–Curriculum Vitae–

Atanu Baksi, PhD Notre Dame, IN, USA

Post-Doctoral Research Fellow, Department of Chemical and Biomolecular Engineering
University of Notre Dame, Notre Dame, Indiana, 46556, USA

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Research Interests

- Mechanistic understanding of chemical transformation pathways in Non-thermal Plasma (NTP) assisted Heterogeneous Catalysis.
- Investigating Liquid-Liquid Phase Separation (LLPS) and self-assembly in proteins and bio-polymers using coarse-grained Molecular Dynamics (MD) simulations.
- Mechanistic understanding of chemical transformation pathways in Non-thermal Plasma (NTP) assisted Heterogeneous Catalysis.

Work Experience

Postdoctoral Researcher with Prof. William F. Schneider July 2025 - Present
Department of Chemical and Biomolecular Engineering,
University of Notre Dame, Notre Dame, IN, USA

Postdoctoral Researcher with Prof. Jonathan K. Whitmer May 2024 - June 2025
Department of Chemical and Biomolecular Engineering,
University of Notre Dame, Notre Dame, IN, USA

Postdoctoral Researcher with Prof. Gül H. Zerze Feb 2022 - April 2024
Department of Chemical and Biomolecular Engineering
University of Houston, Houston, Texas, USA

Education

Ph.D. in Science (Chemical Physics) 2015 - 2021
Jadavpur University, Kolkata, West Bengal, India

Masters in Science - Physics (Condensed Matter Physics) 2012 - 2014
University of Calcutta, Kolkata, West Bengal, India

Undergraduate - Physics (Honors), Chemistry, Maths 2008 - 2012
University of Calcutta, Kolkata, West Bengal, India

Selected Publications and Projects

1. Modeling-Driven Control of Olefin Selectivity in Nonthermal DBD Propane Plasma., *Atanu Baksi*, C. Benaragama, D. Haycock, Jason C. Hicks*, William F. Schneider* (Ongoing Project)

2. Nonthermal-Plasma-Driven Ethane Dehydrogenation: Kinetic Modeling of Known Chemistry, and Future Opportunities., Denver Haycock, Hannah Frankovic, Russell Clarke, *Atanu Baksi*, Jason C. Hicks, William F. Schneider* (To be submitted, 2025)

3. Polyelectrolyte Length Asymmetry Influences the Phase Composition and Viscoelasticity of Polyelectrolyte Complexes., D. Iyer, H. Senebandith, V. Huaco, R. Goh, L. Willey, *A. Baksi,* Jonathan K. Whitmer*, Samanvaya Srivastava* (To be submitted, 2025)

4. Crowded Environments Control the Structure of Polyelectrolyte Coacervates., *A. Baksi,* A. Odenheimer, M. Farshad, I. Knight, N. Nguyen, R. Kayle, Samanvaya Srivastava,* Jonathan K. Whitmer* (To be submitted, 2025)

5. An Explicit Solvent Model of Coacervate Structure and Thermodynamics., *A. Baksi,* K. Alonso, I. Knight, N. Nguyen, M. Farshad, Samanvaya Srivastava, Jonathan K. Whitmer* (To Be Published, JCP, 2025)

6. A Coarse-graining Approach to Model Molecular Liquids for Mesoscale Problems., H. Zerze, A. Gupta,A. Baksi, D. Chakraborty, P. G. Vekilov, J. D. Rimer, Gül H. Zerze., ***AIChE J.*** 2025; 71(3):e18700

7. The Molecular Picture of the Local Environment in a Stable Model Coacervate., *A Baksi*, H Zerze, A Agrawal, A Karim, Gül H Zerze*, ***Commun. Chem.*** 2024, 7, 222

8. Dynamical Anomaly of Aqueous Amphiphilic Solutions: Connection to Solution H-Bond Fluctuation Dynamics?, *Atanu Baksi*, Ranjit Biswas*, ***ACS Omega*** 2022, 7, 13, 10970-10984

9. Does Confinement Modify Preferential Solvation and H-bond Fluctuation Dynamics? A Molecular Level Investigation Through Simulations of Bulk and Confined Three-Component Mixture., *Atanu Baksi*, Ranjit Biswas*, ***J. Phys. Chem. B*** 2020, 124, 11718-11729

10. Dynamic Susceptibility and Structural Heterogeneity of Large Reverse Micellar Water: An Examination of the Core-Shell Model via Probing the Layer-wise Features., *Atanu Baksi*, Pradip K. Ghorai,* and Ranjit Biswas*, ***J. Phys. Chem. B*** 2020, 124, 2848-2863

Skills

Soft Skills: Teaching, Presentation, Collaborative Project Management

Programming Languages: Python, FORTRAN, Bash Scripting

Softwares:

- **Plasma Modeling:** Bolsig++, BOLOS, ZDPlaskin, ChemPlaskin, CHEMKIN, RMG, RMS, VASP

- **Classical MD simulations:** GROMACS, LAMMPS, NAMD

- **Visualization and Analysis:** ASE, VESTA, VMD, OVITO, MDAnalysis, MDTraj, TRAVIS

Awards and Fellowships

1. Eligibility for Junior Research Fellow (CSIR-NET-JUNE-2014) test qualified and a five years Ph.D. Fellowship Grant was provided by CSIR-INDIA.
2. Best POSTER presentation award in BOSE-FEST held in S. N. Bose National Center for Basic Sciences, March-2016.
3. Best POSTER presentation award in DICB conference held in IISC, Bangalore, February-2019.
4. GRC Carl Storm International Diversity Award for attending GRC Liquids 2019 held in Holderness, New Hampshire. USA.

Oral Presentations

1. Oral presentation delivered in 'BOSE FEST' at S. N. Bose National Centre for Basic Sciences, India during 8-10 February 2018.

3. Invited Oral presentation delivered in 'GORDON Research Seminar (GRS) Liquids 2019' held in Holderness School, USA during 1 - 4 August 2019.

4. Oral presentation delivered in 11th Annual Texas Soft Matter Meeting, held at University of Texas at Austin, August 2022.

5. Research presentation delivered in APS March Meeting 2025 held at Anaheim, California.

Reviewing Experience

- Reviewer for Journal of Solution Chemistry (Springer Nature), January 2025.
- Reviewer for ChemistrySelect Journal (Wiley), November 2024.
- Reviewer for ChemistrySelect Journal (Wiley), August 2023.
- Sub-reviewer for Journal of Chemical Physics, done with Prof. Ranjit Biswas, 2020.
- Sub-reviewer for Journal of Physical Chemistry Letters, done with Prof. Ranjit Biswas, 2020.

References

1. **Dr. William F. Schneider (Professor)**
   Department of Chemical and Biomolecular Engineering, University of Notre Dame, USA
   Email: wschneider@nd.edu

2. **Dr. Jonathan K. Whitmer (Associate Professor)**
   Department of Chemical and Biomolecular Engineering, University of Notre Dame, USA
   Email: jwhitme1@nd.edu

3. **Dr. Gül H. Zerze (Assistant Professor)**
   Department of Chemical and Biomolecular engineering, University of Houston, USA
   Email: gzerze@central.uh.edu, h.gul.ozer@gmail.com

4. **Dr. Ranjit Biswas (Professor)**
   Department of Chemical, Biological & Macromolecular Sciences,
   S. N. Bose National Centre for Basic Sciences, India
   Email: ranjit@bose.res.in, rbsnbc@gmail.com