Dr. Tamal Banerjee

Personal Profile

Dr. Tamal Banerjee
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Academic Profile

2007 **Ph.D.** in Chemical Engineering, IIT Kanpur
Thesis Topic: "*Ionic Liquids - Phase Equilibria and Thermodynamic Property Predictions using Molecular Modeling and Dynamics, and their Validation with Experiments*"

2002 **M. Tech**. in Chemical Engineering, IIT Roorkee
Thesis Topic: "*Synthesis and Characterization of Room Temperature Ionic Liquids and its Application to Benzene-Hexane System"*

2000 **B.E** Chemical Engineering, University of Pune

Professional Appointment

- **Professor**, Indian Institute of Technology Guwahati, (Jan 2017-)
- **Associate Professor**, Indian Institute of Technology Guwahati, (Jan 2013-December 2016)
- **Assistant Professor,** Indian Institute of Technology Guwahati, (June 2007-December 2012)
- **Senior Lecturer,** Indian Institute of Technology Guwahati, (December 2006 - May 2007)
- **University Associate**, Curtin University (2020-2024), Perth, Australia
- **Supplemental Faculty**, University of Delaware, USA (2011-2012)

Research Interest

- Computational Chemistry
- Downstream Engineering
- Separations with Deep Eutectic Solvents and Ionic Liquids

Teaching

(a) Courses Taught

- Chemical Engineering Thermodynamics I (CL203)
- Numerical Methods in Chemical Engineering (CL305)
- Mechanical Operations & Thermodynamics Laboratory (CL311)
- Chemical Reaction Engineering (CL303)
- Chemical Engineering Thermodynamics II (CL207)

- Chemical Process Technology (CL 401)
- Advanced Thermodynamics (CL503)
- Molecular Simulations in Chemical Engineering (CL622)
- Applied Statistical Thermodynamics(CL633)
- Characterization of Materials (CL513)
- Computer Aided Process Equipment Design (CL312)
- Process Modelling and Simulation Laboratory (CL652)

(b) **Recent Invited Talks**

1. *Deep Eutectic Solvents as Media for Microextraction and Asphaltene Aggregation Inhibition*. International Conference on Materials Science and Engineering (ICMSE-2025), 11th–12th June **2025**, NIT Jalandhar

2. *Deep Eutectic Solvents for Asphaltene Inhibition: Insights from Quantum Chemistry*. GAZPROM NEFT Russia-India Technological Day, October 24-25,**2024**, St. Petersburg, Russia

3. *Quantum Chemical and Molecular Dynamics Insights in the Extraction of Aromatic moieties from Hydrocarbon and Aqueous Stream using Eutectic Solvents*,5th July,**2023**, University of Twente, Netherlands

4. *Molecular Modelling studies on Deep Eutectic Solvents as Novel Separation Media for Aromatic Extraction,* 38th International Conference on Solution Chemistry (38 ICSC), Belgrade, Serbia, July 9-14, **2023**.

5. *Deep Eutectic Solvents as Novel Separation Media for Aromatic Extraction: Insights from Quantum Chemical and Molecular Dynamics Simulations*. IISC Bangalore. ChemE@IISc Symposium, December 15th and 16th, **2022**

Research Guided

(a) *PhD Thesis* guided

1. **Dr. R. Anantharaj (2008-2012)**
   Thesis title: Simultaneous Desulphurization and Denitrification of Diesel oil using Ionic Liquids with Quantum Chemical Prediction and Validation.
2. **Dr. Ananth Praveen Kumar (2009-2013)**
   Thesis title: Interfacial Dynamics of functional liquids over porous media.
3. **Dr. S. R. Pilli (2010-2015)**
   Thesis title: Extraction of Endocrine–Disrupting Compounds from Aqueous Solutions using Ionic Liquids: Theoretical Predictions and Experimentations using Supported Liquid Membrane
4. **Dr. D. V. Rabari (2012-2015)**
   Thesis title: Experimental, Modelling and Optimization Insights for the Enhancement of Butanol Production using Phosphonium based Ionic Liquids

