Abhinaw Kumar

Department of Chemical Engineering, The University of Arkansas
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Google Scholar Metric (Dec 2025): Total citations: 305, h-index:10

EDUCATION

University of Utah **Department of Chemistry**
PhD in Computational Chemistry 2012–2018

- Dissertation: Self-Assembly of Mesophases and their Role in the Nucleation and Polymorph Selection of Zeolites
- Supervisor: Professor Valeria Molinero
- Areas of Study:
  - Thermodynamics of Self-Assembly of Nanoparticles, Phase Transition using LAMMPS
  - Nucleation of ordered Phases, Transition Path Sampling and Computer Simulation of Zeolite Formation

Indian Institute of Science Education and Research, Pune **Department of Chemistry**
BS/MS Dual Degree with Distinction in Chemistry 2007–2012

- Dissertation: Interaction of Polyethyleneimine with Membrane Bilayer at Different pH: a Molecular Dynamics Study
- Area of Study: Atomistic Simulations of Pore Formation in Polymer-Lipid Bilayer Systems using GROMACS

PROFESSIONAL EXPERIENCE

University of Arkansas at Fayetteville | Department of Chemical Engineering Fayetteville, AR
Postdoctoral Research Associate 2024–Present

- Machine Learning-Based Probabilistic Backmapping for Multiscale Modeling of Phenylalanine Dipeptide Assembly

Texas A&M University | Department of Chemical Engineering College Station, TX
Postdoctoral Research Associate 2023–2024

- Conducted advanced computer simulations focused on protein-DNA condensates to uncover mechanisms of chromatin compaction. Utilized HOOMD for simulation and Python for data analysis.
- Used coarse-grained HPS models to analyze thermodynamic stability and diffusion dynamics of protein and DNA.

University of Texas at Austin | Department of Chemistry Austin, TX
Postdoctoral Research Associate 2019–2023

- Developed computer simulations of intrinsically disordered proteins and liquid-liquid phase separation processes.
- Optimized force fields for Intrinsically disordered proteins, enhancing their structural characterization through SAXS profile.
- Investigated the phase behavior and structural dynamics of FUS protein, revealing insights into fibril formation and the impact of phosphorylation on intrinsically disordered proteins.
- Studied the fibril formation in FUS-LC, discovering distinct core morphologies and elucidating the sequence-dependent stability differences through computational simulations.

PUBLICATIONS (Sorted by Citation Count)

- C. K. Choudhury, **A. Kumar**, and S. Roy, "Characterization of Conformation and Interaction of Gene Delivery Vector Polyethylenimine with Phospholipid Bilayer at Different Protonation States" Biomacromolecules, 2013, 14 (10), 3759 – 3768 (**53 citations,** Based on my BS–MS thesis research)

- **A. Kumar** and V. Molinero, "Self-Assembly of Mesophases from Nanoparticles" J. Phys. Chem. Lett., 2017, 8 (20), 5053-5058, Featured in Most Read Physical Chemistry Articles of the Month in October 2017, (**49 citations, First author**)
- **A. Kumar** and V. Molinero, "Two-Step to One-Step Nucleation of a Zeolite Through a Metastable Gyroid Mesophase" J. Phys. Chem. Lett., 2018, 9 (19), 5692-5697 (**45 citations, First author**)
- **A. Kumar**, A. H. Nguyen, R. Okumu, T. D. Shepherd and V. Molinero, "Could Metastable Mesophases Play a Role in the Nucleation and Polymorph Selection of Zeolites?" J. Am. Chem. Soc., 2018, 140 (47), 16071-16086 (**41 citations, First author**)
- **A. Kumar** and V. Molinero, "Why is Gyroid More Difficult to Nucleate from Disordered Liquids than Lamellar and Hexagonal Mesophases?" J. Phys. Chem. B, 2018, 122 (17), 4758-4770 (**27 citations, First author**)
- **A. Kumar**, D. Chakraborty, M. L. Mugnai, J. E. Straub, D. Thirumalai, "Sequence determines the switch in the fibril forming region of FUS protein and its variants" J. Phys. Chem. Lett., 2021, 12 (37), 9026-9032 (**23 citations, First author**)
- M. L. Mugnai, D. Chakraborty, H. T. Nguyen, F. Maksudov, **A. Kumar**, W. Zeno, J. C. Stachowiak, J. E. Straub, D. Thirumalai, "Sizes, conformational fluctuations, and SAXS profiles for Intrinsically Disordered Proteins using SOP simulations and experiments." Protein Science 2025, e70067 (**17 citations**)
- A. Bertolazzo, **A. Kumar**, C. Chakravarty, and V. Molinero, "Water-like Anomalies and Phase Behavior of a Pair Potential that Stabilizes Diamond" J. Phys. Chem. B, 2015, 120 (8), 1649-1659 (**14 citations**)
- **A. Kumar**, M. Zare, V. Molinero, "Assembly of Zeolitic Crystals From a Model of Mesogenic Patchy Nanoparticles" J. Phys. Chem. C, 2019, 123 (1), 971-978 (**11 citations, First author**)
- M. Marriott, L. Lupi, **A. Kumar**, V. Molinero, "Following the Nucleation Pathway from Liquid to Gyroid" J. Chem. Phys., 2020, 150 (16), 164902 (**8 citations**)
- D. Thirumalai, **A. Kumar**, D. Chakraborty, J. E. Straub, M. L. Mugnai, "Conformational fluctuations and phases in Fused in Sarcoma" Biopolymers 2024, e23558 (**4 citations**)

PEER REVIEW AND JUDGING SERVICE

- Peer reviewer for 17 scientific manuscripts (19 total reviews) for international journals including Molecular Simulation, Frontiers in Soft Matter, Polymers, International Journal of Molecular Sciences, Molecules, Biophysica, Crystals, and Pharmaceuticals.
- Judge, Texas Junior Science and Humanities Symposium (TJSHS): evaluated original student research projects in chemistry and related physical sciences, selecting awardees based on scientific rigor, originality, and technical merit.

