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1400 John R. Lynch Street

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UU	UU	UU	UU		19b. TELEPHONE NUMBER 601-979-3723

RPPR Final Report
as of 24-Mar-2021

Agency Code:

Proposal Number: 75332CHCF **Agreement Number: W911NF-20-1-0009**
INVESTIGATOR(S):

Name: Jerzy Leszczynski
Email: jerzy@icnanotox.org
Phone Number: 6019793723
Principal: Y

Organization: **Jackson State University**
Address: 1400 John R. Lynch Street, Jackson, MS 392170002
Country: USA
DUNS Number: 044507085 EIN: 646000507
Report Date: 31-Jan-2021 Date Received: 16-Mar-2021
Final Report for Period Beginning 01-Nov-2019 and Ending 31-Oct-2020
Title: 27th Conference on Current Trends in Computational Chemistry
Begin Performance Period: 01-Nov-2019 **End Performance Period:** 31-Oct-2020
Report Term: 0-Other
Submitted By: Jerzy Leszczynski Email: jerzy@icnanotox.org
Phone: (601) 979-3723
Distribution Statement: 1-Approved for public release; distribution is unlimited.

STEM Degrees: 4 **STEM Participants:** 73

Major Goals: The major goals of the 27th CCTCC is the dissemination of cutting-edge research in the area of computational chemistry and related fields.

Accomplishments: This year, the ICN, in partnership with Jackson State University and the US Army Corps of Engineers, hosted the 27th International Conference on Current Trends in Computational Chemistry. The Conference was held at the Hilton Hotel of Jackson, Mississippi, on November 8–9, 2019, and hosted over 150 participants from 7 countries including Bulgaria, China, Chile, Belgium, Italy, Ukraine and Poland.
The format of the 27th CCTCC consisted of 6 sessions of (invited) plenary lectures and over 60 poster presentations covering applications as well as theory. Over 40 of the poster presentations were given by graduate and undergraduate students. A total of 9 prizes ranging from first place to honorable mention were awarded for the best undergraduate and graduate poster presentations.

Featured talks involved cutting-edge research regarding Density Functional Theory (DFT) and Machine Learning and Artificial Intelligence to include topics: “The Devil’s Triangle In KSDFT Calculations And How To Fix It,” Rodney Bartlett, University of Florida, FL, USA; “Boosting ab-initio molecular dynamics with machine learning,” Roberto Car, Princeton University, NJ, USA; and “Artificial Intelligence for glass composition design: advances and remaining challenges,” Adama Tandia, Corning Incorporated, NY, USA.

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Other noted scientists who delivered innovative talks included: Donald Truhlar, University of Minnesota, MN, USA; Adriana Pietropaolo, University of Catanzaro, Italy; Jared Delcamp, University of Mississippi, MS, USA; Adam Willard, Massachusetts Institue of Technology, MA, USA; Dean Tantillo, University of California Davis, CA, USA; Davita Watkins, University of Mississippi, MS, USA; Corning Incorporated, NY, USA; Jane Murray, University of New Orleans, LA, USA; Liudmil Antonov, Bulgarian Academy of Sciences, Sofia, Bulgaria; Alicia Mikolajczyk, University of Gdansk, Gdansk, Poland; Minh Tho Nguyen, University of Leuven, Leuven, Belgium; Igor Alabugin, Florida State University, FL, USA and banquet speaker, Robert Wallace, U.S. Army Corps of Engineers, MS USA.

The supporting agencies were the Army Research Office, National Science Foundation (CREST Program, EPSCoR Program); Office of Naval Research; Office of Vice President for Research and Strategic Initiatives, JAS; Parallel Quantum Solutions; Royal Society of Chemistry; Springer; and US Army Corps of Engineers.

Training Opportunities: The 27th CCTCC hosted over 150 participants to include training of 31 graduate, 42 undergraduate, and 3 high school students for a total of 76 students.

Students were able to interact with top professionals in the field and receive feedback on research presentations.

Results Dissemination: The 27th CCTCC proceeding was disseminated to all participants, partners and the public at large.

Honors and Awards: Over five awards for best poster presentations were given to undergraduate and graduate poster presenters. Presenters represented colleges from across the US and Europe.

Protocol Activity Status:

Technology Transfer: Nothing to Report

PARTICIPANTS:

Participant Type: PD/PI
Participant: Jerzy Leszczynski
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Other (specify)
Participant: Shonda Allen
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Other (specify)
Participant: Galina Lobodina
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N

Other Collaborators:

27th Current Trends in Computational Chemistry Conference

November 8-9, 2019

Award No: W911NF-19-1-0009

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Matrix for 27th CCTCC	
Number of participants	159
Number of countries represented	7 countries including Bulgaria, China, Chile, Belgium, Italy, Ukraine and Poland.
Number of female participants	72
Number of AA participants	57
Number of Hispanic participants	3
High School Students	3
Undergraduate Students	42
Graduate Students	31
Total Students	76