## **Kevin Waters**

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## **EDUCATION**

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

#### 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 implemented 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 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 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

#### f 6 Amino-Acid-Conjugated Gold Clusters: Interaction of Alanine and Tryptophan with ${f Au}_8$ and ${f Au}_{20}$

Marwa H. Abdalmoneam, 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

## **PRESENTATIONS & TALKS**

#### Stability and Electronic Properties of Amine Functionalized Boron Nitride

1 Nanostructures

Graduate Research Colloquium (MTU) · February 2017

2 Amino Acids Interaction with Boron Nitride Nanomaterials

American Physical Society March Meeting · March 2016

First Principles Study of Boron Nitride Nanomaterials & Amino Acid

3 Molecules

Physics Graduate Colloquium (MTU) · Feb 2016

Ab Initio Study of the Structural and Electronic Properties of MgV<sub>2</sub>O<sub>4</sub> in its

4 Cubic Phase

Graduate Research Colloquium (MTU) · February 2015

A Theoretical Study of Structural and Electronic Properties of Alkaline-Earth

5 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 & INTERESTS**

#### **PROGRAMING LANGUAGES**

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

#### **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