Maitrayee Ghosh

Postdoctoral Scholar
Stanford University and SLAC National Accelerator Laboratory
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Education

Doctor of Philosophy (PhD) 09/2017 – 12/2023
Frank J. Horton Fellow
Chemistry (Physical Chemistry)
University of Rochester, NY

Master of Science (MS) 09/2017 - 05/2019
Sherman Clarke Fellow
Chemistry
University of Rochester, NY

Master of Science (MSc) 07/2014 – 05/2016
DST INSPIRE Scholar
Chemistry (Theoretical Chemistry)
Indian Institute of Technology (IIT) Bhubaneswar, India

Bachelor of Science (BSc) 07/2011 – 06/2014
First Class Honours, DST INSPIRE Scholar
Chemistry
University of Calcutta, India

Research / Work Experience

01/2024 - Present

Stanford University and SLAC National Accelerator Laboratory
Postdoctoral Scholar

First author works on:

- **Fusion Energy research:** Computational study on the behavior of foams at extreme conditions. We are implementing a mixture of traditional Kohn-Sham DFT-MD and orbital-free DFT to study these foam materials at extreme temperatures in the order of tens of electron volts.
- **Nickel at Martian and Venus cores:** Using on-the-fly machine-learning based DFT-MD simulations, we have estimated the phase diagram of nickel at low pressures and high temperatures. We are also working to incorporate the defects, mechanical stability and transport properties.

PI: **Prof. Siegfried Glenzer and Dr. Arianna E. Gleason-Holbrook**

05/2018 - 12/2023

Laboratory for Laser Energetics (LLE),
University of Rochester
Graduate Research Assistant - Horton Fellow

PhD Thesis: **Intriguing Chemistry of Planetary Materials Under Extreme Conditions**. As a doctoral student, I was involved in studying the chemical behaviors of materials at extreme conditions, relevant to planetary interiors, primarily using **density functional theory molecular dynamics** simulations (DFT-MD).
First author projects worked on:

- **Cooperative diffusion in bcc iron in Earth and super-Earths' inner core conditions:** We clarified the mechanism of diffusion which occurs along energetically favorable direction, its relationship to bcc iron stability, calculated from both mechanical stability criteria and dynamical stability, and correlation with seismological observations like attenuation and P-wave velocity. Performed DFT-MD simulations, calculated equation of state data, phonon spectra (both harmonic and at finite temperature), elastic constants, direction-dependent sound velocities.
- **Near-melting behaviors of aluminum oxide in multi-megabar pressures:** We observed diffusion of oxygen atoms near melting, defined the melt curve till 1000 GPa pressures, and calculated electrical and thermal conductivity, and optical properties near melting.
- **Diamond formation from hydrocarbon mixtures in conditions relevant to ice giant interior conditions:** using a reverse strategy method, we mixed the stable phases of diamond and hydrogen and evolved the mixed system over time using DFT-MD to observe if diamond survives in the thermodynamic conditions investigated. The interface of diamond and hydrogen was modelled by calculating adsorption energies at high pressure, and thermodynamic integration has been used to calculate the free energy of hydrocarbon mixture.

Collaborative works:

- **Development of first principles equation of state in CHON resin:** Being a part of a large collaboration of computational researchers, my job was to perform first-principles simulations along different isochores at low temperatures, and also perform orbital-free DFT MD calculations at higher temperatures (over 1 million K temperatures).
- **Surface chemistry calculations for $MAPbBr_3$ single crystal:** Our experimental collaborators found that oxygen degraded the $MAPbBr_3$ crystal by adsorption on its surface. I performed density of states calculations using Quantum Espresso with oxygen molecule adsorbed on different possible sites on the $MAPbBr_3$ surface.

