Rajendra **Maharjan**

Computational Chemistry · Graduate Research/Teaching Assistant

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Summary

PhD Candidate and Graduate Research/Teaching Assistant at 'Department of Chemistry', Oklahoma State University

Education

Oklahoma State University — *Stillwater, Oklahoma*

PhD Candidate in Computational Chemistry — *2017 - Present*

- Project 1: 'Crystal Seed Assisted Homogeneous Ice Nucleation'
- Project 2: 'Water Order Matrics in liquid, supercooled liquid, and Ice'
- Project 3: 'Estimation of dipole moment of water in condensed phase'
- Project 4: 'Water Ordering due to Hydrophobic Effect of Solvated Hydrophobe'

Tribhuvan University — *Kathmandu, Nepal*

Master of Science (M.Sc.) in Physical Chemistry — *May, 2014*

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

Tri-Chandra Multiple Campus — *Kathmandu, Nepal*

Bachelor of Science (B.Sc.) in Chemistry and Microbiology — *March, 2010*

Research Experience

Oklahoma State University — *Stillwater, OK*

Graduate Teaching/Research Assistant — *Aug. 2017 - Present*

Advisor: Christopher J. Fennell, PhD

Project 1: 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 2: Water Order Matrics in liquid, supercooled liquid, and Ice

- 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 3: Water Ordering due to Hydrophobic Effect of Solvated Hydrophobe

- 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.

Project 4: Estimation of dipole moment 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.

Tribhuvan University *Kathmandu, Nepal*

Graduate Student *Jan. 2011 - Jul. 2014*

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

Oklahoma State University *Stillwater, OK*

Teaching Assistant *Aug. 2017 - Dec. 2021*

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.

Higher Secondary School and Colleges *Kathmandu, Nepal*

Lecturer, Chemistry *Jan. 2014 - Jun. 2017*

- Manakamana Higher Secondary School, Jorpati, 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)

Professional Experience

TechnoMark Solutions Pvt. Ltd. *Kapan, Kathmandu, Nepal*

Research and Development Chemist *Feb. 2012 - Dec. 2012*

- 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.

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, XMGrace, Packmol
- Typesetting/ Document Preparation/Referencing: LaTeX, MS Office, EndNote
- **Others:** GNU Image Manipulation Program (GIMP) and Adobe photoshop for image processing

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.

Manuscripts for Publications

Rajendra Maharjan, Casey Williamson, and Christopher J. Fennell. Assessing Order in Liquid, Supercooled, and Crystalline Water. Ready to Publish.

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.

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 Chemical Society and Tribhuvan University, Kathmandu, Nepal, November, 2014. **Oral**

Workshops Attended

i-CoMSE MD/MC Summer School, Oklahoma State University — *Stillwater, OK*

Hands on Fundamental Concepts in Molecular Dynamics and Monte-Carlo Simulations — *Jul 2022*

Telluride School on Theoretical Chemistry — *Virtual format*

School on Molecular Dynamics, Elect struct, Stat Mech, and Bio Phy — *JUly 19-23, 2021*

Awards & Scholarship

Oklahoma State University

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

Tribhuvan University

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

Referees

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