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14. ABSTRACT
The objective of the multidisciplinary university research initiative (MURI) “Emergent Phenomena at Mott Interfaces” was to establish fundamentally new approaches to predict, understand, and control the wealth of electronic, spin and collective mode excitations associated with Mott metal-insulator transitions at complex oxide interfaces. This report summarizes the main accomplishments over the duration of this MURI.

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The objective of the multidisciplinary university research initiative (MURI) “Emergent Phenomena at Mott Interfaces” was to establish fundamentally new approaches to predict, understand, and control the wealth of electronic, spin and collective mode excitations associated with Mott metal-insulator transitions at complex oxide interfaces. This report summarizes the main accomplishments over the duration of this MURI.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received	Paper
01/07/2011 11.00	Sieu D. Ha, Gulgun H. Aydogdu, Shriram Ramanathan. Metal-insulator transition and electrically driven memristive characteristics of SmNiO3 thin ?lms, Applied Physics Letters, (01 2011): . doi:
01/07/2011 12.00	SungBin Lee, Ru Chen, Leon Balents. Landau Theory of Charge and Spin Ordering in the Nickelates, Physical Review Letters, (01 2011): . doi:
01/18/2013 65.00	Ryan Comes, Man Gu, Mikhail Khokhlov, Hongxue Liu, Jiwei Lu, Stuart A. Wolf. Electron molecular beam epitaxy: Layer-by-layer growth of complex oxides via pulsed electron-beam deposition, Journal of Applied Physics, (01 2013): 23303. doi: 10.1063/1.4774238
01/19/2013 67.00	A. Preston, D. Newby, K. Smith, S. Sallis, L. Piper, S. Kittiwatanakul, J. Laverock, J. Lu, S. Wolf, M. Leandersson, T. Balasubramanian. Photoemission evidence for crossover from Peierls-like to Mott-like transition in highly strained VO_{2}, Physical Review B, (11 2012): 195124. doi: 10.1103/PhysRevB.86.195124
01/19/2013 68.00	Pouya Moetakef, Daniel G. Ouellette, James R. Williams, S. James Allen, Leon Balents, David Goldhaber-Gordon, Susanne Stemmer. Quantum oscillations from a two-dimensional electron gas at a Mott/band insulator interface, Applied Physics Letters, (10 2012): 151604. doi: 10.1063/1.4758989
01/23/2014 97.00	Susanne Stemmer, Andrew J. Millis. Quantum confinement in oxide quantum wells, MRS Bulletin, (12 2013): 1032. doi: 10.1557/mrs.2013.265
02/11/2012 43.00	B. Viswanath, G.H. Aydogdu, S.D. Ha, S. Ramanathan. In situ stress relaxation and diffraction studies across the metal–insulator transition in epitaxial and polycrystalline SmNiO3 thin films, Scripta Materialia, (04 2012): 0. doi: 10.1016/j.scriptamat.2011.12.018
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02/19/2013 73.00	Sang Hyeon Lee, Moonkyung Kim, Sieu D. Ha, Jo-Won Lee, Shriram Ramanathan, Sandip Tiwari. Space charge polarization induced memory in SmNiO3/Si transistors, Applied Physics Letters, (02 2013): 72102. doi:

02/21/2013 75.00 S.-H. Yang, A. X. Gray, A. M. Kaiser, B. S. Mun, B. C. Sell, J. B. Kortright, C. S. Fadley. Making use of x-ray optical effects in photoelectron-, Auger electron-, andx-ray emission spectroscopies: Total reflection, standing-wave excitation,and resonant effects,
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10/12/2010 6.00 Daniel G. Ouellette, SungBin Lee, Junwoo Son, Susanne Stemmer, Leon Balents, Andrew J. Millis, S. James Allen. Optical conductivity of LaNiO3: Coherent transport and correlation driven mass enhancement,
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11/19/2010 7.00 Junwoo Son, James M. LeBeau, S. James Allen, Susanne Stemmer. Conductivity enhancement of ultrathin LaNiO3 films in superlattices,
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11/19/2013 96.00 Clayton A. Jackson, Susanne Stemmer. Interface-induced magnetism in perovskite quantum wells,
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12/02/2010 8.00 Gulgun H. Aydogdu, Dmitry Ruzmetov, Shriram Ramanathan. Metastable oxygen incorporation into thin film NiO by low temperature active oxidation: Influence on hole conduction,
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12/09/2011 40.00 Pouya Moetakef, Tyler A. Cain, Daniel G. Ouellette, Jack Y. Zhang, Dmitri O. Klenov, Anderson Janotti, Chris G. Van de Walle, Siddharth Rajan, S. James Allen, Susanne Stemmer. Electrostatic carrier doping of GdTiO3/SrTiO3 interfaces,
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Physical Review Letters, (12 2011): 0. doi: 10.1103/PhysRevLett.107.256601

