

# Curriculum Vitae

## Maitrayee Ghosh

PhD Candidate  
Department of Chemistry &  
Laboratory for Laser Energetics  
University of Rochester  
Rochester, NY, USA

+1 (585) 451-7373  
mghosh2@ur.rochester.edu  
mg126066@gmail.com  
<https://www.linkedin.com/in/maitrayee-ghosh>  
Google scholar profile

### OBJECTIVE

Application for post-doctoral position with research interests in computational modeling of materials with research interests in materials science and astrochemistry.

### RESEARCH EXPERIENCE

MAY 2018 - PRESENT

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

As a doctoral student, I am 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.
- **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. (Work in progress and in collaboration with experimentalists at LLE, URochester)
- **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 AIMD 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. (Work in progress)

Co-author works include contribution in developing equation-of-state for CHON resin.

**Other skills developed:** crystal structure search, orbital-free DFT.

Research advisors: **Dr. Shuai Zhang** and **Dr. S.X. Hu**,

Thesis advisor: **Prof. David McCamant**

### EDUCATION

- 2017 – PRESENT **Doctor of Philosophy Candidate**  
Chemistry (Physical Chemistry)  
*University of Rochester*
- 2019 **Master of Science**  
Chemistry  
*University of Rochester*
- 2014 – 2016 **Master of Science**  
Chemistry  
*Indian Institute of Technology Bhubaneswar*
- 2011 – 2014 **Bachelor of Science**  
FIRST CLASS HONOURS  
Chemistry  
*University of Calcutta*

### AWARDS

- 2020 **IBM-Zerner Graduate Student Award**  
*60<sup>th</sup> Sanibel Symposium - University of Florida*
- 2018 **Frank J. Horton Graduate Research Fellowship**  
*Laboratory for Laser Energetics*  
*University of Rochester*
- 2017 **Sherman Clarke Fellowship**  
*Department of Chemistry, University of Rochester*
- 2011 **INSPIRE Higher Education Scholarship**  
*Department of Science and Technology, India*

### PUBLICATIONS

- 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](#)
- 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](#)

JULY 2016 - DEC 2016

Indian Association for the Cultivation of Science

### **Intern**

I studied the pseudo Jahn-Teller effect in molecules using computational approaches. PI: **Prof. Ayan Datta**

DEC 2016 - AUG 2017

Indian Association for the Cultivation of Science

### **Junior Research Fellow**

I studied the pseudo Jahn-Teller effect in two dimensional materials: silicene, germanene, and stanene using the orbital vibronic coupling density theory. PI: **Prof. Ayan Datta**

JULY 2015 - MAY 2016

Indian Institute of Technology (IIT) Bhubaneswar

### **Masters' Student**

My Masters' dissertation 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. Thesis: "**Understanding Electronic Transitions Using Semi-classical Dynamics**". PI: **Prof. Kousik Samanta**

DEC 2014 - JAN 2015

Indian Association for Cultivation of Science

### **Intern**

In this winter internship, I went through the basics of electronic structure theory, which formed the basis of later research. PI: **Prof. Debashis Mukherjee**

## TEACHING EXPERIENCE

AUG 2017 - MAY 2019

Department of Chemistry, University of Rochester

### **Graduate Teaching Assistant**

Teaching the fundamentals of general chemistry experiments to undergraduate students and helping them solve relevant chemical problems. Graded the undergraduate students' lab reports and their examination papers, as required.

PI: **Prof. John Olsen**

MAY 2019 - PRESENT

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.

## OUTREACH

University of Rochester Residential Life

### **Graduate Community Assistant**

Served in building the graduate student community by hosting educational, community engagement, arts & culture & diversity events, managing conflicts, and enforcing university policies.

Graduate Students' Association, University of Rochester

### **Travel Grants' Reviewer**

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

CV: [Maitrayee Ghosh](#)

• 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](#)

• 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](#)

• K. Wang, B. Wacker, M. Ghosh, V. V. Karaseiv, S.X. Hu, J. Huang, Y. Gao\*, "Light-enhanced Oxygen degradation of MAPbBr<sub>3</sub> Single Crystal", (*to be submitted*)

• D.A. Chin, P.M. Nilson, J.J. Ruby, M. Signor, G. Bunker, D.T. Bishel, E.A. Smith, M. Ghosh, F. Coppari, Y. Ping, J.R. Rygg and G.W. Collins, "Extended x-ray absorption fine structure cumulant expansion at high-energy-density conditions", (*to be submitted*)

• M. Ghosh, S. X. Hu, T.-A. Suer, S. Zhang\*, "Melting and transport properties of alumina under multi-megabar pressures". (*under preparation*)

• M. Ghosh, S. Zhang, S. X. Hu\*, "Diamond formation from hydrocarbon mixtures in planetary interior conditions". (*under preparation*)

## SELECTED PRESENTATIONS

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)

### 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<sup>th</sup> Sanibel Symposium

Nanodiamond Formation from Hydrocarbon Mixture Under Extreme Pressure-Temperature Conditions - Evidence from First Principles; *Award received* - **IBM Zerner Graduate Student Award**

2019 (ORAL)

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.

### ***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

University of Rochester

### ***Service to the greater university 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.

### ***Service to community at large***

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

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

## COMPUTER SKILLS

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BEGINNER	Quantum Espresso Machine-learning techniques in VASP
INTERMEDIATE	Matlab, FORTRAN 90, L <sup>A</sup> T <sub>E</sub> X Python, USPEX
EXPERT	VASP, Gaussian, VESTA, OVITO

## PROFESSIONAL SOCIETIES

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Graduate student member of:  
*American Geophysical Union (AGU)*,  
*American Physical Society (APS)*

## REFERENCES

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### **Dr. Shuai Zhang**

POSITION	Staff Scientist
EMPLOYER	Laboratory for Laser Energetics <i>University of Rochester</i>
EMAIL	szha@lle.rochester.edu

### **Dr. S. X. Hu**

POSITION	Senior Scientist (Group Leader)
EMPLOYER	Laboratory for Laser Energetics <i>University of Rochester</i>
EMAIL	shu@lle.rochester.edu

### **Prof. David McCamant**

POSITION	Associate Professor
EMPLOYER	Department of Chemistry <i>University of Rochester</i>
EMAIL	david.mccamant@rochester.edu