Nipu Kumar Das

Ph.D - Chemical Engineering
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Education

Degree/Certificate	Institute/Board	CGPA/Percentage	Year
Ph.D. Chemical	Indian Institute of Technology, Guwahati	NA	2025
M.Tech. Petroleum	Indian Institute of Technology, Guwahati	7.39	2017-2019
B.E. Chemical	Assam Engineering College, Guwahati	72.41%	2012-2016
Senior Secondary	AHSEC Board	67.40%	2011
Secondary	SEBA Board	80.67%	2009

Projects

- **Ph.D** *Jan 2020 - 17th June 2025*
  PhD Supervisor-Prof. Tamal Banerjee
  - **Deep Eutectic Mixtures with Graphene and MWCNT Functionalized Nanofluids for Indirect Solar Desalination using Multistage Flash Approach:** This thesis addresses global water scarcity by exploring nanofluids as alternatives for heat transfer and desalination processes. It employs both experimental and computational techniques to study nanofluids dispersed with MWCNT and MWCNT-COOH in various green solvents. Key focus is given to Deep Eutectic Solvents (DES), Natural DES (NADES), and Cyrene-based systems. The work highlights enhanced thermal conductivity, stability, and structural properties of these nanofluids. Spectroscopic and microscopic tools confirm nanoparticle dispersion and conjugation with DES. DFT and MD simulations support observed thermophysical behavior and heat transfer superiority. Proposed applications include BR-MSF desalination and CSP systems using eco-friendly HTFs

- **M.Tech** *July. 2017 - July 2019*
  M.Tech Supervisor-Prof. Pallab Ghosh
  - **Adsorption of Non-ionic Surfactants at Fluid-Fluid Interface and Coalescence of Bubbles in the Presence of Salts**

- **B.Tech** *July. 2012 - August 2016*
  B.Tech Supervisor-Prof. Tapan Sharma
  - **Manufacture of Formaldehyde from Methanol by Metal Oxide Process Investigation of oil storage and movement**

Technical Skills

- **Key Skills**: Molecular Dynamics (MD) Simulations, DFT, COSMO-SAC and Process modelling simulation (Aspen Plus), COMSOL
- **Coding**: Python and Matlab
- **Softwares**: NAMD, LAMMPS, Aspen Plus, VMD, Avogadro, Packmol, Gaussian16, Gauss view, EndNote
- **Operating Systems**: Windows, Linux
- **Languages**: Strong reading, writing, and speaking competencies in Hindi, Assamese (native) and English
- **Miscellaneous**: LATEX, Gnuplot, Origin Pro, Microsoft Word, Microsoft Excel, and Microsoft PowerPoint

Experimental Skills

- Rheometer, TGA, DSC, KD2 Pro, Tensiometer, Densitometer, Delsa nano, FT-IR, XRD, Raman, FETEM, FESEM

Research area

- Green solvents, DES, Thermal energy storage, Organic nanofluids, ionic liquid, nanomaterials and nanofluid, Solubility, Solution Thermodynamics, CFD

Key Subjects

- Heat transfer Operation, Mass transfer operation, Thermodynamics, Chemical Reaction Engineering, Mechanical Operation