TOTAL: **61**

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received Paper

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Received Paper

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Peer-Reviewed Conference Proceeding publications (other than abstracts):

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(d) Manuscripts

Received		Paper
01/14/2013	64.00	G. Conti, A. M. Kaiser, A. X. Gray, S. Nemšák, G. K. Pálsson, J. Son, P. Moetakef, A. Janotti, L. Bjaalie, C.S. Conlon, D. Eiteneer, A.A. Greer, A. Keqi, A. Rattanachata, A.Y. Saw, A. Bostwick, W.C. Stolte, A. Gloskovskii, W. Drube, S. Ueda, M. Kobata, K. Kobayashi, C. G. Van de Walle, S. Stemmer, C. M. Schneider, C. S. Fadley. Band Offsets in Complex-Oxide Thin Films and Heterostructures of SrTiO3/LaNiO3 and SrTiO3/GdTiO3 by Soft and Hard X-ray Photoelectron Spectroscopy, Submitted to J. Appl. Phys. (01 2013)
01/18/2013	66.00	Wing-Ho Ko, Hong-Chen Jiang, Jeffrey G. Rau, Leon Balents. Ordering and criticality in an underscreened Kondo chain, SUBMITTED (01 2013)
01/19/2012	35.00	A. Janotti, D. Steiauf, C. G. Van de Walle. Strain effects on the electronic structure of SrTiO3: Towards high electron mobilities, Submitted to physical review B (01 2012)
01/25/2013	69.00	Sieu D. Ha, R. Jaramillo, D. M. Silevitch, Frank Schoofs, Kian Kerman, John D. Baniecki, Shriram Ramanathan. Hall effect measurements on epitaxial SmNiO3 thin films and implications for antiferromagnetism, SUBMITTED (01 2013)
01/25/2014	98.00	R. Jaramillo, Sieu D. Ha, D. M. Silevitch, Shriram Ramanathan. Origins of bad metal conductivity and the insulator-metal transition in the rare-earth nickelates, Accepted, Nature Physics (12 2014)
01/26/2013	70.00	Sang Hyeon Lee, Moonkyung Kim, Sieu D. Ha, Jo-Won Lee, Shriram Ramanathan, Sandip Tiwari. Space Charge Polarization Induced Memory in SmNiO3/Si transistors, SUBMITTED (01 2013)
02/01/2013	71.00	Jinwoo Hwang, Junwoo Son, Jack Y. Zhang, Anderson Janotti, Chris G. Van De Walle, Susanne Stemmer. Structural origins of the properties of rare earth nickelate superlattices, Submitted (11 2012)
02/15/2014	99.00	Jack Y. Zhang, Clayton A. Jackson, Ru Chen, Santosh Raghavan, Pouya Moetakef, Leon Balents, Susanne Stemmer. Correlation between metal-insulator transitions and structuraldistortions in high-electron-density SrTiO3 quantum wells, Accepted, Physical Review B (01 2014)
02/17/2012	45.00	Sieu D. Ha, Miho Otaki, Rafael Jaramillo, Adrian Podpirka, Shriram Ramanathan. Stable metal-insulator transition in epitaxial SmNiO3 thin films, Submitted (02 2012)
02/21/2013	74.00	R. Jaramillo, Frank Schoofs, Sieu D. Ha, Shriram Ramanathan. High pressure synthesis of SmNiO3 thin films and implications for thermodynamics of the nickelates, SUBMITTED (02 2013)
02/23/2012	49.00	Anderson Janotti, Bharat Jalan, Susanne Stemmer, Chris G. Van de Walle. Effects of doping on the lattice parameter of SrTiO3, Submitted (02 2012)
03/01/2014	01.00	Feng Yan, Frank Schoofs, Jian Shi, Sieu D. Ha, R. Jaramillo, Shriram Ramanathan. Local charge writing in epitaxial SmNiO3 thin films, Journal of Materials Chemistry C (01 2014)

04/23/2013 82.00 Sieu D. Ha, Ulrich Vetter, Jian Shi, Shriram Ramanathan. Electrostatic gating of metallic and insulating phases in SmNiO3 ultrathin films,
SUBMITTED TO Appl. Phys. Lett. (04 2013)

05/17/2011 15.00 Gulgun H. Aydogdu, Sieu D. Ha, B. Viswanath, Shriram Ramanathan. Epitaxy, strain and composition effects on metal-insulator transition characteristics of SmNiO3 thin films,
Journal of Applied Physics (05 2011)

05/17/2012 53.00 Sieu D. Ha, B. Viswanath, Shriram Ramanathan. Electrothermal actuation of metal-insulator transition in SmNiO3 thin film devices above room temperature,
Submitted to J. Appl. Phys. (05 2012)