5. **Dr. Sanjukta Bhoi (2012-2017)**
   Thesis title: Dispersion and Dissolution of Indian Coal in Ionic Liquids: Theoretical Predictions and Experimental Validation
6. **Dr. Anand Bharti (2013-2017)**
   Thesis title: Multiscale Modeling and Experimental studies on Bio-Oil Upgradation
7. **Dr. Mayur Kevat (2013-2018)**
   Thesis title: Simulation Of Chemical Looping Combustion Using Coal and Biomass Mixtures
8. **Dr. Basudhrity Banerjee (2013-2018)**
   Thesis title: Ionic Liquid Supported Thermal Dehydrogenation Of Ammonia Borane
9. **Dr. Rima Biswas (2014-2018)**
   Thesis title: Quantum Chemical and Molecular Dynamics Insights into the Solvent Extraction and Stripping Mechanism of Metal Ions in Aqueous Biphasic Systems
10. **Dr. Mood Mohan (2014-2018)**
    Thesis title: Dissolution of Lignocellulosic Biomass in Ionic Liquids: Insights from Molecular Modeling and Experimental Studies
11. **Dr. Rupesh Verma (2012-2018)**
    Thesis title: Liquid-Liquid Extraction and Process Flow sheeting of Lower Alcohol with Deep Eutectic Solvents
12. **Dr. Debashis Kundu (2015-2019)**
    Thesis title: Development of Cellulose, Hemicellulose and Cyclodextrin based hydrogels for the in-vitro Release of Biomolecules and Metal Ion Adsorption
13. **Dr. Papu Kumar Naik (2014-2019)**
    Thesis title: Molecular Modeling and Thermodynamic Studies on the Selective Extraction of Poly Aromatic Hydrocarbons from Fuel oil using Deep Eutectic Solvent
14. **Dr. Pyarimohan Dehury (2015-2021)**
    Thesis Title: Nanoparticle Dispersed Deep Eutectic Solvents as Low-Cost Heat Transfer fluid for Concentrated Solar Power
15. **Dr. Upasana Mahanta (2016-2021)**
    Thesis Title: Ionic Liquids and Deep Eutectic Solvents as Electrolytes for Energy Efficient Electrical Double Layer Capacitor
16. **Dr. Dhirendra Kumar Mishra (2016-2022)**
    Thesis Title: Experimental and Molecular Modeling Insights on the Thermolytic Dehydrogenation of Amine Boranes with Ionic Liquids and Deep Eutectic Solvents
17. **Dr. Nikhil Kumar (2017-2023)**
    Thesis Title: Solvation and Extraction Mechanism of Aromatic Solutes and Asphaltene utilizing Deep Eutectic Solvents: Experimental and Atomistic Simulation Studies
18. **Dr. Nabendu Paul (2017-2023)**
    Thesis Title: Molecular Modeling and Experimental Insights in the Application of Hydrophobic Deep Eutectic Solvents for Remediation of Micropollutant from Aqueous Systems
19. **Dr. Arindam Dutta (2018-2024)**
    Thesis Title: Investigation of Novel Ionogels and Eutectogels as Electrolytes for Electrochemical Supercapacitors
20. **Dr. Nipu Kumar Das (2019-2025)**

Thesis Title: Deep Eutectic Mixtures with Graphene and MWCNT Functionalized Nanofluids for Indirect Solar Desalination using the Multistage Flash Approach

21. Dr. Raghibul Hussain (2020-2026)

Title: First-Principles Studies on Dioxin and Furan Formation from Organic Halides: Mechanisms, Inhibition, and Prevention Strategies

(b) *MTech Thesis* (24 completed)

(c) *BTech Thesis* (24 completed)

Research and Academic Projects Undertaken

Sponsored Projects **:**

1. **Title**: Design and Development of High capacity and High Voltage Cathodes Derived from Indigenous Minerals for High Energy Density Sodium-ion Batteries
   Duration: 2025-2027
   Funding agency: Indian Space Research Organization (ISRO)

2. **Title**: Development of an automated platform for environmentally safe chemical analysis of food products based on flow methods and deep eutectic solvents
   Duration: 2025-2028
   Funding agency: Department of Science and Technology (DST INDO-RUSSIAN)

3. **Title**: Formulation of membrane based Micro Reactor for decontamination cum denitration of nitrate bearing effluents and conversion to valuable products
   Duration: 2023-2026
   Funding agency: SERB, Department of Science and Technology (DST) (as CO-PI)

4. **Title**: Sustainable, Biodegradable and Affordable Substitutes for 'Single use Plastic' using Castor Oil and Stubble Aggregate
   Duration: 2021-2025
   Funding agency: DST-Waste Management Technology, Department of Science and Technology (DST)

