9314 Cherry Hill Road, College Park, MD, USA
+1 443-255-4012 | www.anmolecule.weebly.com
anmolecule@gmail.com

KUMAR, ANMOL

OBJECTIVE

As a skilled theoretical and computational chemist with expertise in quantum and empirical methods, computer programming, and machine learning, I am committed to advancing the field of chemistry, with a focus on solving structural biology and biochemical problems. I want to educate future scientists while making significant contributions to the body of knowledge in chemistry.

PROFESSIONAL ACHIEVEMENTS

IAS Summer Research Fellowship, IISER TVM, **2010**
CSIR-JRF Chemical Science (Dec-**2010**), All India **57th Rank**
GATE-2011 Chemistry, All India **48th Rank**
CSIR-SRF, Chemical Science, **2013**
Best Poster Presentation Award, **TCS**-2014, NCL-Pune, **2014**
Research Project, Hunan Normal University, China, funded by CGF Award, **2014**
MQM2016 conference, Sweden, funded by DST, **2016**

SKILLS

Strong hold on quantum chemistry, molecular dynamics, QM/MM.
Strong numerical analysis and algorithm development skills.
Proficient in Fortran, Python, C++, Shell script.
Proficient in parallel programming, HPC and version control.
Experience of handling and developing software packages like CHARMM.
Experience in machine learning techniques and deployment.
Strong teaching skills and ability to supervise a scientific idea.
Strong verbal and written communication skills.

EDUCATION

PH.D. IN THEORETICAL AND COMPUTATIONAL CHEMISTRY (2011-2017)
Molecular Electrostatic Potential Topology for Exploring Lone Pairs,
Lone Pair-Π Interactions and Atoms in Molecules
DEPARTMENT OF CHEMISTRY, INDIAN INSTITUTE OF TECHNOLOGY, KANPUR, UP
Thesis Supervisor: Prof. Shridhar R. Gadre and Prof. Nisanth N. Nair

M. SC. IN CHEMISTRY (2009-2011)
SCHOOL OF CHEMISTRY, UNIVERSITY OF HYDERABAD, ANDHRA PRADESH, INDIA
CGPA (7.83); Thesis Grade (A), Rank 3rd

B. SC. CHEMISTRY (Hons.) (2006-2009)
BANARAS HINDU UNIVERSITY, VARANASI, UTTAR PRADESH, INDIA
Grade: 1st Division (74%), Rank 2nd

TEACHING EXPERIENCE

TEACHING ASSISTANT FOR B. TECH. PROGRAM/INT. MS PROGRAM AT IIT KANPUR

Chemical Science, Jan–April (2015)

TEACHING ASSISTANT FOR B. TECH. PROGRAM AT IIT KANPUR

Basic Physical Chemistry, Jan–April (2014)

TEACHING ASSISTANT FOR B. TECH. PROGRAM AT IIT KANPUR

Basic Physical Chemistry, Jan–April (2013)

TEACHING GRADUATE PROGRAM AT SCHOOL OF PHARMACY, UMB, MD USA

Advanced Quantum Chemistry, Jan–April (2022)

WORK HISTORY

POSTDOCTORAL RESEARCH SCIENTIST AT UNIVERSITY OF MARYLAND

BALTIMORE, MARYLAND, USA (Aug 2017 – Aug 2022)

DEVELOPMENT OF FORCE FIELD AND QMMM MOLECULAR DYNAMICS METHODS

Under Supervision of: Professor Alexander D. MacKerell Jr.

POSTDOCTORAL FELLOW AT UNIVERSITY OF MARYLAND

BALTIMORE, MARYLAND, USA (Sep 2022 – OCT 2024)

DEVELOPMENT OF DRUDE POLARIZABLE FORCE FIELD AND SILCS-WATER

Under Supervision of: Professor Alexander D. MacKerell Jr.

RESEARCH ASSOCIATE FACULTY AT UNIVERSITY OF MARYLAND

BALTIMORE, MARYLAND, USA (NOV 2024 – ONGOING)

RESEARCH PROJECTS/ COLLABORATIONS

Drug Design Project on "Direct binding inhibitors of hypoxia-induced factor as an auxiliary cancer treatment" with **Prof. Gregg Semenza (2019 Nobel Prize in Physiology or Medicine**), John Hopkins University, Baltimore, MD, USA-2020.

Collaborative Project work on "Hybrid QTAIM and Electrostatic Potential-Based Quantum Topology Phase Diagrams for Water Clusters" with **Prof. Samantha Jenkins**, Hunan Normal University, Changsha, China-2014.

M. Sc. Project work "Preparation of Graphite Oxide/Sulfonated Polystyrene Nanocomposite" with **Prof. Tushar Jana**, University of Hyderabad-2011.

IAS summer intern project on "Strain effect and structural variation of aromatic rings on metallic substitution" with **Prof. E.D. Jemmis** at IISER Trivandrum-2010.