Other skills developed: crystal structure search, orbital-free DFT, surface chemistry calculations.
Research advisors: **Dr. Shuai Zhang** and **Dr. S.X. Hu**,
Thesis advisor: **Prof. David McCamant**

07/2016 - 08/2017

Indian Association for the Cultivation of Science
Project Junior Research Fellow (Intern)

I studied the pseudo Jahn-Teller effect in two dimensional materials: silicene, germanene, and stanene using the orbital vibronic coupling density theory. Experience working with Gaussian. Published an article in Bulletin of Materials Science. Advisor: **Prof. Ayan Datta**

07/2015 - 05/2016

Indian Institute of Technology (IIT) Bhubaneswar
Masters' Student

My Masters' dissertation "Understanding Electronic Transitions Using Semiclassical Dynamics" involved studying the modification of surface-hopping method, that is used to study non-adiabatic effects on electronic transitions, using a decoherence method. Incorporation of decoherence significantly improved results over the original surface-hopping algorithm. Advisor: **Prof. Kousik Samanta**

Research Interests

Computational modeling of materials at extreme conditions pertaining to:

- Planetary Interiors
- Fusion Energy Research (Inertial Fusion Energy)
- Astrochemistry
- Superconductivity

The toolbox for these simulations involve:

- Molecular dynamics based on:
  - Density-functional theory
  - Classical Mechanics
  - on-the-fly machine-learning
- Quantum Chemistry methods
- Deep learning
- Crystal Structure Search Algorithms

Publications

First-author works:

- M. Ghosh*, A. Gleason-Holbrook, S. Glenzer, "Ab initio coupled with on-the-fly machine learning molecular dynamics unravels high pressure melt curve of nickel at Mars core conditions" *(manuscript under preparation)*
- M. Ghosh*, A. White, A. Gleason-Holbrook, S. Glenzer, "Equation-of-state and transport properties of foam materials at extreme temperatures" *(manuscript under preparation)*
- M. Ghosh, S. X. Hu, E. Blackman, S. Zhang*, "Melting and transport properties of Al_2O_3 at extreme conditions", Phys. Rev. B, **110**, 174107 (2024); DOI: 10.1103/PhysRevB.110.174107; Link to article
- M. Ghosh, S. Zhang, S. X. Hu*, "Direct observation of diamond co-existence with hydrocarbons using large-scale density-functional theory simulations in ice giant interior conditions". *(Under Review)*
- M. Ghosh, S. Zhang*, L. Hu, S.X. Hu, "Cooperative diffusion in body-centered iron in Earth and super-Earths' inner core conditions", J. Phys.: Condens. Matter, **35**, 154002 (2023) ; DOI:10.1088/1361-648X/acba71; Link to article
- M. Ghosh and A. Datta*, "Pseudo Jahn-Teller Effect in silicene, germanene and stanene: a crystal orbital density coupling analysis", Bulletin of Materials Science, **41**(5), 117 (2018).Link to article

Co-authored works:

- M. E. Signor, D.A. Chin, D.T. Bishel, R. Paul, E.A. Smith, M. Ghosh, D.N. Polsin, A. Coleman, F. Coppari, Y. Ping, S. Hu, M. Harmand, J.R. Rygg, G.W. Collins*, "Measuring the melt curve of FeO". *(manuscript under preparation)*
- S. Zhang, A. Panjwani, P. Xiao, M. Ghosh, T. Ogitsu, Y. Ping, S. X. Hu, "Thermal Induced Structural Competitiveness and Metastability of Body-centered Cubic Iron under Non-Equilibrium Conditions", arXiv:2501.00524. Link to article
- D. A. Chin, P. M. Nilson, J. J. Ruby, G. Bunker, M. Ghosh, M.E. Signor, D. T. Bishel, E. A. Smith, F. Coppari, Y. Ping, J. R. Rygg, G. W. Collins, "Parametrized ion-distribution model for extended x-ray absorption fine-structure analysis at high-energy-density conditions", Phys. Plasmas **31**, 042708 (2024). Link to article
- K. Wang, B. Wacker, M. Ghosh, V. V. Karaseiv, S.X. Hu, J. Huang, Y. Gao*, "Light-enhanced Oxygen degradation of MAPbBr3 Single Crystal", Phys. Chem. Chem. Phys, **26**, 5027-5037(2024). Link to article
- S. X. Hu*, L. Ceurvorst, J. L. Peebles, A. Mao, P. Li, Y. Lu, A. Shvydky, V. N. Goncharov, R. Epstein, K. Nichols, R. M. N. Goshadze, M. Ghosh, J. Hinz, V. V. Karasiev, S. Zhang, N. R. Shaffer, D. I. Mihaylov, J. Cappelletti, D. R. Harding, C. K. Li, E. M. Campbell, R. C. Shah, T. J. B. Collins, S. P. Regan, and C. Deeney, "Laser-Direct-Drive Fusion Target Design with a High-Z Gradient-Density Pusher Shell", Phys. Rev. E, **108**(3), 035209, 2023. Link to article
- S. Zhang*, V. V. Karasiev, N. Shaffer, D. I. Mihaylov, K. Nichols, R. Paul, R.M.N. Goshadze, M. Ghosh, J. Hinz, R. Epstein, S. Goedecker, and S. X. Hu, "A first-principles equation of state of CHON resin for inertial confinement fusion applications", Phys. Rev. E, **106** (4), 045207 (2022). Link to article
- S. Zhang* and M. Ghosh, "BCC Iron Cannot Be Refuted at Earth and Super-Earth's Inner-Core Conditions," eLetter [to R. G. Kraus et al., Science 375, 202 (2022)] (16 February 2022).Link to eComment