06/26/2011 17.00 Sieu D. Ha, Gulgun H. Aydogdu, B. Viswanath, Shriram Ramanathan. Electrically-driven metal-insulator transition with tunable threshold voltage in a VO2-SmNiO3 heterostructure on silicon,
(06 2011)

06/26/2011 18.00 A. X. Gray, A. Janotti, J. Son, J. M. LeBeau, S. Ueda, Y. Yamashita, K. Kobayashi, A. M. Kaiser, R. Sutarto, H. Wadati, G. A. Sawatzky, C. G. Van de Walle, S. Stemmer, C. S. Fadley. Insulating State of Ultrathin Epitaxial LaNiO3 Thin Films Detected by Hard X-ray Photoemission,
(06 2011)

06/26/2012 55.00 J. Laverock, A. R. H. Preston, D. Newby, K. E. Smith, S. Sallis, L. F. J. Piper, S. Kittiwatanakul, J. W. Lu, S. A. Wolf, M. Leandersson, T. Balasubramanian. Photoemission evidence for crossover from Peierls-like to Mott-like transition inhighly strained VO2,
SUBMITTED (06 2012)

07/08/2011 19.00 SungBin Lee, Ru Chen, Leon Balents. Metal-insulator transition in a two-band model for the perovskite nickelates,
(07 2011)

07/23/2013 86.00 Man Gu, Stuart A. Wolf, Jiwei Lu. Dimensional-Crossover-Driven Mott Insulators in SrVO3 Ultrathin Films,
SUBMITTED (07 2013)

08/11/2011 20.00 C. G. Van de Walle, A. Janotti, D. Steiauf. Strain effects on the electronic structure of SrTiO3: Towards high electron mobilities,
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08/11/2011 22.00 Menyoung Lee, James R. Williams, David Goldhaber-Gordon, Sipei Zhang, C. Daniel Frisbie. Electrolyte gate-controlled Kondo effect in SrTiO3,
(07 2011)

08/15/2011 24.00 A. M. Kaiser, A. X. Gray, G. Conti, J. Son, A. A. Greer, A. Perona, A. Rattanachata, A. Y. Saw, A. Bostwick, S. Yang, S.-H. Yang, E. M. Gullikson, J. B. Kortright, S. Stemmer, C. S. Fadley. Suppression of near-Fermi level electronic states at the interface in a LaNiO3/SrTiO3superlattice,
(08 2011)

08/15/2012 60.00 S.-H. Yang, A. X. Gray, A. M. Kaiser, B. S. Mun, B.C. Sell, J. B. Kortright, C. S. Fadley. Making use of x-ray optical effects in photoelectron-, Auger electron-,and x-ray emission spectroscopies: total reflection, standing-waveexcitation and resonant effects,
SUBMITTED (08 2012)

08/16/2011 25.00 A.A. Burkov, Leon Balents. Weyl Semimetal in a Topological Insulator Multilayer,
(06 2011)

08/31/2010 3.00 Gulgun H. Aydogdu, Dmitry Ruzmetov, Shriram Ramanathan. Metastable oxygen incorporation into thin film NiO by low temperature active oxidation: Influence on hole conduction,
Journal of Applied Physics (08 2010)

08/31/2010 5.00 Daniel G. Ouellette, SungBin Lee, Junwoo Son, Susanne Stemmer, Leon Balents, Andrew J. Millis, S. James Allen. Optical conductivity of LaNiO3: coherent transport and correlation driven mass enhancement,
Physical Review B (06 2010)

08/31/2010 4.00 SungBin Lee, Ru Chen, Leon Balents. Landau theory of charge and spin ordering in the nickelates, Physical Review Letters (08 2010)

09/08/2013 91.00 Jack Y. Zhang, Clayton A. Jackson, Santosh Raghavan, Jinwoo Hwang, Susanne Stemmer. Magnetism and local structure in low-dimensional, Mottinsulating GdTiO3, Physical Review B (accepted) (08 2013)

09/28/2012 61.00 Pouya Moetakef, Daniel G. Ouellette, James R. Williams, S. James Allen, Leon Balents, David Goldhaber-Gordon, Susanne Stemmer. Quantum oscillations from a two-dimensional electron gas at a Mott/bandinsulator interface, Appl. Phys. Lett. (submitted) (08 2012)

10/16/2011 31.00 Sieu D. Ha, Gulgun H. Aydogdu, Shriram Ramanathan. Examination of insulator regime conduction mechanisms inepitaxial and polycrystalline SmNiO3 thin films, Submission to Journal of Applied Physics (10 2011)

10/19/2011 33.00 Junwoo Son, Bharat Jalan, Adam P. Kajdos, Leon Balents, S. James Allen, Susanne Stemmer. Probing the metal-insulator transition of NdNiO3 byelectrostatic doping, Submited to Applied Physics Letters (10 2011)

