PROF. NILADRI PATRA CURRICULUM VITAE DATE:02/02/2025

Prof. Niladri Patra
Associate Professor (07/2024- present)
Department of Chemistry and Chemical Biology
Indian Institute of Technology (Indian School of Mines) Dhanbad
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EDUCATION:

Education:

Ph.D.: Chemistry, University of Illinois at Chicago, Chicago, IL - 2013.
M.Sc. Chemistry, Indian Institute of Technology Delhi 2008.
B. Sc.: Chemistry (Hons.), Calcutta University, 2006.

ACADEMIC EXPERIENCE:

Associate Professor 7/2024- present
Indian Institute of Technology (Indian School of Mines) Dhanbad

Assistant Professor 12/2017- 7/2024
Indian Institute of Technology (Indian School of Mines) Dhanbad

Brookhaven National Laboratory, Upton, NY
Postdoctoral Associate

Massachusetts Institute of Technology, Cambridge, MA
Postdoctoral Associate

Institute for Theoretical Atomic Molecular and Optical Physics (ITAMP)
Harvard Smithsonian Center for Astrophysics
Predoc Fellow

PROFESSIONAL MEMBERSHIPS AND AWARDS:

- American Chemical Society
- AAMRA Fellowship (2003-2004)
- Hema Prava Debi Memorial Prize (2007)

- PAAREN Graduate Fellowship - University of Illinois at Chicago, Chicago, Illinois (2011-2012)
- Harvard Smithsonian Astrophysical Observatory Fellowship (2012-2013)
- NVIDIA Grant (2018)

PROJECTS:

1. Prediction of MexB efflux inhibitors: A combined Molecular Dynamics Simulations and Machine Learning Approach. PI, Rs. 23.47 Lakhs, DST-SERB

2. Molecular modeling approach to design new binder for low-grade iron ore pelletization, PI, Rs. 10.00 Lakhs,Tata Steel

3. Rational design of amphiphilic self-assembled graft copolymers as drug carriers: experimental and theoretical approach, Co-PI, Rs. 27.87 Lakhs, DST-SERB

4. Foam Assisted Oil-Water Nanoemulsion for Enhanced Oil Recovery: Experimental and Molecular Dynamic Simulation Studies. Co-PI, Rs. 68.95 Lakhs, OIDB

5. A Modular approach for carbon dioxide reduction by nanoparticle, PI, Rs. 2.00 Lakhs, TEQIP III

PhDs Guided: 2

PhD Ongoing: 08

M.Sc. Dissertation supervised: 21

M.Tech. Dissertation supervised: 08

PUBLICATIONS:

50. Diship Srivastava, Shreya Mukherjee, Muskan Begom and Niladri Patra**. Modulation of Gramicidin A's Structural and Dynamical Properties by Cholesterol in the Membrane**. Submitted.

49. Diship Srivastava and Niladri Patra. **Improving the Computational Efficiency of the Adaptive Biasing Force Sampling by Leveraging the Telescopic-Solvation Scheme**. J. Chem. Theory Comput. 2024, 20, 24, 10952–10960.

48. Kanchan Negi, Ashok Kumar, Gourav Chakraborty, Sudhansubala Sahoo, Niladri Patra, Sumanta Kumar Sahu, **Rationally Designed Porous Self-Assembled Nanoparticles for Combinational ChemoPhotodynamic Therapy**, Dalton Trans. Dalton Trans., 2024,53, 17465-17479.

47. Sk. Akhter, Diship Srivastava, Aman Mishra, Niladri Patra, Pankaj Kumar, Sumanta Padhi**, A physicochemical investigation on Cu(II)-based molecular catalysts for the electrochemical reduction of CO_2 to syngas**. Chem. Eur. J. 2024, e202403321.

46. Abhishek Bera, Pritish Joshi, and Niladri Patra. **Delving into Macrolide Binding Affinities and Associated Structural Modulations in Erythromycin Esterase C: Insights into the Venus Flytrap Mechanism**. J. Chem. Inf. Model. 2024, 64, 15, 5964–5976.