Presentations

Invited:

2024 (Oral)

CMAP Seminar Series
Extreme condition behavior of Al_2O_3: from its melting to metallization

Contributed:

2024 (Poster)

American Geophysical Union (AGU) Fall Meeting
Machine-Learning based Study of the Melting of Nickel in Small Terrestrial Planet Core Conditions

2024 (Poster)

NERSC 50th Annual Meeting
Nickel and Foams in Extreme Conditions – Perspectives from Density-Functional Theory and Machine-learning

2023 (Poster)

CMAP Meeting
BCC iron and its exotic behavior at planetary pressure conditions

2022 (Oral)

AGU Fall Meeting
Near-melting Behaviors of Alumina Under Multi-Megabar Pressures – an ab initio study

2022 (Oral)

2022 International Union of Crystallography Meeting
Elucidation of the mechanism of cooperative diffusion in bcc iron in Earth and super-Earths' inner core conditions

2022 (Oral)

American Physical Society (APS) March Meeting
Ab Initio Investigation of the Cooperative Diffusion in Body-Centered Cubic Iron Under Inner Core Conditions of Earth and Super-Earth Exoplanets

2021 (Online Poster)

AGU Fall Meeting
Mechanism of Cooperative Diffusion in BCC Iron under Earth and Super-Earths Inner Core Conditions

2020 (Poster)

60^{th} Sanibel Symposium
Nanodiamond Formation from Hydrocarbon Mixture Under Extreme Pressure-Temperature Conditions - Evidence from First Principles; *Award received* - **IBM Zerner Graduate Student Award: 500 USD**

2019 (Oral)

21st Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter
Diamond Formation from Hydrocarbons in Planetary Conditions: An ab initio Study

Awards

IBM-Zerner Graduate Student Award 2020
60^{th} Sanibel Symposium - University of Florida

Frank J. Horton Graduate Research Fellowship 2018-2023
Laboratory for Laser Energetics
University of Rochester

Sherman Clarke Fellowship 2017
Department of Chemistry, University of Rochester

INSPIRE Higher Education Scholarship 2011-2014
Department of Science and Technology, India

Research Grants and Resources

- Allocation of Computational Resources at High performance Computing facilities
  - **NERSC AY 2025 DOE Mission Science Allocation Award** for the proposal titled *Machine-learning based theoretical investigations of nickel and its mixtures at in terrestrial planetary core conditions.* Principal Investigator (PI): M. Ghosh.
    Award: 19,930 CPU node hours, 4000 GPU node hours
  - **NERSC AY 2025 DOE Mission Science Allocation Award** for the proposal titled *Equation-of-state and conductivity calculations of foams using density-functional theory and machine-learning in inertial fusion energy relevant conditions.* PI: M. Ghosh.
    Award: 20,000 CPU node hours, 5000 GPU node hours