11/02/2013 95.00 Clayton A. Jackson, Susanne Stemmer. Interface-induced magnetism in perovskite quantum wells, Accepted, Physical Review B (Rapid Communication) (07 2013)

11/18/2011 39.00 Pouya Moetakef, Tyler A. Cain, Daniel G. Ouellette, Jack Y. Zhang, Dmitri O. Klenov, Anderson Janotti, Chris G. Van de Walle, Siddharth Rajan, S. James Allen, Susanne Stemmer. Electrostatic carrier doping of GdTiO3/SrTiO3 interfaces, Accepted in Applied Physics Letters (11 2011)

11/29/2012 62.00 B. D. Schultz, S. Ohya, L. Feigl, D. G. Ouellette, A. Kozhanov, C. J. Palmstrøm. Structural and transport properties of epitaxial PrNiO3 thin films grown by molecular beam epitaxy, Submitted to J. Cryst. Growth (11 2012)

12/07/2012 63.00 Man Gu, Jude Laverock, Bo Chen, Kevin E. Smith, Stuart A. Wolf, Jiwei Lu. Metal-insulator transition induced in CaVO3 thin films, Submitted to Journal of Applied Physics (12 2012)

12/12/2010 9.00 Sieu D. Ha, Gulgun H. Aydogdu, Shriram Ramanathan. Metal-insulator transition and electrically-driven memristive characteristics of SmNiO3 thin films, (09 2010)

12/15/2010 10.00 SungBin Lee, Ru Chen, Leon Balents. Landau theory of charge and spin ordering in the nickelates, (12 2010)

12/17/2011 42.00 B. Viswanath, G. H. Aydogdu, S. D. Ha, S. Ramanathan. In-situ stress relaxation and diffraction studies across metal-insulator transition in epitaxial and polycrystalline SmNiO3 thin films, Submitted to Scripta Materialia (12 2011)

TOTAL: 39

Number of Manuscripts:

Books

Received Book

TOTAL:

Received Book Chapter

TOTAL:

Patents Submitted

Patents Awarded

Awards

1) Participating faculty honors:

Charles Fadley:
- Elected foreign member of the Royal Society of Sciences in Uppsala
- Fellow of the American Association for the Advancement of Science
- Elected to Senior Member status in the IEEE
- Visiting Professorship from the French Laboratoires d'Excellence
- Fellow of Elettra (Italian national synchrotron radiation and free electron laser facility)
- Honorary doctorate in Physics, Uppsala University, Sweden
- Senior Distinguished Professorship (Chaire Senior), France
- International Fellow of the Surface Science Society of Japan (SSSJ)
- David A. Shirley Award for Outstanding Scientific Achievement at the Advanced Light Source
- Honorary Member of the International Scientific Committee of the International Vacuum Ultraviolet and X-Ray Physics (VUVX) Conferences, July, 2016

Shriram Ramanathan:
- Robert Lansing Hardy Award, 2011 (Award by TMS to a young scientist annually)
- Kavli Fellow Lecturer, National Academy of Sciences, 2012

Susanne Stemmer:
- Fellow of the American Ceramic Society
- Fellow of the American Physical Society
- Fellow of the Materials Research Society
- Fellow, Microscopy Society of America
- National Security Science and Engineering Faculty Fellow (Department of Defense)

Chris van de Walle:
- Fellow of the American Association for the Advancement of Science

Chris Palmstrom:
- Fellow of the Materials Research Society
- Molecular Beam Epitaxy (MBE) Innovator Award at the North American MBE conference
- National Security Science and Engineering Faculty Fellowship (NSSEFF)

Stuart Parkin:
- 1st Distinguished DGIST Lecturer, Daegu Gyeongbuk Institute of Science & Technology (DGIST)
- Gutenberg Research College Fellowship, University of Mainz
- E.W. Guptill Memorial Lecture, Dalhousie University, Halifax, Nova Scotia, Canada
- Honorary Doctorate awarded by the University of Regensburg
- Election to Honorary Fellow of the Indian Academy of Sciences
- David Adler Lectureship Award from the American Physical Society
- Honorary Doctorate awarded by the Universität Kaiserslautern, Germany,
- Von Hippel Award from the Materials Research Society

Leon Balents:
- Fellow of the American Physical Society

2) Participating student honors:

- Alexander X. Gray: Young Scientist Award of the SPring-8 Used Community in Japan
- Undergraduate James Kally - Worster summer research Fellowship in Physics
- Patrick Gallagher: Stanford Graduate Fellowship for the 2015-16 academic year

