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# Kevin Waters

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## EDUCATION

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### PHD. PHYSICS

August 2013 - Present

*Michigan Technological University (MTU)*

Advisor : Ravindra Pandey

Expected Graduation Date : August 2018

### BACHELOR OF SCIENCE

August 2009 - May 2013

*Indiana State University (ISU)*

Major: Physics

Minors: German, Mathematics

Cum Laude

## RESEARCH EXPERIENCE

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### MICHIGAN TECHNOLOGICAL UNIVERSITY, *Graduate Researcher*

June 2013 - Present

- 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 novel 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 novel long-ranged exchange operators 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.

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## RESEARCH EXPERIENCE (CONT.)

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### 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

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## TEACHING & MENTORING EXPERIENCE

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### 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.

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## TEACHING & MENTORING EXPERIENCE (CONT.)

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### 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

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### 1 **Stability of 3D and 2D Au Clusters on Boron Nitride**

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

### 2 **Absorption and Fluorescence Properties of Eight C4 Substituted 7-Aminocoumarins**

Shraddha Singh, Vaho Begoyan, Marina Tanasova, Kevin Waters, Max Seel, Ravindra Pandey  
Journal of Computational Chemistry, Under Review

### 3 **Dynamics of Self-Assembled Cytosine Nucleobases on Graphene**

Nabanita Saikia, Floyd Johnson, Kevin Waters, Ravindra Pandey  
Nanotechnology, Accepted

### 4 **Stability, elastic and electronic properties of a novel BN<sub>2</sub> sheet with extended hexagons with N-N bonds**

Kevin Waters, Ravindra Pandey  
Journal of Physics: Condensed Matter, Accepted

### 5 **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

### 6 **Amino-Acid-Conjugated Gold Clusters: Interaction of Alanine and Tryptophan with Au<sub>8</sub> and Au<sub>20</sub>**

Marwa H. Abdalmonem, Kevin Waters, Nabanita Saikia, and Ravindra Pandey  
J. Phys. Chem. C, vol. 121 pp. 25585–25593, 2017

### 7 **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

### 8 **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

### 9 **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

### 10 **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

### 11 **Building the Next Pyramid**

Joseph West, Greg Gallagher, Kevin Waters, Stephen Ward, Tia Ward  
arXiv:1502.07319

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## PRESENTATIONS & TALKS

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- 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  $\text{MgV}_2\text{O}_4$  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

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## CONFERENCES ATTENDED

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

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## LEADERSHIP & ENGAGEMENT

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- **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

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## SKILLS & INTERESTS

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### PROGRAMING LANGUAGES

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

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## 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

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- **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