Teaching and Mentoring

Pedagogical Training

Upcoming - 05/2025

SLAC National Accelerator Laboratory
DOE SULI Mentor

Preparations on effective mentoring of the SULI interns through communication, feedback and learning goals

01/2024 - present

Stanford University

- Attended Teaching Commons 2025 Conference at Stanford University
- CIRTL: Stanford Chapter: Teaching Certificate (in progress)
  - IDEAL Pedagogy course offered by Stanford University
  - Pedagogy journal club including leading a session on how to effectively use **Perussal** to better account for pre-readings assigned to students
  - 2024 GradCDI: Course Design Institute: designed syllabus for a graduate level course: "High Energy Density Science"
  - 2024 First Year Faculty Training Certificate Course (offered by **University of Florida**)
  - STEM Course Design: Designed course materials for an undergraduate level course: Introduction to Physical Chemistry
- Mentoring Certificate Tier 1: Stanford University
  - Five hours of training involving understanding different communication styles, giving feedback under stressful situations, understanding different identities of students/mentees.
- Mentoring Certificate Tier 2: Stanford University (in progress)
- Stanford Postdoc Teaching Certificate (in progress)

Mentoring Experience

Upcoming - 06/2025 - 08/2025

SLAC National Accelerator Laboratory
DOE SULI Mentor

Mentee - Carly Chandler

2019 - 2023

Laboratory for Laser Energetics, University of Rochester
Mentor

Teaching undergraduate and high school summer interns the fundamentals of theoretical tools used in our groups' research and high-performance computing.

Teaching Experience

09/2017 - 05/2019

Department of Chemistry, University of Rochester
Graduate Teaching Assistant

Teaching the fundamentals of general chemistry to undergraduate students prior to them performing experiments, and helping the solve relevant chemical problems during office hours. Graded the undergraduate students' lab reports and their examination papers, as required.
Instructor: **Prof. John Olsen**

Outreach

Graduate Students' Association, University of Rochester
Travel Grants' Reviewer

Reviewed several applications for travel grants given to graduate students for their preferred conferences.

Laboratory for Laser Energetics
Efforts in Diversity, Equity and Inclusion (DEI)

Served as the Students' representative in the DEI council to foster connections with DEI groups from other institutions. Also, serving as a member of the planning committee in representing women group (WiSE-LLE) at LLE in improving the website, celebrating Women's History Month by featuring prominent woman scientists in LLE-wide flyers and hosting events for women in science at LLE to create a safe space and foster connections.

03/2022

University of Rochester
Service to professional community

1. **Session chair** at the APS March Meeting 2022 for the session: "Electrons, Phonons, Electron-Phonon Scattering- III", 2. **Reviewer**: jointly reviewed manuscripts with research advisor submitted to journals like Physical Review B

09/2019-12/2019

University of Rochester
Service to the greater University of Rochester community

Served as the graduate students' representative in the Course Evaluation Subcommittee to help make better use of the course evaluation data collected every year. Important recommendation accepted by the committee: request for informal mid-semester evaluation to improve the classes for the current students.

01/2019

University of Rochester
Service to community at large

Volunteered to demonstrate interesting chemistry experiments to high school students to garner their interests in Chemistry. (Teaching Advisor: Prof. John C. Olsen)

References

Dr. Shuai Zhang

Position Staff Scientist
Employer Laboratory for Laser Energetics

University of Rochester
Email szha@lle.rochester.edu

Dr. Arianna E. Gleason-Holbrook

Position Staff Scientist and Deputy Director of HEDS Division @ SLAC
Relationship Postdoctoral Advisor
Employer SLAC National Accelerator Laboratory
Stanford University
Email ariannag@stanford.edu

Prof. Siegfried Glenzer

Position Professor of Photon Science and Director of HEDS Division @ SLAC
Relationship Postdoctoral Advisor and Faculty Sponsor
Employer SLAC National Accelerator Laboratory
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