Graduate Students

NAME	PERCENT_SUPPORTED	Discipline
BROWN-HEFT, TOBIAS	0.02	
CHEN, GANG	0.05	
CHEN, RU	0.04	
FREEZE, CHRISTOPHER R.	0.09	
GOYAL, MANIK	0.14	
IACONIS, JASON J.	0.04	
ISAAC, BRANDON JOSEPH	0.18	
JACKSON, CLAYTON ADAM	0.12	
KAJDOS, ADAM PAUL	0.04	
LEE, SUNGBIN	0.17	
LOGAN, JOHN	0.05	
MIKHEEV, EVGENY	0.01	
MYZAFERI, ANISA	0.02	
OUELLETTE, DANIEL G	0.40	
PENDHARKAR, MIHIR	0.05	
PENNACHIO, DANIEL JOSEPH	0.14	
RAGHAVAN, SANTOSH	0.13	
SON, JUNWOO	0.14	
WILSON, NATHANIEL S	0.04	
Gu, Man	1.00	
Alexander Gray	0.23	
Alexander Saw	0.06	
Albert Greer	0.01	
Catherine Conlon	0.08	
Armela Keqi	0.01	
Arunthai Rattachanata	0.01	
Sam Stanwyck	0.20	
Patrick Gallagher	0.10	
FTE Equivalent:	**3.57**	
Total Number:	**28**	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
ENGEL-HERBERT, ROMAN	0.07
FEIGL, LUDWIG	0.21
HAUSER, ADAM	0.08
JIANG, HONG-CHEN	0.14
RUDAWSKI, NICHOLAS GUY	0.08
SCHUMANN, TIMO	0.04
SON, JUNWOO	0.08
YEE, CHUCK-HOU	0.17
JEONG, JAEWOO	0.48
Ha, Sieu	0.50
Aydogdu, Gulgun	0.50
Alexander Kaiser	0.33
Slavomir Nemsak	0.45
Gunnar Palsson	0.10
Gulgun Aydogdu	0.50
Sieu Ha	0.50
James Williams	0.10
FTE Equivalent:	**4.33**
Total Number:	**17**

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
ALLEN, S. JAMES	0.07	
STEMMER, SUSANNE	0.33	
Wolf, Stuart	0.08	
Lu, Jiwei	0.25	
Fadley, Charles	0.01	
David Goldhaber-Gordon	0.03	
FTE Equivalent:	**0.77**	
Total Number:	**6**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED	Discipline
KALLY, JAMES C	0.20	Physics
Marshall Stycinzski	0.02	Physics
FTE Equivalent:	**0.22**	
Total Number:	**2**	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 2.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:..... 2.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:..... 2.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):..... 2.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:..... 0.00

Names of Personnel receiving masters degrees

NAME
Total Number:

Names of personnel receiving PHDs

NAME	
CHEN, GANG	
CHEN, RU	
JACKSON, CLAYTON ADAM	
KAJDOS, ADAM PAUL	
LEE, SUNGBIN	
OUELLETTE, DANIEL G	
SON, JUNWOO	
Gu, Man	
Alexander Gray	
Albert Greer	
Daria Eiteneer-Harmon	
Patrick Gallagher	
Total Number:	**12**

Names of other research staff

NAME	PERCENT_SUPPORTED
METLITSKI, MAXIM A.	0.07
KOZHANOV, ALEXANDER	0.24
LANGER, MARC JOSEPH	0.02
JACKSON, ANDREW W	0.21
JANOTTI, ANDERSON	0.15
Giuseppina Conti	0.13
David Hemer	0.01
Ray Gerhard	0.02
FTE Equivalent:	**0.85**
Total Number:	**8**

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

See attachment.

Technology Transfer

Final Report

Emergent Phenomena at Mott Interfaces

Multidisciplinary University Research Initiative
W911-NF-09-1-0398

Scientific Progress and Accomplishments

The objective of the multidisciplinary university research initiative (MURI) "Emergent Phenomena at Mott Interfaces" was to establish new approaches to predict, understand and control the wealth of electronic, spin and collective mode excitations associated with Mott metal-insulator transitions at complex oxide interfaces. Research focused on electronic and atomic structure and correlation physics of oxide interfaces comprised of perovskite titanates, rare earth nickelates, and vanadates. Here we briefly summarize the main accomplishments.

Thin Films and Interfaces in Rare Earth Nickelates

The MURI focused on interfaces with Mott materials with only one electron or hole in either e_g or t_{2g}. This configuration maximizes interpretability and quantum effects. For the e_g systems, we focused on the rare earth nickelates, $RNiO_3$ (R = rare earth, i.e., La or Nd). Ni^{3+} has a $3d^7$ configuration with a filled t_{2g} band and one electron in the e_g multiplet. These orbitals show a strong hybridization with the adjacent oxygen $2p$ orbitals. The overlap determines the bandwidth W, which is a critical parameter of the Mott transition, and can be tuned by film strain or interface proximity effects.

