

Tanmoy Pal

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EDUCATION

Boston University

PhD Candidate in Computational Chemistry

Boston, MA

Spring 2018 –

University of Wisconsin-Madison

Master of Science in Chemistry

Madison, WI

Fall 2016 – Fall 2017

Indian Institute of Science

Bachelor of Science (Research)

Bengaluru, India

Fall 2012 – Spring 2016

Major: Chemistry | Special focus: Computational Chemistry

Thesis: Ab-initio Molecular Dynamics Studies of Carborane Clusters

PUBLICATIONS

1. Qiang Cui, Tanmoy Pal, and Luke Xie. “Biomolecular QM/MM Simulations: What Are Some of the “Burning Issues”?” In: *The Journal of Physical Chemistry B* 125.3 (2021). PMID: 33401903, pp. 689–702. DOI: [10.1021/acs.jpcb.0c09898](https://doi.org/10.1021/acs.jpcb.0c09898)
2. Interfacial Polarization and Ionic Structure at the Ionic Liquid-Metal Interface Studied by Vibrational Spectroscopy and Molecular Dynamics Simulations, *Matthew J. Voegtle, Tanmoy Pal, Anuj K. Pennathur, Sevan Menachekanian, Joel G. Patrow, Sohini Sarkar, Qiang Cui, and Jahan M. Dawlaty*, J. Phys. Chem. A, Submitted

RESEARCH

- Boston University | University of Wisconsin-Madison Spring 2017 –
Advisor: Prof. Qiang Cui
 - QM/MM Simulations of Mechanism of Proton Transfer in Cytochrome c Oxidase
 - Study of Two-body and Three-body Energies of Water using Semi-empirical Models, Calculation of Second Virial Coefficients of Small Molecules
 - Multidimensional DFTB3 Free Energy Calculations using Reinforcement Learning
 - Interfacial Polarization and Ionic Structure at the Ionic Liquid-Metal Interface Studied by Vibrational Spectroscopy and Molecular Dynamics Simulations
 - Machine Learning Assisted High-accuracy Multidimensional Free Energy Surfaces
- Indian Institute of Science, Bengaluru
 - Ab-initio Molecular Dynamics (CPMD) and Ab-initio Computational Modelling of Carboranes
Advisor: Prof. E D Jemmis Summer 2015 - Spring 2016
 - Generating Formula for Condensed Polyhedral Boranes and its Computer Implementation
Advisor: Prof. E D Jemmis Summer 2014
 - Generation of Promoter:Reporter Constructs to Study Cytokinin Distribution Profile in Rice (*Oryza sativa*)
Advisor: Prof. Usha Vijayraghavan Summer 2013
- Indian Institute of Science Education and Research, Kolkata
 - Quantum Harmonic Oscillator: A Special Case of Quasi-exactly Solvable Equations
Prof. Prasanta K Panigrahi Summer 2012

TEACHING

- [BU] Mathematical Methods for Molecular Sciences CH 225 Fall 2020
- [BU] Mathematical Methods for Molecular Sciences CH 225 (Grader) Spring 2020
- [BU] General Chemistry for Engineering Sciences CH 131 Fall 2019
- [BU] General Chemistry CH 102 Spring 2019
- [UWMadison] General Chemistry Chem 104 Spring 2017
- [UWMadison] General Chemistry Chem 103 Fall 2016

TECHNICAL EXPERIENCE

- Programming Languages
 - Python, Linux shell, L^AT_EX, C/C++, Javascript, OpenMP, MPI, OpenACC, CUDA, Wolfram Language, MySQL
 - Python Packages: TensorFlow/Keras, Bokeh, Matplotlib, NumPy, SciPy, Pandas, cuDF, Requests
- [HackerRank](#)
- Computational Chemistry Software
 - CHARMM, Gaussian, CPMD, CP2K, Quantum Espresso, GROMACS, ASE, SchNetPack, DeePMD
- Art and Design
 - Adobe Photoshop, Illustrator, InDesign, Muse, Edge Animate, Premiere Pro
 - Procreate [Procreate Portfolio](#)

RELEVANT COURSEWORKS AND WORKSHOPS

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|---|-------------|
| • Telluride School on Theoretical Chemistry at Telluride Science Research Center, Telluride, CO
Project: <i>Programming Davidson's Diagonalization Method</i> | Summer 2017 |
| • [BU] Machine Learning by Prof. Kate Saenko
Project: <i>Classification of Bacteriophage Genome with Harvard Innovation Lab's XGENOMES</i> | Fall 2018 |
| • [UWMadison] High Performance Computing for Engineering Applications by Prof. Dan Negrut
Project: <i>Parallel Implementation of Davidson's Diagonalization Method: Comparison of Performance Between Eigen C++, OpenMP, NumPy, and cuSolver</i> | Fall 2017 |
| • [UWMadison] Molecular Dynamics and Monte Carlo Simulations in Materials Science | Spring 2017 |
| • [BU] Advanced Molecular Quantum Mechanics by Prof. David Coker | Spring 2018 |
| • [UWMadison] Special Topics in Physical Chemistry by Prof. Qiang Cui | Spring 2017 |
| • [IISc] Computational Modeling of Materials | Spring 2014 |
| • [IISc] Organic Electronics | Spring 2015 |
| • [IISc] Introduction to Electronics and Electrical Engineering | Spring 2013 |
| • [IISc] Algorithms and Programming | Fall 2012 |

CERTIFICATIONS

- DeepLearning.AI TensorFlow Developer Certification
 - [Introduction to TensorFlow for Artificial Intelligence, Machine Learning, and Deep Learning](#)
- IBM Data Science Professional Certificate
 - [Machine Learning with Python](#)
 - [Data Science Methodology](#)
 - [Data Science Orientation](#)
 - [Data Visualization with Python](#)
 - [Open Source Tools for Data Science](#)
 - [Python for Applied Data Science](#)

HONORS AND AWARDS

- Delegate at 22nd Session of Youth Assembly (formerly Youth Assembly at the United Nations)
- Hirschfelder Prize Graduate Fellowship at Theoretical Chemistry Institute, Department of Chemistry, University of Wisconsin-Madison (2016)
- Nominated by Ministry of Human Resource Development, India for Commonwealth Scholarship for PhD in the United Kingdom (2015)
- National Initiative on Undergraduate Science (NIUS) Chemistry fellow (batch IX 2012-14)
- KVPY National Fellowship (India) (2011)