Kevin Waters

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EDUCATION

PHD. PHYSICS August 2013 - August 2018
Michigan Technological University (MTU)
Advisor : Ravindra Pandey

BACHELOR OF SCIENCE August 2009 - May 2013
Indiana State University (ISU)
Major: Physics
Minors: German, Mathematics
Cum Laude

RESEARCH EXPERIENCE

U.S. ARMY RESEARCH LABORATORY, *Postdoctoral Scholar* October 2018 - Present

- Proposed and investigated new 2D polymers for advantageous mechanical properties using state-of-the-art electronic structure software on high performance computing platforms.
- Developed frameworks and libraries in python to perform high-throughput calculations augmented with machine learning to predict material properties.
- Worked in an interdisciplanary collaboration of experimental and theoretical chemists, engineers and physicists to address U.S. Army R&D goals.

MICHIGAN TECHNOLOGICAL UNIVERSITY, *Graduate Researcher* June 2013 - August 2018

- Performed quantum mechanical simulations (density functional theory) on various systems of interest on high performance computing architectures.
- Designed and implemented computational analysis tools using Python.
- Communicated findings through documentation, presentations and publications to academic journals and professional conferences.
- Collaborated on the NASA Ultra-Strong Composites by Computational Design study investigating polymers and nanomaterials.
- Mentored undergraduate, graduate, post-doctoral students and visiting faculty members on research methodologies, utilizing the linux-unix environment, and harnessing high performance computing facilities.

DOE SCIENCE GRADUATE FELLOWSHIP, *Graduate Researcher* January 2018 - June 2018

- Collaborated with Eric Bylaska to implement features into the ab initio computational chemistry package NWChem at the Pacific Northwest Laboratory.
- Derived theoretical framework and obtained results to implement a novel numerical method for a long-ranged exchange operator in a plane-wave setting.
- Prototyped and implemented long-ranged exchange operator into the framework of NWChem.
- Performed ab intio molecular dynamics simulations on the nanomaterial and biological interface to gain insight on the chemistry and physics for the next generation of biosensors.

AIR FORCE RESEARCH LABORATORY, *Graduate Researcher* June 2017- August 2017

- Collaborated with Ruth Pachter investigating the potential functionalization of boron-nitride nanomaterials using first principles methods.
- Investigated the effects of defects on the physical and electronic properties of boron-nitride monolayers and nanotubes.
- Analyzed the effects of chirality of boron nitride nanotubes on the electronic and mechanical properties.

RESEARCH EXPERIENCE (CONT.)

INDIANA STATE SUMMER RESEARCH, *Undergraduate Researcher* May 2012 - Aug 2012

- Derived theoretical and experimental methods with Joseph West for moving large pyramid type blocks.
- Developed numerical models using python to modify n-sided (3-n) polygons to decrease work required for rotation.
- Implemented the numerical methods to modify concrete blocks and tracked motion to test models.
- Communicated results in monthly presentations to peers and professors in the summer undergraduate research program.

INDIANA STATE SUMMER RESEARCH, *Undergraduate Researcher* May 2010 - Aug 2011

- Analyzed electrocardiograms (ECGs) with Guo-ping Zhang using Fourier transforms in an attempt to diagnose heart conditions.
- Utilized the university's supercomputer to perform analysis on data obtained from the MIT-BIH Arrhythmia Database.
- Communicated results in monthly presentations to peers and professors in the summer undergraduate research program.
- Presented results at the American Physical Society March Meeting 2013

TEACHING & MENTORING EXPERIENCE

INSTRUCTOR, *Michigan Technological University* Fall 2016, 2017

- Developed the course curriculum for PH4390, Computational Methods in Physics, for senior undergraduates and new graduate students.
- Instructed students on the fundamentals of coding, numerical methods and scientific computing.
- Implemented a laboratory section for the class to create a supervised learning environment for students writing, developing, testing and documenting their programming assignments in a linux-unix environment.

