

Rajendra Maharjan

COMPUTATIONAL CHEMISTRY · VISITING ASSISTANT PROFESSOR

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Summary

I am currently a Visiting Assistant Professor at Grinnell College. I am teaching Physical Chemistry and General Chemistry. I received PhD in Computational Chemistry from the Department of Chemistry at Oklahoma State University in the Fall of 2023. My research is focused on the molecular level organization of water in pure water and in presence of hydrophobic particle. Additionally, I also investigate to study the dipole moment distribution of water in condensed phase with response to different environmental factors.

Education

Oklahoma State University

PHD CANDIDATE IN COMPUTATIONAL CHEMISTRY

Stillwater, Oklahoma

Aug, 2017 - Dec, 2023

- Project 1: 'Assessing Order in Liquid, Supercooled, and Crystalline Water'
- Project 2: 'Estimation of Dipole Moment Distribution of Water in Condensed Phase'
- Project 3: 'Crystal Seed Assisted Homogeneous Ice Nucleation'
- Project 4: 'Water Ordering in Response to the Solvated Hydrophobic Particle'

Tribhuvan University

MASTER OF SCIENCE (M.Sc.) IN PHYSICAL CHEMISTRY

Kathmandu, Nepal

May, 2014

- Thesis: 'Preparation and Characterization of Solid-State Electrochemical Sensor for the Determination of Ni(II)'

Tri-Chandra Multiple Campus

BACHELOR OF SCIENCE (B.Sc.) IN CHEMISTRY AND MICROBIOLOGY

Kathmandu, Nepal

March, 2010

Research Experience

Oklahoma State University

GRADUATE TEACHING/RESEARCH ASSISTANT

Stillwater, OK

Aug, 2017 - Dec, 2023

Advisor: Christopher J. Fennell, PhD

Project 1: Assessing Order in Liquid, Supercooled, and Crystalline Water

- Developed an algorithm (nucleation_tracker written in both C++ and Python) to study network topology analysis and water structural ordering using an order parameter.
- Monitor closed rings distribution in liquid and supercooled water using different empirical potential water models at different temperatures.
- Studied intrinsic hydrogen bonded polygons in different known ice polymorphs and render the Pov-Ray image unique to each ice polymorphs.
- Studied tetrahedral order parameter for water ordering in liquid, supercooled liquid, and ice.

Project 2: Estimation of Dipole Moment Distribution of Water in Condensed Phase

- Determine the dipole moment distribution of water in liquid and ice using quantum approach (QM) and ab-initio molecular dynamics (AIMD).
- Studied the polarization effect from the environment on enhancing the dipole moment of gas phase water in condensed system.
- Developed an algorithm based on tabulated quantum calculation to determine the dipole moment of water at different temperatures that is comparable to pure QM calculations.
- Employed ice Ih and ice VII as a toy model to study moment distribution dependent on density, quality of hydrogen bonds, and hydrogen bond distance.

Project 3: Crystal Seed Assisted Homogeneous Ice Nucleation

- Stochastic growth of ice using crystal seed and direct coexistence method from pure water.
- Network topology analysis and water structural ordering during molecular dynamics (MD) simulation.
- Study of crystal defects during ice formation.

Project 4: Water Ordering in Response to the Solvated Hydrophobic Particle

- Studied how the hydrophobic particle enhance the water ordering using 'nucleation_tracker' program
- Carefully monitor the constructive interference behavior of two hydrophobic particles on water ordering.
- Studied chaotropic effect of ions on water ordering.

Advisor: Amar Prasad Yadav, PhD

Project: Preparation and Characterization of Solid-State Electrochemical Sensor for the Determination of Ni(II)

- Development of electrochemical sensor and improve its detection limit.
- Used alkaline medium to prepare the nano-disc sensor and tested its performance in different solutions.
- Used potentiometer to monitor the response of the sensor to the solution.

