategic planning and implementation called for in the Proceedings. By the time one implements the total accountability noted above, one has to address a host of related steps delineated in the Proceedings. They include metrics for technology infusion and evaluation and incentive systems for instruction, research, and services. If and when every administrator is not held fully accountable, solutions will be thwarted. Both Dr. James Hefner and Dr. Eugene Jones made clear *"the inescapable fact that technology infusion within our institutions is no longer an option; it is an absolute necessity for our survival," let alone our competitiveness.* As Dr. James Hefner stated at the opening of the first conference, *"let us cut the chase and get on with these solutions."*