Work in the **Balents** group involved a combination of fundamental theory and collaboration with experiment in modeling and interpreting measurements. The most significant two accomplishments included a *spin density wave* interpretation and theory of spin and charge order in the RNiO$_3$ nickelates. The work predicted the quenching of charge order in ultra-thin films, proving that in the more itinerant nickelates, the spin density wave is the driving instability. The work on heterostructures led to some of the very first theoretical work on Weyl semimetals (which appear naturally in the theory of heterostructures of topological insulators) and their properties. Collaborations with experimentalists in the MURI included modeling of transport and optical response of the nickelates, which showed that main features of the conductivity could be understood from a minimal two-band model of e_g symmetry states, and their intra- and inter-band contributions.

Experiments on RNiO$_3$ nickelate thin films focused on unconventional (non-Fermi liquid) metallic behavior, metal-insulator transitions, and pseudogaps, and how these are influenced by film strain, film thickness, and orbital polarization that is tuned by these parameters. One of the first sets of experiments concerned the electrical resistivity and magnetotransport of thin, epitaxial $LaNiO_3$ films. The **Stemmer** group, in collaboration with **Allen** and **Balents**, showed that *d*-band transport is inhibited as the layers progress from compression to tension. Increasing tensile strain causes the film resistivity to increase, causing strong localization to appear below a critical thickness. Optical conductivity by **Allen** of these films signal the approach to the quantum phase transition. The spectral weight in the Drude tail exposes a mass enhancement as large as 2-3 times the band mass and which depends on the compressive/tensile strain. The strain dependent mass enhancement correlates with strain dependent electron-electron contribution to transport scattering. A divergent mass is a signature of the Mott critical point.

The **Palmstrøm** group performed in-situ scanning tunneling spectroscopy of $LaNiO_3$ films grown by molecular beam epitaxy on Nb-doped $SrTiO_3$ substrates. The results show an observable gap in the density of states ranging in size from 200-400 meV for $LaNiO_3$ films $\leq$5 unit cells thick, and a transition to a metallic density of states with a pseudo gap at a thickness of 7 unit cells. The presence of an observable gap in the density of states is evidence that disorder and Anderson localization is not the source of the metal to insulator transition observed in thin films of $LaNiO_3$.

The **Fadley** group combined soft and hard x-ray photoemission with synchrotron radiation. Using standing-wave photoemission, including tuning over strong core-level resonances, unique depth resolution for composition and electronic structure at buried interfaces are obtained. For $LaNiO_3$, the insulating state of ultrathin epitaxial $LaNiO_3$ thin films was detected by hard x-ray photoemission and also verified a suppression of near-Fermi level electronic states at the interface in a $LaNiO_3/SrTiO_3$ superlattice grown by the **Stemmer** group. Soft- and hard- x-ray standing-wave angle-resolved photoemission were used to determine the depth-resolved composition and electronic structure of buried layers and interfaces in a $LaNiO_3/SrTiO_3$ superlattice.

A second set of experiments concerned $NdNiO_3$, which in bulk form shows a temperature induced metal-insulator transition. This system proved to be especially fruitful for studies of the origins of unconventional metallic behavior. Tunneling spectroscopy by **Allen** on samples by **Stemmer** of the electron states in Nd and La nickelate strongly suggest that the metal-insulator phase transition is quantum critical. $NdNiO_3$ exhibits a well-developed gap at low temperatures, with an energy scale that is in quantitative agreement with the transition temperature. The behavior begs a comparison with tunneling experiments in superconductors. $LaNiO_3$ is metallic to the lowest temperatures but develops a pseudogap in the tunneling conductance with a width that is approximately the same as the gap in the insulating $NdNiO_3$: it presages the development of the Mott insulating state. The results point to both types of gaps arising from a common origin, namely, a quantum critical point associated with the T = 0 K metal-insulator transition. The results support theoretical models of the quantum phase transition in terms of spin and charge instabilities of an itinerant Fermi surface, as suggested by theory.

The **Stemmer** group applied epitaxial strains to study the effect of suppressing the metal-insulator transition in the rare earth nickelate $NdNiO_3$. The results allowed insights into "bad metal" behavior that is found also in other strongly correlated systems. Accounting for resistivity saturation was key to correctly describe the electrical transport behavior. The resistivity saturation limit was found to be sensitive to strain, and this was interpreted in terms of the degree of e_g orbital polarization, which is varied by the film strain. Accounting for saturation clarifies many aspects of the epitaxial strain-film thickness phase behavior and the quantum critical point in the $RNiO_3$ system. In particular, an abrupt crossover between classic Landau Fermi liquid (LFL) and non-Fermi liquid (NFL) metallic regimes occurs with the suppression of the temperature-driven MIT. The metallic phase is a LFL in all cases where a robust MIT is present. The non Fermi liquids exponent was $n \approx 5/3$, for all NFLs. We also clarified the conditions leading to Anderson

localization in this system, namely a second, disorder-driven MIT: it appears when the 0-K resistivity approaches the saturation resistance.

