Tanmoy Pal

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Education

Boston University — Boston, MA
PhD Candidate in Computational Chemistry — Spring 2018 –

University of Wisconsin-Madison — Madison, WI
Master of Science in Chemistry — Fall 2016 – Fall 2017

Indian Institute of Science — Bengaluru, India
Bachelor of Science (Research) — Fall 2012 – Spring 2016
Major: Chemistry | Special focus: Computational Chemistry
Thesis: Ab-intio 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
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. B, Accepted

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 Leaning 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, LaTeX, 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

Relevent Courseworks and Workshops

- Telluride School on Theoretical Chemistry at Telluride Science Research Center, Telluride, CO — Summer 2017
  Project: *Programming Davidson's Diagonalization Method*
- [*BU*] Machine Learning by Prof. Kate Saenko — Fall 2018
  Project: *Classification of Bacteriophage Genome with Harvard Innovation Lab's XGENOMES*
- [*UWMadison*] High Performance Computing for Engineering Applications by Prof. Dan Negrut — Fall 2017
  Project: *Parallel Implementation of Davidson's Diagonalization Method:*
  Comparison of Performance Between Eigen C++, OpenMP, NumPy, and cuSolver
- [*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 22^{nd} 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)