GRADUATE TEACHING ASSISTANT, *Michigan Technological University* Fall 2013 - Fall 2016

- Assisted in class instruction, directed laboratory sections and provided feedback to students ranging from freshman to graduate students.
- Facilitated the following classes: Introduction to Scientific Programming for Physicists, Computational Methods in Physics, Honors Physics I, and Introductory Astronomy.
- Proctored University Physics I and II exams.

PHYSICS LEARNING COACH, *Michigan Technological University* Spring 2015

- Worked with a diverse population of students in group and one-on-one settings.
- Assisted students with concepts and problems for University Physics I and II.

UNDERGRADUATE TEACHING ASSISTANT, *Indiana State University* Fall 2010 - Spring 2013

- Assisted in the instruction of the College and University Physics I and II.
- Aided in the set-up, breakdown and maintenance of the laboratory.

PHYSICS LEARNING CENTER TUTOR, *Indiana State University* Fall 2010 - Spring 2013

- Worked with a diverse population of students in group and one-on-one settings.
- Assisted students with concepts and problems for College and University Physics I and II.

TEACHING & MENTORING EXPERIENCE (CONT.)

ACADEMIC PEER ADVOCATE, *Indiana State University* Fall 2011 - Spring 2012

- Assisted a floor of 40 freshman, organized floor programs, and advised residents on academic issues.
- Mentored first years students during their transition to college.
- Worked the front desk as a customer service representative to answer phone calls, set up meetings, and address needs of residents and staff.

PUBLICATIONS

1 **Two-Dimensional Gold Quantum Dots with Tunable Bandgaps**
Shiva Bhandari, Boyi Hao, Kevin Waters, Chee Huei Lee, Juan-Carlos Idrobo, Dongyan Zhang, Ravindra Pandey, Yoke Khin Yap
ACS Nano 13, 44347-4353, 2019

2 **Multiscale Modeling of PEEK using Reactive Molecular Dynamics Modeling and Micromechanics**
William A. Pisani , Matthew S. Radue , Sorayot Chinkanjanarot, Brett A. Bednarcyk, Evan J. Pineda, Kevin Waters, Ravindra Pandey, Julia A. King, Gregory M. Odegard
Polymer 163, 96-105, 2019

3 **Coumarins: Spectroscopic measurements and first principles calculations of C4-substituted 7-aminocoumarins**
Shraddha Singh, Vaho Begoyan, Marina Tanasova, Kevin Waters, Max Seel, Ravindra Pandey
Journal of Physical Organic Chemistry 31 (9), e3852, 2018

4 **Dynamics of Self-Assembled Cytosine Nucleobases on Graphene**
Nabanita Saikia, Floyd Johnson, Kevin Waters, Ravindra Pandey
Nanotechnology, vol. 29 pp. 19560, 2018

5 **Stability, elastic and electronic properties of a novel BN_2 sheet with extended hexagons with N-N bonds**
Kevin Waters, Ravindra Pandey
Journal of Physics: Condensed Matter, vol. 29 pp.195601, 2018

6 **Hierarchical Self-Assembly of Noncanonical Guanine Nucleobases on Graphene**
Nabanita Saikia, Kevin Waters, Shashi P. Karna, Ravindra Pandey
ACS Omega, vol. 2. pp. 3457, 2017

7 **Amino-Acid-Conjugated Gold Clusters: Interaction of Alanine and Tryptophan with Au_8 and Au_{20}**
Marwa H. Abdalmoneam, Kevin Waters, Nabanita Saikia, and Ravindra Pandey
J. Phys. Chem. C, vol. 121 pp. 25585–25593, 2017

8 **Electronic Properties of Acetaminophen Adsorbed on 2D Clusters: A First Principles Density Functional Study**
Ujjal Saikia, Nabanita Saikia, Kevin Waters, Ravindra Pandey, Munima Bora Sahariah
ChemistrySelect vol. 2 pp. 3613, 2017