Teaching Experience

Grinnell College

VISITING ASSISTANT PROFESSOR

Teaching Physical Chemistry (Chm 363) and General Chemistry (Chm 129) with labs

Grinnell, IA

Aug. 2024 - Dec. 2025

Oklahoma State University

TEACHING ASSISTANT

Labs: Chem 1314 and Chem 1515

Lecture Class: Physical Chemistry-1

- Conducted laboratory experiments
- Provided grades and comments on student's assignments, lab reports and exams.
- Held office hours to review material and answer students' questions.

Stillwater, OK

Aug. 2017 - Dec. 2021

Higher Secondary School and Colleges

LECTURER, CHEMISTRY

- Jaya Multiple Campus, Gokarneshwor, Kathmandu, Nepal. (Duration: April, 2014 - April, 2016)
- Janasewa Higher Secondary School, Kirtipur, Kathmandu, Nepal. (Duration: June 2016 - June, 2017)
- Classic Academy Higher Secondary School, Chabahil, Kathmandu, Nepal. (Part time)
- Jubilant College and Research Center, Kalimati, Kathmandu, Nepal. (Part time)
- Shankarapur Hospital and Academy, (CTEVT program) Jorpati, Kathmandu, Nepal (Part time)

Kathmandu, Nepal

Jan. 2014 - Jun. 2017

Professional Experience

TechnoMark Solutions Pvt. Ltd.

RESEARCH AND DEVELOPMENT CHEMIST

- Conducted the project on 'Chlor-alkali PEM fuel cell'
- Prepared and fabricated a fuel-cell model and tested its efficiency and durability in alkaline medium.

Kapan, Kathmandu, Nepal

Feb, 2012 - Dec, 2012

Skills

- **Programming Skills:** Python Programming for numerical calculations, Basic C++ programming, Basic Matlab programming, R-programming, Linux/Unix Programming
- **Software Carpentry Certified Instructor:** Instructor and helper for software carpentry workshops for 'Unix Shell', 'Python Programming', and 'Version Control'
- Statistical data analysis and data visualization in Python, R, and Advanced MS Excel
- **Molecular Dynamics Simulation:** Used GROMACS and OpenMD packages for MD simulations
- **Quantum Mechanics:** Used 'Gaussian/g16' and NWChem for pure QM calculations and 'CP2K' for ab-initio molecular dynamics (AIMD)
- **Computational tools:** Used Chimera, Jmol, and Avogadro for molecule visualization and modeling, Inkscape for creating vector images, XM-Grace, Packmol
- Typesetting/ Document Preparation/Referencing: LaTeX, MS Office, EndNote
- **Others:** GNU Image Manipulation Program (GIMP) and Adobe photoshop for image processing, Version Control: Git, GitHub

Seminar

Chem-6011: Hidden Structures and the Dipole Moment Distribution in Liquid Water and Ice. Department of Chemistry Seminar, May 23, 2023.

Chem-5011: Potentiometric Sensor Development for quantification of Cd(II) and other Heavy Metal Ions. Department of Chemistry Seminar, March 26, 2019.

Publication and Manuscripts

Maharjan R, Williamson C, and Fennell C. Assessing Order in Liquid, Supercooled, and Crystalline Water. ChemRxiv. 2025; doi:10.26434/chemrxiv-2025-7pc7f.

Rajendra Maharjan and Christopher J. Fennell. Dipole Moment Distribution Analysis in Liquid Water and Ice. Manuscript in Preparation.

Rajendra Maharjan, Sarah Foy, Ibrahim Asad, and Christopher J. Fennell. Seeding Ice Crystallization in Molecular Simulations. Manuscript in Preparation.

Maharjan, R.; Nakarmi, K. B.; and Yadav, A. P. Preparation and Characterization of Solid-State Electrochemical Sensor for the Determination of Ni(II). *J. Nepal Chem. Soc.* **2016**, 35, 104–112. <https://doi.org/10.5281/zenodo.15787601>.

