Ommair Ishaque

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Personal Profile

Ph.D. physicist specializing in first-principles–driven modeling of liquid water and related molecular systems. I design and fit explicit two-body, three-body, and polarization terms to high-level *ab initio* (e.g., CCSD(T), SAPT, DFT) data and develop high-performance MD workflows in Fortran/Python/C++. My simulation stack spans rigid models (quaternion rigid-body integrators, Ewald electrostatics, induction; NVE/NVT/NPT) and flexible water potentials with path-integral MD (i-Pi) to capture nuclear quantum effects. These capabilities support prediction of thermodynamic, structural, and transport properties from ambient to supercooled regimes and generalize to biomolecular force-field parameterization and simulations (e.g., solvent models, protein–ligand and ion–solvent interactions, interfacial behavior). Beyond water, I have contributed to crystal-structure prediction (CCDC BT7). An experienced instructor and collaborator, I communicate complex theory clearly and translate rigorous computation into practical insight for academic and industrial R&D.

Education

Ph.D. **University of Delaware**, Physics — Dec 2025 (expected)
- **Thesis**: Explaining Anomalous behavior of Water from first-principle-based quantum simulations

M.S. **University of Delaware**, Physics — Sept. 2015 - Dec 2018
- **non-Thesis**

M.Phil. **University of Karachi**, Physics — Sept. 2012 - Dec 2014
- **Thesis**: Inflation in the Era of Precision Cosmology

M.Sc. **University of Karachi**, Physics — Jan. 2005 - Dec 2006
- I interned at Karachi Institute of Power Engineering and learned the interactive, scriptable Physics Analysis Workstation (PAW) for HEP data analysis and graphical presentation.
- **Project**: Data analysis of electric power situation in Pakistan

B.Sc.(H) **University of Karachi**, Physics — Jan. 2003 - Dec 2005

Research Experience

First-principles–based water force fields & MD (rigid body) — Newark, DE, USA
University Of Delaware, Ph.D. Research — Sept 2018 - Dec 2025
- Developed and validated a rigid-monomer water model from CCSD(T)/SAPT data; refit the 3B term and quantified the range of exchange with switching sensitivity.
- Reproduced key anomalies and equation-of-state behavior from ambient to supercooled conditions with size/timestep convergence.
- Benchmarked RDFs, and diffusion data; demonstrated transferability across ensembles/pressures and released reproducible protocols.

Path-integral MD (i-Pi) with flexible water potentials — Newark, DE, USA
University Of Delaware, Ph.D. Research — Jan 2022 - Dec 2025
- Implemented fully flexible, first-principles water potentials (explicit 2B/3B + induction) in i-Pi to include nuclear quantum effects.
- Computed RDFs, diffusion, and related observables; assessed impacts of flexibility and quantum effects on liquid properties.

Force-field development & Crystal Structure Prediction (CSP) Newark, DE, USA
University Of Delaware, Ph.D. Research; CCDC BT7 collaboration Sept 2020 - Dec 2024

- Derived intermonomer force fields using SAPT; refitted flexible terms for an agrochemical (System XXXI).
- Ran UPACK-based CSP (generation $\rightarrow$ ranking) and MD-assisted minimization; contributed to BT7 "generation" and "ranking" publications.

Alchemical solvation (BAR) in TIP4P water Newark, DE, USA
University Of Delaware, CHEM 874 course Sept - Dec 2017

- Computed solvation free energies of methane/argon in water using GROMACS and the Bennett Acceptance Ratio (BAR) method.

Teaching Experience

University Of Delaware, Graduate Teaching Assistant (DPA & ISLL) Newark, DE, USA
Sept 2015 - May 2025

- Led a team of TAs; organized review sessions for PBL/EBL formats; managed grading and course logistics.
- Taught/assisted: Circuit Theory and Problems (Phys245), Introductory Physics I/II (Phys201/Phys202), Fundamentals of Physics I/II (Phys207/Phys208), Physical Science & Astronomy.
- Facilitated small-group problem solving with emphasis on physical reasoning and quantitative modeling.

University Of Karachi, Lecturer (Department of Physics) Karachi, Pakistan
Nov 2009 - May 2015

- Lectured junior/senior undergraduate courses: Mechanics, Thermodynamics, Waves & Oscillations, Mathematical Physics I/II, Relativity & Cosmology, Introductory Quantum.
- Designed lab materials and assessments; coordinated senior-lab operations; helped organize conferences/workshops.