The relative roles of disorder and strong correlations are among the least understood in metal-insulator transitions. Disorder due to defects can alter the extent of interactions between electrons leading to drastic modification of the insulator-metal transition properties. The **Ramanathan** group studied the role of point defects in influencing the electronic properties of rare-earth nickelates. Thorough analysis of temperature-dependent FTIR measurements were performed on epitaxial $SmNiO_3$ films with varying oxygen content. The measurements spanned the insulator-metal phase transition at 400 K, and they provided original insight into the mechanism of the phase transition in the rare-earth nickelates. We showed that polaronic conduction in the metallic phase is derived from electrons coupling to the Ni-O stretching and bending mode phonons. Analysis of the optical conductivity with extended Drude analysis revealed that the scattering rate and effective mass of SNO remain surprisingly constant across the phase transition. In addition, we observe that the integrated spectral weight, which is a qualitative measure of free carrier density, tracks the temperature dependence of the conductivity from insulating to metallic phases quite well. We also showed that increasing disorder (reduced oxygen content) has a similar effect on carrier density and conductivity as temperature. We also showed that the surface of epitaxial oxides, while stable to ambient, can be chemically modified reversibly and repeatedly using AFM.

Perovskite Titanates

For the t_{2g} Mott systems, the MURI focused on the titanates and vanadates, in which Ti^{3+} and V^{4+} have the $3d^1$ configuration, with one electron in t_{2g}. The series of $RTiO_3$ with R = La, Pr, Nd, Sm, Y are prototypical Mott-Hubbard materials, with decreasing bandwidth W from La down to Y. This is due to the progressive decrease in the Ti-O-Ti bond angle from ~ 157° in $LaTiO_3$ to ~ 140° in $YTiO_3$. $GdTiO_3$ shows ferromagnetism, whereas $LaTiO_3$ and $SmTiO_3$ show antiferromagnetism. As discovered during this MURI project, when interfaced with the band insulator $SrTiO_3$, a high-density, two dimensional electron liquid is formed. In this MURI we showed that this electron liquid exhibits a plethora of strongly correlated phenomena that can be finely tuned by the heterostructure parameters.

For example, the **Stemmer** group, in collaboration with the **Goldhaber-Gordon** and **Allen** groups, showed that ferromagnetism appears at low temperatures in the electron liquid confined in narrow quantum wells bound by $GdTiO_3$, as evidenced by a hysteresis in the magnetoresistance. The longitudinal and transverse magnetoresistance are consistent with anisotropic magnetoresistance, and thus indicative of induced ferromagnetism in the $SrTiO_3$ (a material that is paramagnetic in the bulk), rather than a nonequilibrium proximity effect. Scaling the electron liquid to extreme limit of a 1-2 SrO layers thickness embedded in $GdTiO_3$ thermally activated transport is observed. The **Allen** group used optical conductivity to show that it quantitatively agrees with predictions of small polaron transport. The delta doping produces an extremely high, two-dimensional density, 7.3×10^{14} cm^{-2}. Unlike transport in randomly doped 3D Mott insulators, the delta-doped layer is potentially free of disorder and introduces a new arena in which to explore the effect of electron correlations, polaron transport and dimensionality.

The **Fadley** group used resonant angle-resolved photoemission to directly view the critical thickness for electron liquid formation in $SrTiO_3$ embedded in $GdTiO_3$, and standing-wave soft- and hard- x-ray photoemission to determine the energetic, spatial, and momentum character of the 2D electron liquid at a buried $GdTiO_3/SrTiO_3$ interfaces.

Advanced first-principles methods, such as LDA+*U* and hybrid functionals by the **Van de Walle** group were used to address problems related to electronic structure, defects, doping, and band alignments in the titanate heterostructures. The effects of strain on the energetic ordering and effective mass of the lowest conduction-band states in $SrTiO_3$ were explored. It was found that biaxial stress in the (001) or (110) planes results in the lowest-energy conduction-band state having significantly smaller electron mass in the in-plane directions compared to the unstrained $SrTiO_3$, suggesting that pseudomorphic growth is a promising route to increasing the electron mobility in epitaxial films. Another study (in collaboration with experiments by **Stemmer**) focused on the effects of incorporation of high concentrations of donor impurities on the lattice parameter. The observed increase in lattice parameter was attributed to two causes: impurity-size and electronic effects, and both were quantified. Band alignments were calculated that aided in the interpretation of hard x-ray photoemission measurements by **Fadley**.