NOTEWORTHY WORKSHOPS/ CONFERENCES

Oral presentation at **'ACS Fall 2024 Elevating Chemistry",** Denver, CO, USA, 2024 and **"ACS Spring 2023 Crossroad of Chemistry'**, Indianapolis, IN, USA, 2023.

Poster presentation selected for SciMix at **'ACS Spring 2023 Crossroad of Chemistry'**, Indianapolis, IN, USA, 2023.

Oral presentation at **'Tinker Software Developer Workshop'**, NIH Bethesda, MD, USA, 2022.

Online poster presentation at **"The 2021 ISQBP President's Meeting"**, 2021.

Online poster presentation at **"ACS Spring 2020 National Meeting"**, 2020.

Oral presentation at **'CHARMM Mini Meeting'**, NIH Bethesda, MD, USA, 2020.

Poster presentation at **"Biophysical Society Meeting"**, Baltimore, MD, USA, 2019.

Oral presentation at **"XXVII IUPAP Conference on Computational Physics"**, IIT Guwahati, 2015.

Poster presentation at **"Theoretical Chemistry Symposium"**, NCL-Pune, 2014.

Poster presentation at **"International workshop on Theoretical and Computational Chemistry (TCC-III)"** Hunan Normal University, Changsha, China, 2014.

Poster presentation at **"National Symposium on Crystallography (NSC)"**, IISER Mohali, 2014.

Poster presentation at **"Dynamics of Complex Chemical and Biological Systems (DCCBS)"**, IIT Kanpur, 2014.

Poster presentation at **"Current Trends in Theoretical Chemistry (CTTC)"** BARC Mumbai, 2013.

SELECTED PUBLICATIONS

1. **Kumar A.**, Goel H., Yu W., Zhao M., MacKerell A.D., Modeling Ligand Binding Site Water Networks with Site-Identification by Ligand Competitive Saturation: Impact on Ligand Binding Orientations and Relative Binding Affinities, *J. Chem. Theory Comput.* **2024**, 20, 24, 11032–11048.
2. Nordquist E., Zhao M., **Kumar A.**, MacKerell A.D., Combined physics- and machine-learning-based method to identify druggable binding sites using SILCS-Hotspots, *J. Chem. Inf. Model.* **2024**, 64, 19, 7743–7757.
3. **Kumar A.**, MacKerell A.D., FFParam-v2.0: A Comprehensive Tool for CHARMM Additive and Drude Polarizable Force-Field Parameter Optimization and Validation, *J. Phys. Chem. B*, **2024**, 128, 18, 4385–4395.
4. Yu Y., Venable R., Thirman J., Chatterjee P., **Kumar A.**, Pastor R., Roux B., MacKerell A.D., Klauda J., Drude Polarizable Lipid Force Field with Explicit Treatment of Long-Range Dispersion: Parametrization and Validation for Saturated and Mono-unsaturated Zwitterionic Lipids, *J. Chem. Theory Comput.*, **2023,** 19, 9, 2590–2605.
5. **Kumar A.**, Pandey P., Chatterjee P., MacKerell, A.D., Deep Neural Network Model to Predict the Electrostatic Parameters in the Polarizable Classical Drude Oscillator Force Field, *J. Chem. Theory Comput.*, **2022**, 18, 3, 1711–1725.
6. Chatterjee P., Sengul, M., **Kumar A.**, MacKerell A.D., Harnessing Deep Learning for Optimization of Lennard-Jones Parameters for the Polarizable Classical Drude Oscillator Force Field, *J. Chem. Theory Comput.*, 2022, 18, 4, 2388–2407.
7. **Kumar A.**, Lopez R., Martinez F., Ramırez G., Ema I., Zorrilla D., Yeole S.D., Gadre S.R., DAMQT 3: Advanced suite for the analysis of molecular density and related properties in large systems. *Comput. Phys. Comm.*, **2022**, 279, 108460.
8. Croitoru A., Park S., **Kumar A.**, Lee J., Im W., MacKerell, A.D., Aleksandrov A., Additive CHARMM36 Force Field for Nonstandard Amino Acids, *J. Chem. Theory Comput.*, **2021**, 17, 6, 3554–3570.
9. **Kumar A.**, Yoluk O., MacKerell Jr A.D., FFParam: Standalone package for CHARMM additive and Drude polarizable force field parametrization of small molecules, *J. Comput. Chem.*, **2020**, 41 (9), 958-970.