Research Publications

1. **Nipu Kumar Das**, Somtirtha Santra, Papu Kumar Naik, Maureen Shama Vasa, Rishi Raj, Suryasarathi Bose, Tamal Banerjee. " Evaluation of Thermophysical Properties and Thermal Performance of Amine-Functionalized Graphene Oxide/Deep Eutectic Solvent Nanofluids as Heat-Transfer Media for Desalination System." **ACS Sustainable Chemistry Engineering**, March 27, 2023, https://doi.org/10.1021/acssuschemeng.2c06325
2. **Nipu Kumar Das**, Dhirendra Kumar Mishra, Papu Kumar Naik, Pyarimohan Dehury, Suryasarathi Bose, Tamal Banerjee. "Dihydrolevoglycosenone as a novel bio-based nanofluid for thermal energy storage: Physiochemical and quantum chemical insights". **Journal of energy storage**, 59(2023): 106365, https://doi.org/10.1016/j.est.2022.106365.
3. **Nipu Kumar Das**, Papu Kumar Naik, Dhileep N. Reddy, Bhabani S. Mallik, Suryasarathi Bose, and Tamal Banerjee. "Experimental and molecular dynamic insights on the thermophysical properties for MWCNT-Phosphonium based eutectic thermal media." **Journal of Molecular Liquids**, 354 (2022): 118892, https://doi.org/10.1016/j.molliq.2022.118892
4. **Nipu Kumar Das**, Raghibul Hussain, Anoop Kishore Vatti, Tamal Banerjee. "Thermal Performance of Bio-Nanofluid Dihydrolevoglucosenone: Experimental and Atomistic Simulation Investigations". **AIChE journal** (https://doi.org/10.1002/aic.18718)
5. Nikhil Rahul Dhongde, **Nipu Kumar Das**, Tamal Banerjee, Prasanna Venkatesh Rajaraman. "Synthesis of carbon quantum dots from rice husk for anti-corrosive coating applications: Experimental and theoretical investigations".**Industrial Crops and Products**, 212(2024): 118329
6. Nikhil Rahul Dhongde, **Nipu Kumar Das**, Jenasree Hazarika, Jin-Goo Park, Tamal Banerjee, Prasanna Venkatesh Rajaraman. "Azoles as corrosion inhibitors in alkaline medium for Ruthenium chemical mechanical planarization applications: Electrochemical and Theoretical analysis". **Journal of molecular structure**, 1320 (2024), 139651)
7. Rifat Muradymov, Nabendu Paul, **Nipu Kumar Das**, Tamal Banerjee, Andrey Shishov. " Quasi-hydrophobic deep eutectic solvents for simultaneous automated determination of polar and non-polar dyes in food products". **Microchemical Journal**, 206 (2024), 111510
8. Andrey Shishov, Ulyana Markova, Valeriia Mulloyarova, Peter Tolstoy, Natalya Shkaeva, Dmitry Kosyakov, **Nipu Kumar Das**, Tamal Banerjee. " Deep eutectic solvent as stationary phase for flow analysis: automated trace metal determination in food products". **Analytica Chimica Acta**, 1332 (2024), 343356
9. Andrey Shishov, Ulyana Markova, Valeriia Mulloyarova, Peter Tolstoy, Natalya Shkaeva, Dmitry Kosyakov, **Nipu Kumar Das**, Tamal Banerjee. " 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 (2025), 127079
10. Andrey Shishov, Sergey Savinov, **Nipu Kumar Das**, Tamal Banerjee, Andrey Bulatov. "Automated simultaneous determination of mercury and copper in edible oils by reversed-phase column-based extraction with deep eutectic solvent". **Journal of Food Composition and Analysis**, 137(A) (2025), 106919
11. Pratyashee Barukial, Benzir Ahmed, Basanta Singha, Pankaj Chetia, **Nipu Kumar Das**, Samir Thakur, Upasana Bora Sinha, Bipul Bezbaruah. " Some Co (II)-Schiff base complexes as promising anticancer agents: A DFT and molecular docking study". **Indian Journal of Biochemistry and Biophysics (IJBB)**, 61 (2024), 354-370
12. Mangal Mangal,Chebrolu Venkateswara Rao, '**Nipu Kumar Das**, Suryasarathi Bose, Tamal Banerjee. "Impact of cellulose enrichment on castor oil polyurethane sheets: A path to greener materials". **Journal of Applied Polymer Science** , 142 (2025), e56364
13. Pratyashee Barukial, Rajib Nandi, **Nipu Kumar Das**, Rituraj Barman, Benzir Ahmed, Gunolla Nagendraprasad, Tamal Banerjee, Bipul Bezbaruah. "Synergistic in silico exploration of some pyrazole-based potential anticancer agents: a DFT, molecular docking, and molecular dynamics study". **Journal of Molecular Modeling** , 31 (2025), 1-19
14. Nipom Sekhar Das and **Nipu Kumar Das**, "Improvement of non-volatile resistive memory behaviour in post-annealed rGO-SnS2 embedded PMMA polymer nanocomposites film". **ournal of Materials Science: Materials in Electronics** , 36 (2025), 1-19