Conference Presentations

Sarah Foy, **Rajendra Maharjan**, and Christopher J. Fennell. Ice Crystal Growth in Solutions. Annual Undergraduate Research Symposium, Conoco-Phillips Alumni Center, Oklahoma State University, April, 2023. **Poster**

Rajendra Maharjan and Christopher J. Fennell. Dipole Moment Distribution Analysis in Liquid Water and Ice. ACS Southwest Regional Meeting (SWRM), Baton Rouge, LA, November, 2022. **Poster**

Rajendra Maharjan and Christopher J. Fennell. Order in Water and its Range in Hydrophobic Solvation. ACS Midwest Regional Meeting (MWRM), Springfield, MO, October, 2021. **Poster**

Rajendra Maharjan and Christopher J. Fennell. Algorithmic Investigation of Order in Liquid, Crystalline, and Supercooled Water. Molecular Modeling and Materials Design (M3D) Conference, Department of Chemical Engineering, Oklahoma State University, July, 2020. **Oral**

Rajendra Maharjan and Christopher J. Fennell. Identification and Quantification of Water Ordering in Liquid, Crystalline, and Supercooled Water. The 2019 Annual Southwest Theoretical and Computational Chemistry Meeting, Norman, OK, September, 2019. **Poster**

Rajendra Maharjan and Christopher J. Fennell. Mapping Order in Liquid and Crystalline Water. ACS Midwest Regional Meeting (MWRM), Wichita, Kansas, October, 2019. **Poster**

Rajendra Maharjan, Casey Williamson, and Christopher J. Fennell. Seeding Ice Crystallization in Molecular Simulations. Department of Chemistry, Oklahoma State University, May, 2019. **Poster**

Rajendra Maharjan, Casey Williamson, and Christopher J. Fennell. Seeding Ice Crystallization in Molecular Simulations. 64th Pentasectional Meeting of the Oklahoma Sections of the ACS (Norman, OK), February, 2019. **Poster**

Rajan Timilsina, Krishna Badan Nakarmi, **Rajendra Maharjan**, and Amar Prasad Yadav. Effect of Back Contact on the response of Ni(II) Ion-Selective Electrodes. NAST - Nepal Academy of Science and Technology (7th National Conference of Science and Technology), O-PY-1-821, 2016. **Oral**

Rajendra Maharjan, Amar P. Yadav. Preparation and Characterization of Solid-State Electrochemical Sensor for the Determination of Ni(II). Advanced Materials and Nanotechnology for Sustainable Development, Nepal Chemi-

Workshops Attended

i-CoMSE MD/MC Summer School, Oklahoma State University

HANDS ON FUNDAMENTAL CONCEPTS IN MOLECULAR DYNAMICS AND MONTE-CARLO SIMULATIONS

Stillwater, OK

Jul 2022

Telluride School on Theoretical Chemistry

SCHOOL ON MOLECULAR DYNAMICS, ELECT STRUCT, STAT MECH, AND BIO PHY

Virtual format

July 19-23, 2021

Awards & Scholarship

OKLAHOMA STATE UNIVERSITY

- 2023 **Graduate Abstract Writing - Honorable Mention**, Graduate College, OSU
2021 **Graduate Technical Abstract Writing - 2nd position**, Graduate College, OSU
2019 **Outstanding Poster Award - 2nd position**, Department of Chemistry, OSU

Stillwater, OK

Stillwater, OK

Stillwater, OK

TRIBHUVAN UNIVERSITY

- 2014 **University Grants Commission**, Department of Chemistry, TU
2012 **Academic Excellence Scholarship (Partial Tuition Waiver) for the M.Sc Chemistry**, Department of Chemistry, TU
2010 **Academic Excellence Scholarship (Partial Tuition Waiver) for the M.Sc Chemistry**, Department of Chemistry, TU

Kathmandu, Nepal

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References

Christopher J. Fennell, PhD

Associate Professor, Modeling and Computational Chemistry
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Frank D. Blum, PhD

Regents Professor, Polymer, Physical, Colloid, and Materials Chemistry
Department of Chemistry
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Jeffery L. White, PhD

Professor, Heterogeneous catalysis, Heterogeneous polymeric materials, Nuclear magnetic resonance spectroscopy, diffusometry
Department of Chemical Engineering
Oklahoma State University, Stillwater 74075
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Elaine Marzluff, PhD

Professor, Protein structure and dynamics in solution and gas phase
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