45. Kousik Kumar Bhanja, Niladri Patra. **Discovery of Fourth-Generation Allosteric Inhibitors Targeting EGFR T790M/L858R/C797S and T790M/L858R Mutations: A Combined Machine Learning and Molecular Dynamics Approach.** submitted

44. Rakesh Kumar Roy, Madhur Sharma and Niladri Patraa. **SARS-CoV-2 Spike Protein Variants and Bebtelovimab: Immune Escape Mechanisms Revealed by Computational Studies**, Phys. Chem. Chem. Phys., 2024,26, 29929-29939.

43. Gourav Chakraborty, Niladri Patra. **Targeting 14-3-3ζ: α-Synuclein Complexation: Identification of Allosteric Sites and Development of Modulatory Inhibitors.** submitted

42**.** Gourav Chakraborty, Keka Ojha, Ajay Mandal, Niladri Patra, **Effect of spacer group variation of gemini surfactants on the detachment of oil from silica surfaces with different hydrophobicity: a molecular dynamics study**,Phys. Chem. Chem. Phys. Accepted

41. Kousik Kumar Bhanja, Madhur Sharma, Niladri Patra. **Computational Design of Allosteric Tyrosine Kinase Inhibitors Targeting Non-Small Cell Lung Cancer.** submitted.

40. Avigyan Naskar, Rakesh Roy, Niladri Patra. **Decoding Inhibitor Egression from Wild-Type and G2019S Mutant LRRK2 Kinase: Insights into Unbinding Mechanisms for Precision Drug Design in Parkinsons Disease,** J. Phys. Chem. B 2024, 128, 28, 6657–6669.

39. Gourav Chakraborty, Niladri Patra. **Elucidating the Molecular Basis of 14-3-3 Interaction with -Synuclein: Insights from Molecular Dynamics Simulations and the Design of a Novel Protein-Protein Interaction Inhibitor.** J. Phys. Chem. B 2024, 128, 29, 7068-7085.

38. Rakesh Roy, Abhishek Bera, Niladri Patra, **Insights into Allosteric Inhibition of AcrB Efflux Pump: Role of Distinct Binding Pockets, Protomer Preferences, and Crosstalk Disruption**, J. Phys. Chem. B 2024, 128, 29, 7068-7085.

37. Gourav Chakraborty, Mahima Sudhir Kolpe, Ambily Nath I.V, Avlokita Tiwari, Praapti Jayaswal, Niladri Patra, **Computational structure-guided approach to simulate delamanid and pretomanid binding to mycobacterial F420 redox cycling proteins: identification of key determinants of resistance**, Journal of Biomolecular Structure & Dynamics, accepted.

36. Debayan Basu, Barshali Ghosh, Diship Srivastava, Niladri Patra and Hari Pada Nayek, **Mononuclear Organogermanium(IV) Catalysts for [3+2] Cycloaddition Reaction,** Dalton Trans., 2024,53, 5648-5657.

35. Abhishek Bera, Shreya Mukherjee, Niladri Patra. **Exploring the Transmembrane Allostery in MexB: DB08385 Variant as Promising Inhibitor like Candidate Against Pseudomonas aeruginosa Antibiotic Resistance – A Computational Study, Phys. Chem. Chem. Phys., 2024, 26, 17011-17027.**

34. Diship Srivastava, Niladri Patra, **Elucidating Daptomycins Antibacterial Efficacy: Insights into the Tripartite Complex with Lipid II and Phospholipids in Bacterial Septum Membrane**, J. Phys. Chem. B 2024, 128, 18, 4414–4427.

33. Diship Srivastava, Biswajit Saha, Niladri Patra, **Design of Saccharide Based Organic Binder for Low-grade Iron Ore Pelletization using Atomistic Simulations and Machine Learning Methods,** J. Mol. Graphics Modell. 2024.

32. Abhishek Bera, Rakesh Roy, Pritish Joshi, Niladri Patra, **Machine Learning-Guided Discovery of AcrB and MexB Efflux Pump Inhibitors**, J. Phys. Chem. B 2024, 128, 3, 648–663.

31. Aman Mishra, Diship Srivastava, Niladri Patra, Sumanta Padhi, **Formate Dehydrogenase Activity by a Cu(II)-based Molecular Catalyst and Deciphering the Mechanism by DFT studies,** Dalton Trans., 2024,53, 1209-1220.