Book Chapter

- **Nipu Kumar Das**, Papu Kumar Naik, and Tamal Banerjee, "Green Nanomaterials for Energy Conversion in *Green Synthesis of Nanomaterials for Environmental Remediation*" API press (ebook ISBN No. 9781779643841, paperback ISBN 9781779643834), PP est 466pp w/ index (In Production)

Industrial collaboration work

- Design a new organic solvent through molecular modeling and database (In-silico approach) for targeting the solubilization of solid organic filters, 2024 (Collaboration work with L'Oréal Cosmetic Company)

Conferences

1. **Nipu Kumar Das**, Papu Kumar Naik, and Tamal Banerjee, "Evaluation of thermo-physical properties of amine functionalized graphene oxide/Deep Eutectic Solvent nanofluids as heat transfer media for solar desalination system" International Conference on Emerging Trends in Nanomaterials Science and Technology, 27-29 January 2022, NIT Nagaland, India
2. **Nipu Kumar Das**, Papu Kumar Naik, and Tamal Banerjee, "Thermophysical properties for MWCNT based Phosphonium Eutectic Nanofluid: An Emerging Heat Transfer Media for Solar Desalination System" 1st International Conference on Advances in Water Treatmentand Management (ICAWTM-22) March 25-26, 2022, Pandit Deendayal Energy University, Gandhinagar, Gujarat, India (Virtual)
3. **Nipu Kumar Das**, Papu Kumar Naik, and Tamal Banerjee, "Investigation on thermal performance of Carbon based Nanoparticle with Cyrene as Nanofluid: A Green Heat Transfer Media for Solar Desalination System" International conference on Desalination and Water Treatment: Recent Technological Advancement, Challenges and Opportunities (InDACON-2022), March 26–27, 2022, MBM University in association with Indian Desalination Association (InDA) and DRDO, Jodhpur (Virtual)
4. **Nipu Kumar Das**, and Tamal Banerjee, "Evaluation of thermal performance of bio-based nanofluids comprising of dihydrolevoglycosenone and functionalised carbon nanotube" International conference on Biotechnology for Sustainable Bioresources and Bioeconomy (BSBB-2022), December 7–11, 2022, Indian Institute of Technology Guwahati, Assam
5. **Nipu Kumar Das**, and Tamal Banerjee, "Characteristics and computational studies of bio-based Nanofluids as Thermal Energy Storage Media for Heat Transfer Application" 16th Complex Fluids Symposium 2022 (CompFlu-2022), Indian Society of Rheology Indian Institute of Technology Kharagpur, Kharagpur-721302
6. **Nipu Kumar Das**, and Tamal Banerjee, DAE-BRNS national workshop on "Atomistic Modeling of Molecules and Materials (AMMM-2023), Anushaktinagar, BARC, Mumbai, December 11-14, 2023
7. **Nipu Kumar Das**, and Tamal Banerjee, Thermophysical Properties and Dispersion behaviour of Menthol-Based Deep Eutectic Solvent with Carboxylate-Functionalized MWCNT Nanofluids: Evaluating Thermal Efficiency and DFT Insights to Enhance Thermal Energy Storage Capacity, International Conference on New Frontiers in Chemical, Energy and Environmental Engineering (INCEEE-2023) 24-25 Nov., 2023, NIT Warangal, India

Achievements

- **Anundoram Barooah Award** from Assam Government, 2009
- **NEC Scholarship** from Assam Government, 2013-15
- **GATE Qualified**, 2017 and 2019
- **INSC Young Researcher Award**, 2023
- **Chief Minister of Assam Scholarship**, 2018
- **Participated in the National Workshop on "Deep Eutectic Solvents for Environmental Remediation and Energy Storage"**, MHRD, Government of India, 2020
- **Miscellaneous**: Guided 4 Btech students and 6 internship students
- **Miscellaneous**: Teaching Assistant at NPTEL 2023 and 2024

References

1. **Prof. Tamal Banerjee** (PhD Supervisor)
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