
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

- Investigated 2D polymer properties for mechanical properties using state-of-the-art electronic structure software on high performance computing platform.
- Developed and utilized frameworks and libraries in python to perform high-throughput simulations and analysis.
- Worked in a interdisciplinary collaboration of experimental and theoretical chemists, engineers and physicists to address the 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 initio 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 **Stability and Electronic properties of of Gold Quantum Dots on Boron Nitride Nanotubes**

Kevin Waters, Shiva Bhandari, Yoke Khin Yap, Ravindra Pandey

In Preparation

2 **Multiscale Modeling of PEEK using Reactive Molecular Dynamics Modeling and Micromechanics**

William A. Pisani , Matthew S. Radue , Sorayot Chinkanjanarot, Brett A. Bednarczyk, Evan J. Pineda, Kevin Waters, Ravindra Pandey, Julia A. King, Gregory M. Odegard

In Preparation

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, 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 BN₂ 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 Au₈ and Au₂₀**

Marwa H. Abdalmonem, 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)
- 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