30. Gourav Chakraborty, Ambily Nath I.V, Mukta Sharma, Jigar Sheth, Mahima Korib, Avlokita Tiwari, Niladri Patra, **In silico structural and mechanical insights into bedaquiline resistance associated with high-grade non-synonymous mutations in atpE, mmpR5, and pepQ**, Journal of Biomolecular Structure & Dynamics, 0, 1-13, 2023.

29. Avigyan Naskar, Kousik Kumar Bhanja, Rakesh Roy, Niladri Patra, **Structural insight into G2019S mutated LRRK2 kinase and brain- penetrant Type I inhibitor complex: A Molecular dynamics approach.** Journal of Biomolecular Structure & Dynamics, 1-21,2023.

28. Rakesh Roy, Niladri Patra, **Probing the pH Sensitivity of OprM: Insights into Metastable States and Semi-Open Conformation**, J. Phys. Chem. B 2024, 128, 3, 622–634.

27. Diship Srivastava, Niladri Patra, **Telescoping-Solvation-Box Protocol based Umbrella Sampling Method for Potential Mean Force Estimation**, J. Chem. Inf. Model. 2023, 63, 19, 6109–6117.

26. Diship Srivastava, Niladri Patra, **Enhanced Uptake of Anticancer C6-Pep Dimer in Tumor Membrane Caused by Differential pKa in Acidic Tumor Microenvironment**, J. Phys. Chem. B 2023, 127, 45, 9747–9758.

25. Kousik Kumar Bhanja, Madhur Sharma, Niladri Patra, **Uncovering the structural and binding insights of dual inhibitors simultaneously targeting two distinct sites on EGFR kinase**, J. Phys. Chem. B 2023, 127, 50, 10749–10765.

24. Avigyan Naskar, Kousik Kumar Bhanja, Rakesh Roy, Niladri Patra, Role of the Residue Q1919 in Increasing Kinase Activity of G2019S LRRK2 Kinase: A Computational Study. **ChemPhysChem** 2023, e202300306.

23. Rakesh Roy, Abhishek Bera, and Niladri Patra. Encapsulation of testosterone and dihydrotestosterone into chiral carbon nanotubes: A molecular dynamics study. **J. Mol. Liq.** 376 (2023) 121426.

22. Diship Srivastava and Niladri Patra. Self-Uptake Mechanism of Polymyxin-Based Lipopeptide against Gram-Negative Bacterial Membrane: Role of the First Adsorbed Lipopeptide. **J. Phys. Chem. B** 2022, 126, 41,8222-8232.

21. Kalipada Manna, Priyapratim Patra, Arpita Roy, Rakesh Kumar Roy, Krishna Chaitanya Sunka, Santanu Dhara, Niladri Patra, Sagar Pal, Amino Acid Inspired Alginate-Based pH Sensitive Polymeric Micelles via Reversible Addition–Fragmentation Chain Transfer Polymerization. **ACS Applied Polymer Materials.** 2022, 4, 6, 4432-4444.

20. RK Roy, N Patra. Prediction of COMT Inhibitors Using Machine Learning and Molecular Dynamics Methods. **J. Phys. Chem. B** 2022, 126, 19, 3477–3492.

19. P Bhattacherjee, M Roy, A Naskar, HC Tsai, A Ghosh, N Patra, RP John, Photoinduced generation of the active chloride-phosphate anionophore from its inactive proanionophore. **Applied Organometallic Chemistry** 36 (1), e6459.

18. Subhasis Dey, Soumya Chatterjee, Anjali Patel, Nirmalya Pradhan, Diship Srivastava, Niladri Patra, Arindam Bhattacharyya, Debasis Manna. Photoresponsive transformation from spherical to nanotubular assemblies: anticancer drug delivery using macrocyclic cationic gemini amphiphiles, **Chem. Comm.** 57 (38), 4646-4649.

17. Rakesh Roy, Niladri Patra, Configuration Flipping in Distal Pocket of Multidrug Transporter MexB Impacts the Efflux Inhibitory Mechanism, **ChemPhysChem,** 21 (23), 2516-2524.