5. **Title:** Deep Eutectic Mixtures with Graphene Functionalized Nanofluids for Indirect Solar Desalination using Multistage Flash Approach
   Duration: 2020 - 2023
   Funding agency: SERB, Department of Science and Technology (DST)

6. **Title:** Development of Novel Deep Eutectic Solvents for the Extraction of Aromatics for Production of Food Grade Hexane and Straight run Kerosene using COSMO-SAC Screening.
   Duration: 2019 - 2021
   Funding agency: Hindustan Petroleum Corporation Limited, HP-Green

7. **Title:** Hydrophobic Deep Eutectic Solvent for Remediation of Antifugal and Antiobiotics in Waste water.

Duration: 2019 - 2021
Funding agency: Scheme for Promotion of Academic and Research Collaboration (SPARC) MHRD, Govt. of India

8. **Title:** Ionic Liquid and deep eutectic solvents as electrolytes for energy efficient electrochemical double layer capacitor.
   Duration: 2016 - 2019
   Funding agency: RESPOND-ISRO, Govt. of India

9. **Title:** Nanoparticle Dispersed Deep Eutectic Solvents as Low Cost Heat Transfer fluid for Concentrated Solar Thermal Power Plant.
   Duration: 2017 - 2020
   Funding agency: IMPRINT India, MHRD, Govt of India

10. **Title**: GIAN course on "Integration of Molecular Design to Process Simulation for the Development of Industrial Chemical Products and Processes
    Duration: 12-17th December 2016
    Funding agency: Ministry of Human Resource and Development, Government of India

11. **Title:** Quantum Chemical Understanding of Solvent Extraction Mechanism of Metal Ions in Novel Ionic Liquid Medium.
    Duration: 2013 - 2016
    Funding agency: Board of Research in Nuclear Sciences (BRNS), Govt of India

12. **Title:** Ionic Liquid assisted Thermal Dehydrogentation of Ammonia Borane.
    Duration: 2013 - 2016
    Funding agency: SERB, Department of Science and Technology (DST)

13. **Title:** Dispersion and Dissolution of Coal in Ionic Liquids: Theoretical Predictions and Experimental Validation.
    Duration: 2012 - 2015
    Funding agency: Council of Scientific and Industrial Research (CSIR)

14. **Title:** Simultaneous Desulphurization and Denitrification of Diesel oil using Ionic Liquids with Quantum Chemical Prediction and Validation.
    Duration: 2008 - 2011
    Funding agency: Fast Track Scheme, Department of Science and Technology (DST)

Consultancy Projects **:**

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1 **Title:** Natural Deep Eutectic Solvent (NADES) green solvent design framework by predictive modeling stimulation tools for solubilization of solid organic UV filters **(2024)**
Funding Agency: L,Oreal India Limited

2 **Title:** Designing of Process Flow Diagram, Engineering diagrams and P&ID Diagram for Laboratory Developed Process for Separation of Carbon Nanotubes and Graphene from Shunghite ore **(2023)**
Funding Agency: Nisarga Ispat

3 **Title:** Conversion of Wood Chips to Wood Alcohol **(2021)**
Funding agency: Sheenlac Paints,Chennai

4 **Title:** Investigation of Thermodynamic Properties of Kerosene Samples (**2014**)
Funding agency: Jyothy Labarotories, Mumbai

Educational Projects **:**

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1. **Title:** NPTEL-MOOCS Course on **"**Applied Statistical Thermodynamics" (January 2024-April 2024)
   Funding agency: Ministry of Education, Govt. of India
   Link: https://onlinecourses.nptel.ac.in/noc24_ch34/preview

2. **Title:** NPTEL-MOOCS Course on **"**Chemical Process Technology" (January 2023-April 2023)
   Funding agency: Ministry of Education, Govt. of India
   Link: https://onlinecourses.nptel.ac.in/noc23_ch16/preview

3. **Title:** NPTEL-MOOCS Course on **"**Physical and Electrochemical Characterizations in Chemical Engineering" (January 2022-March 2022)
   Funding agency: Ministry of Education, Govt. of India
   Link: https://onlinecourses.nptel.ac.in/noc22_ch23/preview

4. **Title:** Co-developer for NPTEL web course entitled "Molecular Simulation in Chemical Engineering" (**2012**)
   Funding agency: Ministry of Human Resource and Development, Government of India
   Link: http://nptel.ac.in/courses/103103036/