POSTER PRESENTATIONS

- "Clathrates, Zeolites and Liquid-Crystals in Binary Solutions of Water and Simple Isotropic Solutes", **A. Kumar**, A. Nguyen, R. Okumu, T. Shepherd, and V. Molinero; Gordon Research Conference on Chemistry and Physics of Liquids, Plymouth, NH, Aug 2013
- "Tuning the Dimensionality of Water and Solute Networks in Binary Solutions of Water and Simple Isotropic Solutes", **A. Kumar**, A. Nguyen, and V. Molinero, American Conference of Theoretical Chemistry, Telluride, CO, July 2014.
- "Liquid Crystals from Spherical Particles", **A. Kumar** and V. Molinero, 90th ACS Colloid & Surface Science Symposium, Harvard University, Cambridge, MA, June 2016
- "Sequence determine the switch in the fibril forming regions of FUS protein" **A. Kumar**, D. Chakraborty, M. L. Mugnai and D. Thirumalai, Protein Folding Consortium Workshop, June 2021

TALKS

- "Liquid Crystals from Spherical Particles", **A. Kumar** and V. Molinero, Gordon Research Seminar: Chemistry & Physics of Liquids, Plymouth, NH, Aug 2015
- "Could the monomer dynamics predict the aggregation propensity of FUS protein", **A. Kumar**, D. Chakraborty, and D. Thirumalai, Protein Folding Consortium Workshop, St. Louis University, June 2019

- "Sequence Determines the Switch in the Fibril forming Regions in FUS Protein", **A. Kumar**, D. Chakraborty, M. L. Mugnai and D. Thirumalai, 6th Midwest Single Molecule Protein Workshop, Omaha, NE, Aug 2022
- Self-assembly of mesophases and their role in nucleation and polymorph selection of zeolite, **A. Kumar**, Department Seminar, Indian Institute of Technology, Bombay, India, Oct 2022
- "Early Stages of FUS protein aggregation", **A. Kumar** and D. Thirumalai American Physical Society Meeting, Las Vegas, NV, Mar 2023
- "HP1-DNA condensate dynamics: Insight into chromatin compaction mechanism", **A. Kumar**, DS Devarajan, TM Phan, J. Mittal, Biophysical Society Meeting, Philadelphia, Feb 2024
- "Machine Learning-Based Probabilistic Backmapping for Multiscale Modeling of Phenylalanine Dipeptide Assembly", **A. Kumar**, S. Paschall, and J. Monroe, American Institute of Chemical Engineers Annual Meeting, Boston, Nov 2025

ACADEMIC HONORS AND AWARDS

- Graduate Student Travel Award to Attend the Gordon Research Conference on Chemistry and physics of Liquids, 2015.
- Graduate Student Travel Award to Attend the American Conference on Theoretical Chemistry, 2014.
- INSPIRE DST Fellowship (Department of Science and Technology, India) 2008-2012. It is given to Top 1% student in India to pursue Science as Career.
- UKIERI (UK India Research Initiative) Fellowship to Conduct Summer Project at the University of Surrey, UK, 2011. It was awarded to only one student in chemistry department from my Institute.
- Summer Research Fellowship from DAAD (Deutscher Akademischer Austausch Dienst/ German Academic Exchange Service), 2010. This award was given to a total of 25 Students in Science Discipline from India to work in Germany in that year.
- Academic Excellence Award in the Undergraduate Program, 2010. It was awarded for achieving a perfect GPA of 10.0 in that semester.

UNDERGRADUATE PROJETS AND INTERNSHIPS

- "Hartree–Fock Theory to Calculate Electronic Properties of Small Molecules" under Prof. Sourav Pal (National chemical laboratory, Pune), 2008
- "Monte Carlo Simulations to Calculate Gas Adsorption in Metal-Organic Frameworks" under Prof. Sudip Roy (National Chemical Laboratory, Pune), 2009
- "Comparing the Structure of Nanoclusters" under Prof. Michael Springborg (Saarland University, Saarbruecken, Germany), 2010
- "Electronic Circular Dichroism Spectra Study of Neuropeptides: A TD-DFT Study" under Prof. Brendan Howlin (University of Surrey, Guildford, UK), 2011

PROFESSIONAL REFERENCES

Prof. Valeria Molinero
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Email: valeria.molinero@utah.edu

Prof. Dave Thirumalai
Department of Chemistry
The University of Texas at Austin
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The University of Arkansas
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Prof. Michael Gruenwald
Department of Chemistry
The University of Utah
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