

SURAJIT KALITA



Department of Chemical Sciences, Tezpur University, Napaam, Tezpur, Assam - 784028, India

Email: skalita@tezu.ernet.in

Date: 8th Sept 2025

ASSISTANT PROFESSOR

Department of Chemical Sciences, Tezpur University

(August/2025 – Present)

POSTDOCTORAL EXPERIENCE

Michigan Technological University

MI, USA (April – August, 2025)

Advisor: Prof. Christo Z. Christov and Prof. Tatyana G. Karabenchewa-Christova

Research Area: Conformational dynamics and mechanism of non-heme iron enzymes

The Hebrew University of Jerusalem

Israel (July/2022 – Jan/2025)

Advisor: Prof. Sason Shaik

Research Area: Oriented External Electric Field Theory, Alzheimer's Disease, Quantum Tunneling/Eckart Method and Ice Nucleation.

EDUCATION

Shiv Nadar Institution of Eminence Deemed to be University

UP, India

Ph.D. Student at Molecular Simulation Lab

August/2018 – July/2022

Advisor: Dr. Kshatresh D. Dubey and Co-Advisor: Prof. Parthapratim Munshi

Thesis Title: Mechanistic Study of Cytochrome P450 Enzymes: A Computational Insight.

Gauhati University

Guwahati, India

M.Sc. in Chemistry (CGPA: 7.8)

2015 – 2017

Advisor: Dr. Dhruva Jyoti Kalita

Dissertation: Tuning the Triphenylamine Based Organic Dyes for their Potential Applications in Dye Sensitized Solar Cells.

B. Borooah College

Guwahati, India

B.Sc. in Chemistry (CGPA: 8.4)

2012 – 2015

Advisor: Dr. Pradyumna Majumdar

Dissertation: Optimization and Spectral Analysis of Amino Acids: A Theoretical Study

Anundoram Borooah Academy

Pathsala, India

Class 12 (Board: AHSEC)

2010 – 2012

Science (Percentage: 84.6; Chemistry Mark: 90 [out of 100])

Anundoram Borooah Academy

Pathsala, India

Class 10 (Board: SEBA)

2010

DISTINCTION with all Subjects Letter Marks (Percentage: 85%)

SUMMER RESEARCH

IAS-INSANA-SI Summer Research, Indian Institute of Technology Bombay, Mumbai 2015

Advisor: Prof. Ramaswamy Murugavel

Report Title: Synthesis and Characterization of Schiff Base Phosphonate Complexes.

PUBLICATIONS

Corresponding and First Author:

1. **Kalita, S.***; Danovich, D.; Shaik, S.* Origins of the Superiority of Oscillating Electric Fields for Disrupting Senile Plaques: Insights from the 7-Residue Fragment and Full-length A β -42 Peptide. *J. Am. Chem. Soc.* **2025**, *147*, 3, 2626-2641 ([link](#))
2. Yadav, S.#; **Kalita, S****; Dubey, K. D.* Mechanism of a Novel Metal-Free Carbonic Anhydrase, *Phys. Chem. Chem. Phys.*, **2024**, *26*, 28124-28132 (# = Equal contribution [link](#)).

First Author:

3. **Kalita, S.**; Danovich, D.; Shaik, S. Local Electric Fields Originate Unusual Kinetic Isotope Effects in the Hydrogen Abstraction Reactions of the Functionally-Analogous P450 and TauD Enzymes. *J. Am. Chem. Soc.* **2025 (Just Accepted)**.
4. **Kalita, S.**; Bergman, H.; Dubey, K. D.; Shaik, S. How Can Static and Oscillating Electric Fields Serve in Decomposing Alzheimer's and Other Senile Plaques? *J. Am. Chem. Soc.* **2023**, *145*, 6, 3543-3553 ([link](#))
5. Javitt, L. F.#; **Kalita, S.#**; Dubey, K. D.; Ehre, D.; Shaik, S.; Lahav, M.; Lubomirsky, I. Electro-freezing of Supercooled Water is Induced by Hydrated Al³⁺ and Mg²⁺ Ions: Experimental and Theoretical Studies *J. Am. Chem. Soc.* **2023**, *145*, 34, 18904-18911. (# = Equal contribution) ([link](#))
6. **Kalita, S.**; Shaik, S.; Dubey, K. D. Mechanistic Conundrum of C-C Cleavage by CYP51. *ACS Catal.* **2022**, *12*, 5673-5683. ([link](#))
7. **Kalita, S.**; Shaik, S.; Dubey, K. D. MD Simulations and QM/MM Calculations Reveal the Key Mechanistic Elements Which are Responsible for the Efficient C-H Amination Reaction Performed by a Bioengineered P450 Enzyme. *Chem. Sci.* **2021**, *12*, 14507-14518. ([link](#))
8. **Kalita, S.**; Shaik, S.; Kisan, H. K.; Dubey, K. D. A Paradigm Shift in the Catalytic Cycle of P450: The Preparatory Choreography during O₂ Binding and Origins of the Necessity for Two Protonation Pathways. *ACS Catal.* **2020**, *10*, 11481-11492. ([link](#))