5. **Title:** Co-developer for Course entitled "Numerical Methods for Chemical Engineering" under the project entitled "Developing suitable pedagogical methods for various classes, intellectual calibres and e-learning"(**2011**)
   Funding agency: Ministry of Human Resource and Development, Government of India
   Link: http://www.ide.iitkgp.ernet.in/Pedagogy_view/example.jsp?USER_ID=178

Research Publications

(a) Books

1. Dhirendra Kumar Mishra, Nikhil Kumar, Nabendu Paul, Nipu Kumar Das and Tamal Banerjee. *Quantum Chemical and Molecular Dynamics Simulations for Beginners*. CRC Press, ISBN: 9781032619286 (In Press)
2. Papu Kumar Naik, Nikhil Kumar, Nabendu Paul, Tamal Banerjee. *Deep Eutectic Solvents in Liquid-Liquid Extraction Correlation and Molecular Dynamics Simulation* (**2022**).ISBN: 9781003231158.CRC Press.
3. Tamal Banerjee, Anand Bharti, Debashis Kundu and Dharamashi Rabari. *Phase Equilibria in Ionic Liquid Facilitated Liquid–Liquid Extractions* (**2017**). ISBN: 9781498769488.CRC Press.
4. Tamal Banerjee and Ramalingam Anantharaj. *Desulphurization and Denitrification of Diesel Oil using Ionic Liquids* (**2015**). ISBN: 978-0-12-801347-2.Elsevier,MA, USA

(b) Book Chapter

5. Paul, N., Banerjee, T. (**2023**). Water Decontamination Through Thiamethoxam Removal Using DL-Menthol/Octanoic Acid Deep Eutectic Solvent: Molecular Dynamics Insights. In: Mazumder, D. (eds) Sustainable Advanced Technologies for Industrial Pollution Control. ATIPC 2022. Springer Proceedings in Earth and Environmental Sciences. Springer, Cham. https://doi.org/10.1007/978-3-031-37596-5_1
6. Sushma P. Ijardar, Arvind Kumar, Debashis Kundu, Tamal Banerjee, and Naved I. Malek, Application of Thermodynamic Model for Prediction of Experimental Solubility of Alkali Metal Halides in Aqueous Organic Solvent in book "Theoretical Models and Experimental Approaches in Physical Chemistry Research Methodology and Practical Methods" (**2018**). Apple Academic Press, ISBN: 9781771886321, pp 83-114.

(c) Patent:

1. *Eutectic Mixture-Based Process for Selective Fluoride Removal from Contaminated Water.* Indian Patent Office, 202631021295 dated 23rd February **2026 (Filed)**

2. *Enhancing Thermal Energy Storage with MentholDES/Carboxylate MWCNT Nanofluids*. Indian Patent Office, Patent No. 202631022013,24th February **2026 (Filed)**

3. *Alumina based Deep Eutectic Solvent comprising Benzophenone and Biphenyl as Heat Transfer Media*, Indian Patent Office, Patent No. 430369, 16th May **2022 (Granted)**

4. *A Deep Eutectic solution as heat transfer fluid comprising Diphenyl Ether and Benzophenone*, Indian Patent Office, Patent No. 387491, 30th December **2020 (Granted)**

(d) **International Journals (total 174 SCI Published Journals with 7400 citation and h-index of 47)**

For full list: https://scholar.google.co.in/citations?user=iSwkMbMAAAAJ&hl=en (See Annexure II)

