305 West Fayette Street, Baltimore, MD, USA
+1 443-255-4012 | www.anmolecule.weebly.com
anmolecule@gmail.com

KUMAR, ANMOL

OBJECTIVE

Experienced computational chemist with strong hold on *ab initio* quantum chemical methods as well as molecular dynamics. Aim to develop improved *in silico* drug design using quantum mechanical and machine learning techniques. Seeking to utilize my working knowledge of chemistry and teaching skills as a faculty member in the field of Theoretical and Computational Chemistry.

PROFESSIONAL ACHIEVEMENTS

Selected for IAS Summer Research Fellowship, 2010
Secured 57th Rank in CSIR-JRF (Dec-2010)
Secured 48th Rank in GATE-2011
Senior Research Fellowship by CSIR, 2013
Best Poster Presentation Award at TCS-2014, NCL-Pune
One Month Project with 2013-Chinese Government Friendship Award, 2014

SKILLS

Excellent knowledge and understanding of quantum chemistry and molecular dynamics.
Strong numerical analysis and algorithm development skills.
Excellent programming skills in Fortran, Python, C++ and bash.
Proficient in parallel programming with OPENMPI and OPENACC.
Experience of handling and developing huge software packages like CHARMM.
Experience of GUI development and machine learning techniques.
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 SCIENTIST AT UNIVERSITY OF MARYLAND

BALTIMORE, MARYLAND, USA (2017 – ONGOING)

DEVELOPMENT OF FORCE FIELD AND QMMM MOLECULAR DYNAMICS METHODS

Under Supervision of: Professor Alexander D. MacKerell Jr.

RESEARCH PROJECTS/ COLLABORATIONS

Ongoing Project work on "Drug design to control the role of HIF protein in cancer" with Prof. Gregg Semenza (received 2019 Nobel Prize in Physiology or Medicine), John Hopkins University, Baltimore, MD, USA-2020.

Ongoing Project work on "Molecular level insights into FPOP method: A powerful structural proteomics tool" with Dr. Lisa Jones, University of Maryland, Baltimore, MD, USA-2021.

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.

WORKSHOPS/ CONFERENCES

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 (BPS)**", Baltimore, MD, USA, 2019.

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

Poster presentation at "**Theoretical Chemistry Symposium (TCS)**", 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.

PUBLICATIONS

1. **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.
2. 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**.
3. 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.
4. Srivastava P., Verma M., **Kumar A.**, Srivastava P., Mishra R. Sri S., Patra A.K., Luminescent Naphthalimide-Tagged Ruthenium(II)-Arene Complexes: Cellular Imaging, Photocytotoxicity and Transferrin Binding, *Dalton Trans.*, **2021**, 50, 3629-3640.
5. Diethelm-Varela B., **Kumar A.**, Lynch C., Imler G., Deschamps J., Xia M., MacKerell Jr. A.D., Xue F. Stereoisomerization of human constitutive androstane receptor agonist CITCO, *Tetrahedron*, **2021**, 79, 131886.
6. Nedyalkova M., Vasighi M., Sappati S., **Kumar A.**, Madurga S., Simeonov V., Inhibition Ability of Natural Compounds on Receptor-Binding Domain of SARS-CoV2: An In Silico Approach, *Pharmaceuticals*, **2021**, 14 (12), 1328.
7. **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.
8. Turchi M., Kognole A.A., **Kumar A.**, Cai Q., Lian G., MacKerell Jr A.D., Predicting Partition Coefficients of Neutral and Charged Solutes in the Mixed SLES–Fatty Acid Micellar System, *J. Phys. Chem. B*, **2020**, 124 (9), 1653-1664.
9. 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.
10. Gadre S.R., **Kumar A.**, Bonding and Reactivity Patterns from Electrostatic Landscapes of Molecules, *J. Chem. Sci.* **2016**, 128, 1519–1526.
11. **Kumar A.**, Gadre S.R., Molecular Electrostatic Potential based Atoms in Molecules: Shielding Effects and Reactivity Patterns, *Aust. J. Chem.*, **2016**, 69, 975-982.

12. **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.
13. **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.
14. **Kumar A.**, Gadre S.R., On the electrostatic nature of electrides, *Phys. Chem. Chem. Phys.*, **2015**, 17, 15030-15035.
15. **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.
16. **Kumar A.**, Gadre S.R., Mohan N., Suresh C.H., Lone Pairs: An Electrostatic Viewpoint, *J. Phys. Chem. A.*, **2014**, 118, 526-532.
17. Sarmah S., Guha A.K., Phukan A.K., **Kumar A.**, Gadre S.R., Stabilization of Si (0) and Ge (0) compounds by different silylenes and germylenes: a density functional and molecular electrostatic study, *Dalton Trans.*, **2013**, 42, 13200-13209.
18. 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.
19. 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.*, (Under Review.)
20. Goel H., **Kumar A.,** MacKerell, A.D., Accounting for Role of Water in Protein-Ligand Binding Free Energy Estimation using SILCS. (Manuscript under 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.

CONFERENCE ABSTRACTS

Kumar A., MacKerell A.D., Use of Cyano Probes in QM/MM Simulations to Study the Effect of Ion Concentration and Temperature of the Environment on a Uracil Nucleotide and DNA, Biophys. J. 116 (3), 357a, **2019**.

Kumar A., Simmonett A., MacKerell A.D., Introduction of Polarized Embedding QMMM Technique in CHARMM with PSI4, Biophys. J. 120 (3), 175a-176a, **2021**.

Goel H., **Kumar A.**, MacKerell A.D., Capturing Water Networks during Ligand Binding with the Site-Identification by Ligand Competitive Saturation-Monte Carlo Approach, Biophys. J. 120 (3), 265a **2021**.

REVIEWED JOURNALS

Living Journal of Computational Molecular Science

Electronics

International Journal of Environmental Research and Public Health

OUTREACH ACTIVITIES

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.

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

Mentored high-school summer science intern, Frank Horrigan from **Montgomery County Public School**, on his project on **computer-aided drug design**, 2020-2021.

Served as **public relations secretary in Indian Association, UMB**, 2018-2019.

SOFTWARES/ PACKAGES

FFParam: Force-Field Parametrization Package with GUI

CHARMM-PSI4: Interface for QMMM Simulation

DAMQT-2.0: A package for the analysis of electrostatic potential in molecules

DAMQT-3.2.0: A renewed package with advanced visualization and GUI assisted plugin for the fast optimization of non-covalently bonded molecular clusters.

REFERENCES

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

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

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

Professor E. D. Jemmis

IPC Department, Indian Institute Of Science
Bangalore 560 012, Karnataka, India
Phone No: +91 8022933347
Email: jemmis@gmail.com

Professor Anunay Samanta

School of Chemistry, University of Hyderabad
Hyderabad 500046, Telangana, India
Phone no: +91 4023134813
Email: anunay.samanta@gmail.com

Dr. P. Balanarayan

Chemical Sciences, IISER Mohali
Knowledge city, Sector 81, SAS Nagar, Manauli
Phone no: +91 1722293
Email: balanarayan@iisermohali.ac.in