10. López R., Rico J.F., Ramírez G., Ema I., Zorrilla D., **Kumar A.**, Yeole S.D., Gadre S.R., Topography of Molecular Electron density and electrostatic potential with DAMQT, *Comput. Phys. Comm.*, **2017**, 214, 207-215.
11. **Kumar A.**, Gadre S.R., Exploring the Gradient Paths and Zero Flux Surfaces of Molecular Electrostatic Potential, *J. Chem. Theory Comput.*, **2016**, 12, 1705–1713.
12. **Kumar A.**, Yeole S.D., Gadre S.R., López R., Rico J.F., Ramírez G., Ema I., Zorrilla D., DAMQT 2.1.0: A new version of the DAMQT package enabled with the topographical analysis of electron density and electrostatic potential in molecules, *J. Comput. Chem.*, **2015**, 36, 2350-2359.
13. **Kumar A.**, Gadre S.R., On the electrostatic nature of electrides, *Phys. Chem. Chem. Phys.*, **2015**, 17, 15030-15035.
14. **Kumar A.**, Gadre S.R., Chenxia X., Tianlv X., Kirk S.R., Jenkins S., Hybrid QTAIM and electrostatic potential-based quantum topology phase diagrams for water clusters, *Phys. Chem. Chem. Phys.*, **2015**, 17, 15258-15273.
15. **Kumar A.**, Gadre S.R., Mohan N., Suresh C.H., Lone Pairs: An Electrostatic Viewpoint, *J. Phys. Chem. A.*, **2014**, 118, 526-532.
16. Mohan N., Suresh C.H., **Kumar A.**, Gadre S.R., Molecular electrostatics for probing lone pair–π interactions, *Phys. Chem. Chem. Phys.*, **2013**, 15, 18401-18409.
17. Croitoru A., **Kumar A**., Lambry J-C., Lee J., Sharif S., Yu W., et al. Increasing the Accuracy and Robustness of the CHARMM General Force Field with an Expanded Training Set. ChemRxiv. **2025.**
18. Sharif S., **Kumar A.**, MacKerell A. D., Non-Covalent Molecular Interaction Rules to Define Internal Dimer Coordinates for Quantum Mechanical Potential Energy Scans. ChemRxiv. **2025**.
19. Shaima Salman S., Huang T. Y., Hwang Y., **Kumar A.**, et al., Targeted, dual destruction of HIF-1a and HIF-2a: a powerful anti-cancer strategy. Under Review, **2025**.

*One other manuscripts under review, two in preparation.

BOOK CHAPTER

Gadre S.R., **Kumar A.**, Understanding Lone Pair-π Interactions from Electrostatic Viewpoint. In: Scheiner S. (eds) Noncovalent Forces. Challenges and Advances in Computational Chemistry and Physics, **2015**, vol 19. Springer, Cham.

REVIEWED JOURNALS

J. Chem. Theory Comput. (3), J. Phys. Chem. (4), J. Comp. Chem. (3), J. Comp Aid. Mol. Desig. (1), J. Mol. Model (1), Front. Chem. (1), Molecules (8), Pharmaceutics (1), DDC (1)

OUTREACH ACTIVITIES

Delivered **webinar** highlighting the capabilities of the **SILCS-WATER** program, **2024.** https://youtu.be/wrTJOzMrH2w?si=aBGd0OBmMh6j_UTL

Teaching Assistant and **Core Member** in summer school: **"Advanced Molecular Dynamics"**, jointly organized by IISER Pune and Kathmandu University, **2021**.

Teaching Assistant and **Resource Person** in winter school on **"Electronic structure and molecular dynamic simulations using open source softwares: from theory to practice"**, organized by Kathmandu University, **2020**.

Organizer, Workshop **"FFParam: Simplifying Parametrization of force-field"**, at School of Pharmacy, University of Maryland, MD, USA, **2019**.

Public Relations Secretary in **Indian Association, UMB, 2018-2019**.

SOFTWARES/ PACKAGES

FFParam: Force-Field Parametrization Package with GUI. ***Copyright transferred to UMB.***

DAMQT: A GUI Assisted Package for The Analysis of Electron Density and Electrostatic Potential in Molecules with Plugin for The Fast Optimization of Non-Covalently Bonded Molecular Clusters.

pyDGenFF: Package for Generating Drude Force Field Parameters for Drug-Like Molecules

SILCS-WATER: SILCS Plugin for capturing water contributions in protein-ligand binding. ***Copyright transferred to UMB.***

CHARMM-PSI4: Interface for QM/MM Simulation

REFERENCES

Professor Alexander D. MacKerell Jr.
(Postdoc Supervisor)
School of Pharmacy, University of Maryland Baltimore
20 Penn Street Baltimore, MD 21201, USA
Phone no: +1 4107067441
Email: alex@outerbanks.umaryland.edu

Professor Nisanth N. Nair
(Thesis Supervisor)
Department of Chemistry,
Indian Institute of Technology Kanpur
Kanpur, 208016, India
Phone no. +91 5122596311
Email: nnair@iitk.ac.in

Emeritus Professor Shridhar R. Gadre
(Thesis Supervisor)
Department of Scientific Computing, Modeling & Simulation, Savitribai Phule Pune University, Pune 411007, India
Phone no. +91 9960624664
Email: gadresr007@gmail.com

Professor Rafael López
(Research Collaborator)
Department of Chemical Physics Applications,
Faculty of Science, Autonomous University of Madrid
28049 Madrid, Spain
Phone no: +34 914978642
Email: rafael.lopez@uam.es