16. Priyapratim Patra, Niladri Patra, Sagar Pal, Opposite swelling characteristics through changing the connectivity in a biopolymeric hydrogel based on glycogen and glycine, **Polym. Chem.** 11, 2630-2634 (2020).

15. Surajit Mondal, Niladri Patra, Hari Nayek, Sumit Hira, Soumit Chatterjee, Swapan Dey, Unusual absence of FRET in triazole bridged coumarin-hydroxyquinoline, an active sensor for Hg2+ detection, **Photochem. Photobiol. Sci.,** 2020,19, 1211-1221.

14. Priyapratim Patra, Venkata Sundeep Seesala, Saundry Raj Soni, Rakesh Kumar Roy, Santanu Dhara, Animesh Ghosh, Niladri Patra, and Sagar Pal. Biopolymeric pH-Responsive Fluorescent Gel for in-vitro and in-vivo Colon Specific Delivery of Metronidazole and Ciprofloxacin; **Eur. Polym. J.** 114, 255 (2019).

13. Niladri Patra and Alexie V. Tkachenko, Programmable self-assembly of diamond polymorphs from chromatic patchy particles, **PRE** 98, 032611 (2018).

12. Niladri Patra and Alexie V. Tkachenko, Layer-by-layer Self-assembly of Patchy Particles as a Route to Complex Lattice Structure, **PRE** 96, 022601 (2017).

11. Niladri Patra, Efthymios I. Loannidis and Heather J. Kulik. Computational Investigation of the Interplay of Substrate Positioning and Reactivity in Catechol O-Methyltransferase. **PLOS ONE,** 11, 1 (2016).

10. Niladri Patra, Petr Král, and Hossein. R. Sadeghpour. Nucleation and Stabilization of Carbon-Rich Structures in Interstellar media, **ApJ,** 785, 6 (2014).

9. Irena Yzeiri, Niladri Patra, and Petr Král, Porous Carbon Nanotubes: Molecular Absorption, Transport, and Separation. **J. Chem. Phys. 1**40, 104704 (2014).

8. Niladri Patra, Dominic A. Esan, and Petr Král, Dynamics of Ion Binding to Graphene Nanostructures, **J. Phys. Chem. C 1**17, 10750 (2013), cover page.

7. Ryan M. Pearson, Niladri Patra, Hao-jui Hsu, Sayam Uddin, Petr Král, and Seungpyo Hong, Positively Charged Dendron Micelles Display Negligible Cellular Interactions. **ACS Macro Letters** 2, 77 (2013).

6. Jin Woo Bae, Ryan M. Pearson, Niladri Patra, Suhair Sunoqrot, Lela Vuković, Petr Král, and Seungpyo Hong, Dendrons-mediated Self-assembly of highly PEGylated block copolymers: a modular nanocarrier platform, **Chem. Comm.** 47, 10302 (2011).

5. Niladri Patra and Petr Král, Controlled Self-assembly of filled Micelles on Nanotubes, **J. Am. Chem. Soc.** 133, 6146 (2011).

4. Petr Král, Lela Vuković, Niladri Patra, Boyang Wang, Kyaw Sint, and Alexey Titov, Control of Rotary Motion at the Nanoscale: Motility, actuation, self-assembly, **J. Nanosci. Lett.,** 1, 128, (2011). (Cover page)

3. Niladri Patra, Yuanbo Song, and Petr Král, Self-Assembly of Graphene Nanostructures on Nanotubes,

ACS Nano 5, 1798 (2011).

2. Goutam Mukherjee, Niladri Patra, Poranjyoti Barua, and Bhairav Jayaram, Fast Empirical GAFF Compatible Partial Atomic Charge Assignment Scheme for Modeling Interactions of Small Molecules with Biomolecular Targets, **J. Comp. Chem.** 32, 893 (2010).

1. Niladri Patra, Boyang Wang, and Petr Král, Nanodroplet Activated and Guided Folding of Graphene Nanostructures, **Nano Lett.** 9, 3766 (2009).