Using complex oxides in nanoscale circuitry opens up the possibility of utilizing electron-electron correlations to create novel functionality in devices, which were explored in the titanates by the **Goldhaber-Gordon** group. Under this MURI, they developed a method to locally pattern carrier accumulation in the common complex oxide $SrTiO_3$ and used it to create tunable lateral Josephson junctions in $SrTiO_3$. These junctions show two surprising characteristics: (i) They have ballistic single-mode transport as they are first opened up. (ii) This single-mode transport is spin-polarized (Fig. 1). This is likely connected to the strong spin-orbit coupling in $SrTiO_3$, and it may eventually help us understand the various measurements of apparently carrier-induced magnetism in $SrTiO_3$, mentioned above. The **Goldhaber-Gordon** group also developed a method to electrolyte gate using a barrier layer to achieve large carrier density modulations while preventing chemical reactions. They applied this approach to achieve high-mobility 2D electron system at surface of $SrTiO_3$ (and now use it for a range of materials).

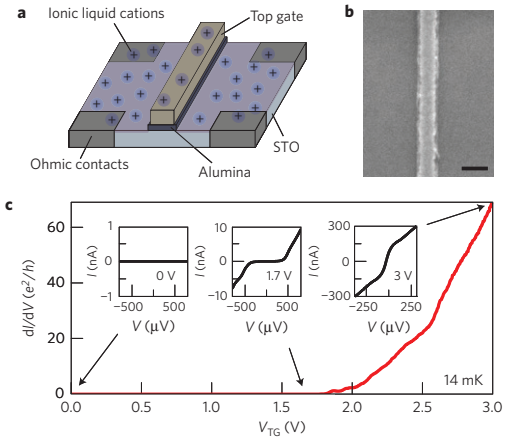

Figure 1. Device properties. a, Schematic of the device, which is submerged in ionic liquid. Cations are drawn to the sample by a positively charged electrode (not shown) that is also

immersed in the liquid, accumulating electrons at the exposed $SrTiO_3$ surface (lavender shading). The top gate defines a channel of low electron density by spacing and screening the cations. **b**, Scanning electron micrograph of a top gate of nominal length 60 nm. The scale bar is 100 nm. The alumina dielectric laterally protrudes 5–10 nm (faint edge around top gate). **c**, Electronic properties versus top gate voltage V_{TG} at 14 mK. Main panel: differential conductance at zero source–drain bias. Insets: *IV* curves from the insulating, tunneling, and superconducting regimes.

Vanadates

The vanadates $CaVO_3$ and $SrVO_3$ are metallic, with $CaVO_3$ being closest to a Mott metal-insulator transition. The **Lu**/**Wolf** groups used electron-beam deposition to study the Mott transitions in the vandates, in particular, dimensional confinement in the quantum well, chemical doping, and superlattice structures. For example, vanadate films with thicknesses over 20 nm are metallic, following the T^2 law corresponding to a Fermi liquid system. A temperature driven metal-insulator transition was induced in vanadate ultrathin films. The induced metal-insulator transition can be attributed to the dimensional crossover from a three-dimensional metal to a two-dimensional Mott insulator, as the resulting reduction in the effective bandwidth *W* opens a bandgap at the Fermi level. The magnetoresistance measurements also confirmed the metal-insulator transition is due to the electron-electron interactions other than disorder-induced localization. B-site doping in $SrVO_3$ with Ti^{4+} was investigated. The transport study revealed a temperature-driven metal-insulator transition. Films with higher vanadium concentration were metallic, and the ones with lower vanadium concentration were semiconducting following Mott's variable range hopping mechanism. The mechanisms behind the observed metal-insulator transition are complicated due to completing effects among electron correlation, disorder, and percolation. $SrVO_3/SrTiO_3$ (SVO/STO) superlattices showed a pronounced enhancement in the conductivity, which is a further indication of electronic phase separation in the vanadate ultrathin layers and can be described as percolation phenomena.

The **Parkin** group investigated electric field induced metallization of insulating oxides as a means of exploring and creating novel electronic states. However, the electric fields created by conventional field effect transistor devices are generally not sufficient to achieve the necessary carrier densities in correlated oxides. Large electric fields from polar surfaces and electric double layers have been used to create emergent metallic, superconducting and magnetic states in insulating oxides. However, the electric fields needed are so high that the possibility of atomic reconfigurations at the interface and motion of atoms and vacancies at and beyond the interface cannot be ruled out. To address these issues, the **Parkin** group carried out a wide range of systematic studies on prototype titanates and vanadates. The found clear evidence that the electrolyte gate induced suppression of the metal-insulator transition is largely due to the electric field induced formation of oxygen vacancies in the VO_2 channel. Electrolyte gating of VO_2 leads to the removal of oxygen from the top portion of the film and this oxygen is forced back into the film by reverse gating.