1. Pratyashee Barukial, Rajib Nandi, Manazira Ahmed, Rituraj Barman, Tamal Banerjee and Bipul Bezbaruah. Computational insights into Ru(ii)–coumarin complexes as potential anticancer agents: a DFT, QTAIM, NCI-RDG, molecular docking and molecular dynamics approach. *Phys. Chem. Chem. Phys.*, 2026,28, 1447-1462
2. Mangal, M., Goswami, R.N., Boruah, P.J. *et al.* Synthesis and characterization of linseed oil-derived polyurethane composites via epoxidation and ring-opening pathway: Structure–property relationships and DFT insights. *Bull Mater Sci* **49**, 46 (2026). https://doi.org/10.1007/s12034-026-03574-y
3. Barukial, P., Nandi, R., Das, N. K., Barman, R., Ahmed, B., Nagendraprasad, G., Banerjee, T., & Bezbaruah, B. (2025). Synergistic in silico exploration of some pyrazole-based potential anticancer agents: A DFT, molecular docking, and molecular dynamics study. *Journal of Molecular Modeling, 31*(6), 167. https://doi.org/10.1007/s00894-025-0590-0
4. Dutta, A., Kundu, D., Sharma, S., Silvester, D. S., & Banerjee, T. (2025). Investigating the electrochemical properties of ionic-liquid-mediated inorganic eutectogels derived from carboxylic-acid-based hydrophobic natural deep eutectic solvents. *Journal of Solution Chemistry*, 1–16. https://doi.org/10.1007/s10953-025-01301-2
5. Hussain, R., Pugazhenthi, G., Banerjee, T., Ali, S. M., & Chakraborty, B. (2025). Transition metal-decorated biphenylene sheet for dioxin detection: A first-principles investigation. *The Journal of Physical Chemistry B, 129*(19), 4818–4831. https://doi.org/10.1021/acs.jpcb.4c01344
6. Kakati, N., Paul, N., Dubey, S., Mahanta, J., Lakshmi, A. R., Banerjee, T., & Bandyopadhyay, D. (2025). Microrheology of ionic liquid doped mucus for an efficient delivery of protein-based oral drugs. *Small, 21*(14), 2500403. https://doi.org/10.1002/smll.202500403
7. Mangal, M., Rao, C. V., Das, N. K., Bose, S., & Banerjee, T. (2025). Impact of cellulose enrichment on castor oil polyurethane sheets: A path to greener materials. *Journal of Applied Polymer Science, 142*(3), e56364. https://doi.org/10.1002/app.56364
8. Nandi, R., Paul, N., & Banerjee, T. (2025). Molecular dynamics insights of CO_2 capture through phosphonium-based deep eutectic solvents for direct air capture. *ACS Sustainable Chemistry & Engineering*. https://doi.org/10.1021/acssuschemeng.5c03036
9. Shishov, A., Markova, U., Mulloyarova, V., Tolstoy, P., Shkaeva, N., Kosyakov, D., Das, N. K., & Banerjee, T. (2025). 1-(o-Tolyl) thiourea-based deep eutectic solvent as a stationary phase in flow injection analysis system for mercury and copper determination in edible oils. *Talanta, 282*, 127079. https://doi.org/10.1016/j.talanta.2024.127079
10. Vatti, A. K., & Banerjee, T. (2025). Atomistic investigation of stability and thermal conductivity of cyrene nanofluid: A molecular dynamics study. *Journal of Molecular Liquids, 422*, 126844. https://doi.org/10.1016/j.molliq.2024.126844

Achievements/Awards and Other Details

- Guest Editor for Special Issue on " Data-Driven and Computationally Enabled Composites", Journal of Material Chemistry: Composites (Springer)**2026**
- Editorial Board Member, Journal of Solution Chemistry (Springer)**(2025-)**
- Associate Editor, Thermal Advances (Elsevier) (**2024-)**
- Editorial Board Member of *Fluid Phase Equilibria*(**2020-**), Elsevier.
- Guest Editor for Special Issue on "Thermodynamics and Thermal Analysis of Deep Eutectic Solvents", Chemical Thermodynamics and Thermal Analysis(Elsevier)**2023**
- Guest Editor for Special Issue titled “Ionic liquids and Deep Eutectic Solvents: two contrasting options or opposite sides of the same coin?” Frontiers in Chemistry **2022**
- Fellow of Indian Chemical Society (FICS),2**021**
- Fellow of Royal Society of Chemistry(FRSC),**2021**
- Local Organizer, SESTEC 2016, BARC held at IIT Guwahati from 17th to 20th May **2016**
- Certificate of Excellence in Reviewing from Fluid Phase Equilibria (Elsevier) **2013**
- Recipient of "*INDO-US Fellowship*" in Engineering Sciences, **2011** from the INDO-US Science and Technology Forum(IUSSTF)
- Certificate of Appreciation from American Chemical Society(ACS),December **2011** as the most valuable reviewer
- Highest Cited Article titled “Quantum Chemical Studies on the Simultaneous Interaction of Thiophene and Pyridine with Ionic Liquid” of **2010** for American Journal of Chemical Engineers (AIChEJ)

(**Tamal Banerjee**)