Skills

Programming Languages: C++, C, Fortran, Python

Softwares: MATHEMATICA, MATLAB

Libraries and Tools: Sklearn, Pandas, Numpy, Git, LaTEX, Origin, Microsoft Office, Visual Studio Code

Quantum Chemistry Tools: VASP, Quantum Espresso, ORCA, Avogadro, MERCURY, UPACK, AUTOPES

Molecular Dynamics simulation Tools: DLPOLY, LAMMPS, Gromacs, I-Pi, Home Grown MD package

Publications

Dust-acoustic solitary waves in plasmas with nonthermal–nonextensive electrons and Boltzmannian ions. Sept. 2025

A. A. Abid, K. Qamer, N. Ahmad, M. S. Hussain, M. N. S. Qureshi, S. Ali,
Ommair Ishaque, Xiaojie Li, Guang-Rui Yao, Yan-Fang Ji

J. Korean Phys. Soc., https://doi.org/10.1007/s40042-025-01499-z

Magnetospheric multiscale observations of electromagnetic ion cyclotron waves associated with cold ion heating in the Earth's magnetosphere July. 2025

AA Abid, K Qamar, Nisar Ahmad, A Waheed, MS Hussain, MNS Qureshi, Amin Esmaeili, BM Alotaibi,
Ommair Ishaque, Xiaojie Li, Guang-Rui Yao, Yan-Fang Ji.

AIP Advances, https://doi.org/10.1063/5.0287326

Molecular Dynamics Simulation Code for the Rigid CCPol23+ Water Model Using Quaternion-Based Rigid Body Dynamics Mar. 2025

Ommair Ishaque

Zenodo, https://doi.org/10.5281/zenodo.14968189

The Seventh Blind Test of Crystal Structure Prediction: Structure Generation Methods Dec. 2024

Hunnisett et al.

J. Acta Cryst. B80, https://doi.org/10.1107/S2052520624007492

The Seventh Blind Test of Crystal Structure Prediction: Structure ranking Methods Dec. 2024

Hunnisett et al.

J. Acta Cryst. B80, https://doi.org/10.1107/S2052520624008679

Crystal structure predictions for molecules with soft degrees of freedom using inter-monomer force fields derived from first principles Dec. 2024

R. Nikhar, R. Podeszwa, A. Rehman, O. Ishaque, A. Jing, J. Melkumov, K. Szalewicz et al.

Acta Crystallographica Section B, https://doi.org/10.1107/S2052520624010837

Quantum smearing in hybrid inflation with chaotic potentials Jan. 2016

Waqas Ahmed, Ommair Ishaque, Mansoor Ur Rehman

International Journal of Modern Physics D 25 (03), 1650035 https://doi.org/10.1142/S0218271816500358

Publications (In progress)

How long-range are three-body exchange interaction in liquid water?

O. Ishaque, K. Szalewicz.

in progress (complete)

How important is monomer flexibility for predictions of properties of liquid water?

O. Ishaque, K. Szalewicz

in progress (almost complete)

Effects of monomer flexibility and of nuclear quantum effects on properties of liquid water

O. Ishaque, K. Szalewicz

in progress

Open-Source Software

CCpol23+ Rigid-Water MD (Quaternion-Based Rigid Body Dynamics) Mar. 2025

Ommair Ishaque — Zenodo DOI: 10.5281/zenodo.14968189

- Fortran-based MD engine implementing quaternion rigid-body integration (NVE/NVT/NPT), Ewald electrostatics, polarization/induction, and explicit 2B/3B terms for water.
- Validated against high-level *ab initio* data (e.g., CCSD(T), SAPT); includes switching/smoothing for long-range 3B behavior and reproducible input decks.
- Parallel-ready and HPC-oriented; documented workflows for analysis and benchmarking; example cases cover ambient–supercooled regimes.

Professional Memberships

American Chemical Society (ACS) Member 2025 - present

Division of Physical Chemistry and Theoretical Chemistry, engaging in computational and molecular science research.

ACS Member Number – 32104424

Certifications and Workshops

Quantum-Mechanical, Data-Driven and Multi-Scale Simulations of Complex Systems (QDMS) at UC San Diego. Jul. 2025

- Hands-on experience in advancing computational science through high-performance quantum simulations, machine-learning-enhanced modeling, and multiscale techniques to solve complex problems in molecular and materials modeling(link)

Computational Biophysics Dec. 2024

- 62nd Hands-On Workshop on Computational Biophysics, presented by the NIH Center for Macromolecular Modeling and Visualization of the University of Illinois at Urbana-Champaign (link)

Udemy Sept. 2024

- The Complete Introduction to LAMMPS (link)

Schrodinger courses Jun. 2023

- Introduction to Molecular Modeling in Drug Discovery (link)

DeepLearning.AI Aug. 2023

- Supervised Machine Learning: Regression and Classification (link)

IBM Data Science Professional Certificate(link) Aug. 2023

- Python for Data Science Project(link)
- Data Science and Machine Learning Capstone Project(link)
- Machine Learning with Python: A Practical Introduction(link)
- Visualizing Data with Python(link)
- Analyzing Data with Python(link)
- Python Basics for Data Science(link)

Course work

Electromagnetic Theory I and II, Special topics in Physical Chemistry (Practical introduction to Molecular dynamics Simulations), Quantum Statistical Mechanics, Advanced Quantum Mechanics, Advanced treatment selected topics (Advanced Molecular Science)

Interests

Playing Cricket: I have been the playing Delaware Premier League (DPL), Delaware United Cricket League (DUCL) and Greater Cricket Cricket League (GDCL) for last 7 years.

Fittness: I enjoy going to the gym because it helps me stay fit and toned.