Co-Author:

9. Dubey, K. D.#; Stuyver, T.#; **Kalita, S.**; Shaik, S. Solvent Organization and Rate Regulation of a Menshutkin Reaction by Oriented External Electric Fields are Revealed by Combined MD and QM/MM Calculations. *J. Am. Chem. Soc.* **2020**, *142*, 9955-9965. ([link](#)) (# = equal contribution)
10. Siddiqui, S. A.; Shaik, S.; **Kalita, S.**; Dubey, K. D. A Porphyrin-Based Molecular Cage Guided by Designed Local-Electric Field is Highly Selective and Efficient. *Chem. Sci.* **2023**, *14*, 10329-10339. ([link](#))
11. Kardam, V.; **Kalita, S.**; Dubey, K. D. Computations Reveal a Crucial Role of an Aromatic Dyad in the Catalytic Function of Plant Cytochrome P450 Mint Superfamily. *J. Inorg. Biochem.* **2022**, *237*, 111990. ([link](#))
12. Yadav, S.; Shaik, S.; Siddiqui, S. A.; **Kalita, S.**; Dubey, K. D. Local Electric Fields Dictate Function: The Different Product Selectivity Observed for Fatty Acids Oxidation by Two Deceptively Very Similar P450-Peroxygenase OleT and BSbeta. *J. Chem. Inf. Model.* **2022**, *62*, 1025-1035 ([link](#))
13. Dutta, R.; **Kalita, S.**; Kalita, D. J. Tuning of Some Novel Triphenylamine-Based Organic Dyes for Their Potential Application in Dye-Sensitized Solar Cells: A Theoretical Study. *Comput. Theor. Chem.* **2018**, *1142*, 39-44. ([link](#))

Manuscripts Under Revision:

14. Shaik, S.; Danovich, D.; **Kalita, S.**; Dubey, K. D. Oriented Electric Fields – Universal Catalysts. (Revision submitted in *Acc. Chem. Res.*: **ar-2025-005087**)

SKILLS

Computational Methods: Quantum chemical DFT calculations, DFT and forcefield based hybrid quantum mechanics/molecular mechanics (QM/MM) calculations, Electronic structure calculations, Molecular orbital theory, TD-DFT, Catalysis in the presence or absence of oriented external electric field (OEEF), Eckart method/Quantum tunnelling, Molecular dynamics (MD) simulations, Non-equilibrium MD (NEMD) in the presence of static/time-varying external electric fields, Free energy calculations, Molecular docking, Enhanced sampling techniques: umbrella sampling and adaptive steered MD, Learning *ab-initio* MD simulation and meta-dynamics.

Software Tools: AMBER, GROMACS, CHEMSHELL, TURBOMOLE, GAUSSIAN, ORCA, TITAN, AutoDock Vina, CP2K, Various visualization and analysis tools, including Microsoft based software.

Programming Language: Python and Shell scripting

AWARDS & ACHIVEMENTS

- Qualified for Council of Scientific and Industrial Research, India (CSIR) Junior Research Fellowship and **National Eligibility Test (NET) for Assistant Professor in Chemical Sciences, NET-JRF-2019 (All India Rank 99)**.
- Achieved the Associate Membership of the **Royal Society of Chemistry (AMRSC)** for the year 2023.
- **Independent Reviewer** of the Scientific Journals: Journal of Cellular Physiology, Discover Chemistry, PLOS ONE and Ecotoxicology and Environmental Safety.
- **Assistant Reviewer (via supervisor):** All leading scientific journals from American Chemical Society (ACS), Royal Society of Chemistry (RSC), Elsevier, Wiley, etc.
- Awarded **IAS-INSANA-SI Summer Research Fellowship 2015**, Indian Institute of Technology Bombay, Mumbai, India.
- Selection for National Initiative on Undergraduate Sciences (**NIUS) Workshop 2012 in Chemistry**, Tata Institute of Fundamental Research (TIFR), Mumbai, India.
- Qualified for Joint Admission Test for M.Sc., **JAM-2015**.

INVITED LECTURE

Kalita, S. Assessing the Potential of Static and Oscillating Electric Fields for Treating Alzheimer's Disease. *National Seminar on Science for Sustainable Development (SSD-2025)*, Organized by Department of Chemistry, B. Borooah College, **January 2025**.

INVITED WEBINAR

Kalita S. Static and Oscillating Electric Fields to Disrupt Alzheimer's Plaques: Insights from Molecular Dynamics Simulations. Organized by *Bio-electrodynamics Research Team, Institute of Photonics and Electronics, Academy of Sciences of the Czech Republic*, **June 2025**.