ABHINAW KUMAR Curriculum Vitae

CONTACT INFORMATION

Texas A&M University
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EDUCATION

University of Utah Department of Chemistry
Ph.D. Degree *Aug 2012 – Aug 2018*

- Supervisor: **Professor Valeria Molinero**
- Dissertation: **"Self-Assembly of Mesophases and their Role in the Nucleation and Polymorph Selection of Model Zeolites"**
- Area of Study:
  - Thermodynamics of Self-Assembly of Nanoparticles, Phase Transition
  - Nucleation of Order from Disordered Phases, Transition Path Sampling
  - Computer Simulation of Zeolite Formation

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

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

EMPLOYMENT

Texas A&M University Department of Chemical Engineering
Postdoctoral Research Associate *May 2023 – Current*

- Area of Study:
  - Computer simulation of protein-DNA condensates

University of Texas at Austin Department of Chemistry
Postdoctoral Research Associate *Mar 2019 – April 2023*

- Area of Study:
  - Computer simulation of Intrinsically disordered proteins, Liquid-liquid phase separation of proteins

PUBLICATIONS

1. D. Thirumalai, **A. Kumar,** D. Chakraborty, J. E. Straub, M. L. Mugnai, "Conformational fluctuations and phases in Fused in Sarcoma" *Biopolymers* 2023, e23558

2. **A. Kumar**, D. Chakraborty, M. L. Mugnai, J. E. Straub, D. Thirumalai, "Sequence determine the switch in the fibril forming region of FUS protein and its variants" ***J. Phys. Chem. Lett.,*** 2021, 12 (37), 9026-9032

3. M. Marriott, L. Lupi, **A. Kumar**, V. Molinero, "Following the Nucleation Pathway from Liquid to Gyroid" ***J. Chem. Phys.,*** 2020, 150 (16), 164902

4. **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

5. **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

6. **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

7. **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

8. **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
   http://axial.acs.org/2017/11/20/physical-october-2017/

9. 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

10. 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

11. M. L. Mugnai, D. Chakraborty, **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"

12. **A. Kumar,** D. Thirumalai "Early stages of FUS protein aggregation"

TALKS AND POSTER PRESENTATIONS

1. "Clathrates, Zeolites and Liquid-Crystals in Binary Solutions of Water and Simple Isotropic Solutes" (poster) **A. Kumar**, A. Nguyen, R. Okumu, T. Shepherd, and V. Molinero; Gordon Research Conference on Chemistry and Physics of Liquids, Plymouth, NH, Aug 2013

2. "Tuning the Dimensionality of Water and Solute Networks in Binary Solutions of Water and Simple Isotropic Solutes" (poster) **A. Kumar**, A. Nguyen, and V. Molinero, American Conference of Theoretical Chemistry, Telluride, CO, July 2014.

3. "Liquid Crystals from Spherical Particles" (oral), **A. Kumar** and V. Molinero, Gordon Research Seminar: Chemistry & Physics of Liquids, Plymouth, NH, Aug 2015

4. "Liquid Crystals from Spherical Particles" (poster), **A. Kumar** and V. Molinero, 90th ACS Colloid & Surface Science Symposium, Harvard University, Cambridge, MA, June 2016

5. "Could the monomer dynamics predict the aggregation propensity of FUS protein" (oral), **A. Kumar,** D. Chakraborty, and D. Thirumalai, Protein Folding Consortium Workshop, St. Louis University, June 2019

6. "Sequence determine the switch in the fibril forming regions of FUS protein" (poster) **A. Kumar**, D. Chakraborty, M. L. Mugnai and D. Thirumalai, Protein Folding Consortium Workshop, June 2021

7. "Sequence Determines the Switch in the Fibril forming Regions in FUS Protein" (oral) **A. Kumar,** D. Chakraborty, M. L. Mugnai and D. Thirumalai, 6th Midwest Single Molecule Protein Workshop, Omaha, NE, Aug 2022

8. "Early Stages of FUS protein aggregation" (oral) **A. Kumar** and D. Thirumalai American Physical Society Meeting, Las Vegas, NV, Mar 2023

UNDERGRADUATE PROJECTS 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

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COMPUTATIONAL SKILLS

- Programming Languages: FORTRAN, PYTHON, MPI, OpenMP, CUDA, and MATLAB

- Softwares: LAMMPS, GROMACS, AMBER, HOOMD, GAUSSIAN, and TOWHEE

- Molecular Dynamics, Monte-Carlo, and Brownian Dynamics

- Classical Nucleation Theory, Nonclassical Nucleation, and Phase Diagram

- Transition Path Sampling, Maximum Likelihood Optimization, and Order Parameters

- Coursera courses on Machine learning and Deep learning Specialization

ACADEMIC HONORS AND AWARDS

- Academic Excellence Award in the Undergraduate Program, 2010.

- Summer Research Fellowship from DAAD (Deutscher Akademischer Austausch Dienst/ German Academic Exchange Service), 2010.

- UKIERI (UK India Research Initiative) Fellowship to Conduct Summer Project at the University of Surrey, UK, 2011.

- INSPIRE DST Fellowship (Department of Science and Technology, India) 2008-2012.

- Graduate Student Travel Award to Attend the American Conference on Theoretical Chemistry, 2014.

- Graduate Student Travel Award to Attend the Gordon Research Conference on Chemistry and physics of Liquids, 2015.

NAME AND ADDRESSES OF REFERES

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Prof. Dave Thirumalai
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