9 **Amino Acid Analogue-Conjugated BN Nanomaterials in a Solvated Phase : First Principles Study of Topology-Dependent Interactions with a Monolayer and a (5,0) Nanotube**
Kevin Waters, Ravindra Pandey, Shashi P. Karna
ACS Omega vol. 2, pp. 76−83, 2017

10 **Thermoelectric Properties of SnSe Nanoribbons: A Theoretical Aspect**
Kriti Tyagi, Kevin Waters, Gaoxue Wang, D. Haranath, Bhasker Gahtori, Ravindra Pandey
Materials Research Express, vol. 3 pp. 35013, 2016

11 **A Theoretical Study of Structural and Electronic Properties of Alkaline-Earth Fluoride Clusters**
Ratnesh Pandey, Kevin Waters, Sandeep Nigam, Haiying He, Subhash Pingle, Avinash Pandey, Ravindra Pandey.
Computation and Theoretical Chemistry, vol. 1043, pp. 24–30, 2014

12 **Building the Next Pyramid**
Joseph West, Greg Gallagher, Kevin Waters, Stephen Ward, Tia Ward
arXiv:1502.07319

PRESENTATIONS & TALKS

1 **Stability and Electronic Properties of Amine Functionalized Boron Nitride Nanostructures**
Graduate Research Colloquium (MTU) · February 2017

2 **Amino Acids Interaction with Boron Nitride Nanomaterials**
American Physical Society March Meeting · March 2016

3 **First Principles Study of Boron Nitride Nanomaterials & Amino Acid Molecules**
Physics Graduate Colloquium (MTU) · Feb 2016

4 **Ab Initio Study of the Structural and Electronic Properties of MgV_2O_4 in its Cubic Phase**
Graduate Research Colloquium (MTU) · February 2015

5 **A Theoretical Study of Structural and Electronic Properties of Alkaline-Earth Fluoride Clusters**
American Physical Society March Meeting · March 2014

6 **Computational Analysis of Electrocardiograms**
American Physical Society March Meeting · March 2013

CONFERENCES ATTENDED

- **American Physical Society March Meeting** · March 2016
- **Supercomputing** · November 2014
- **American Physical Society March Meeting** · March 2014
- **American Physical Society March Meeting** · March 2013

LEADERSHIP & ENGAGEMENT

- **MTU Graduate Student Government: Department Representative** · 2014-2015
- **Friends of the Van Pelt Library Board Member** · 2016-2017
- **Reviewer for MTU Summer Undergraduate Research Fellowship** · 2016-2017
- **MTU Graduate Student Government: Friends of the Van Pelt Library Liaison** · 2014-2016
- **MTU Graduate Student Government: IT Governance Group Representative** · 2015
- **MTU Summer Graduate School Softball Team Manager** · 2014-Present
- **ISU Society of Physics Students President** · 2012-2013
- **ISU Phi Gamma Delta Academic Chair** · 2012-2013
- **ISU Residential Life Academic Peer Advocate** · 2012-2013

SKILLS

PROGRAMING LANGUAGES

- Python (5+ years)
- C/C++ (3 years)
- Fortran (2 year)
- Matlab/Octave (1 year)

ATOMIC SIMULATION SOFTWARE

- Vienna Ab-initio Simulation Package (VASP) (5 years)
- Gaussian09 (5 years)
- CP2K (1 year)
- NWChem (1 year)

OPERATING SYSTEMS

- Linux/Unix
- Mac OS
- Microsoft Windows

AWARDS

- **Department of Energy Science Graduate Fellowship** · 2017
- **John Miles Physics End Fellowship** · 2017
- **Traditions of Giving Fellowship** · 2013
- **Physics Outstanding Graduating Senior** · 2013
- **Outstanding Physics Teaching Assistant** · 2013
- **John McCarthy Outstanding Junior Award** · 2012
- **Boy Scouts of America Eagle Scout** · 2007