PROCEEDINGS:

- Petr Král, Lela Vuković, Niladri Patra, Boyang Wang, and Alexey Titov, Control of Rotary Motion at the Nanoscale: Motility, Actuation, Self-assembly, Proceedings of the Beilstein Symposium on Functional Nanoscience, Bozen, June, 2011.
- Niladri Patra, Petr Král, and Hossein. R. Sadeghpour. Dynamics of Synthesis of Large Carbon Structures in Interstellar Medium. Proceedings IAU Symposium 297: The diffuse interstellar bands. Netherlands, May, 2013.
- Ryan M Pearson, Jin Woo Bae, Niladri Patra, Suhair Sunoqrot, Sayam Uddin, Lela Vukovic, Petr Král, Seungpyo Hong, Synthesis and self-assembly of highly PEGylated dendron-coils: A potential nanocarrier platform. Cancer Research, Vol. 72, 1954-1954.

BOOK CHAPTERS:

- John Russell, Boyang Wang, Niladri Patra, Petr Král, Water Nanodroplets: Molecular Drag and Self-assembly. Nanodroplets, Lecture Notes in Nanoscale Science and Technology, Volume 18 2013, ISBN: 978-1-4614-9471-3.

CONFERENCES ATTENDED:

- 237th American Chemical Society National Meeting and Exposition, spring 2009, Salt Lake, Utah, March 22–26, 2009.
- 41st Midwest Theoretical Chemistry Conference, Carbondale, Illinois, May 28-30, 2009.
- International Institute for Nanotechnology Symposium, October 29, 2009
- 239th American Chemical Society National Meeting and Exposition, spring 2010, San Francisco, March 21–25, 2010.
- 42nd Midwest Theoretical Chemistry Conference, Purdue University, Indiana, May 20-22, 2010.
- International Institute for Nanotechnology Symposium, October 21, 2010.
- Workshop on Self-Assembled Bio-Inspired Materials for Energy, Argonne National Laboratory, February 4-5, 2011.
- 241st American Chemical Society Meeting and Exposition, spring 2011, Anaheim, March 27–31, 2011.
- 243rd American Chemical Society National Meeting and Exposition, spring 2012, San Diego, March 25–29, 2012.
- 44 th Midwest Theoretical Chemistry Conference, Wisconsin, Madison, June 7-9, 2012.
- 245th American Chemical Society National Meeting and Exposition, spring 2013, New Orleans, April 7–11, 2013.
- Gordon Research Conference: Complex Active and Adaptive Material Systems. Ventura, January 29th, 2017 - 3rd February, 2017
- RTCST, IIT Patna, 2024
- MD@60. JNCSAR Bangalore, 2024

PRESENTATIONS:

- Niladri Patra, Boyang Wang, and Petr Král, Nanodroplet Activated and Guided Folding of Graphene Nanostructures, 239th American Chemical Society National Meeting and Exposition, spring 2010, San Francisco, March 21–25, 2010.
- Niladri Patra, Boyang Wang, Yuanbo Song, and Petr Král, Activated and Guided Self-assembly of Graphene Nanostructures, 241th American Chemical Society National Meeting and Exposition, spring 2011, Anaheim, March 27–31, 2011
- Niladri Patra, Yuanbo Song, and Petr Král, Controlled Self-Assembly of Nanostructures on Nanotubes, 243rd American Chemical Society National Meeting and Exposition, spring 2012, San Diego, March 25–29, 2012.
- Niladri Patra, Dominic A. Esan, and Petr Král, Scanned Quantum Molecular Dynamics Simulations: Ion Binding to Graphene Nanostructures, 245th American Chemical Society National Meeting and Exposition, spring 2013, New Orleans, April 7-11, 2013.
- Niladri Patra, Petr Král, and Hossein. R. Sadeghpour, Self-assembly of Carbon Atoms in Interstellar Space and Formation Mechanism of Naphthalene from Small Precursors: A Molecular Dynamics Study, CFA symposium, SAO, Harvard University, April 26th, 2013.
- Niladri Patra and Alexie V. Tkachenko, Layer-by-layer Self-assembly of Patchy Particles as a Route to Complex Lattice Structure, Brandeis University, Waltham, MA, September 23, 2016.

SOFTWARE:

- Brownian Dynamics Simulation software

JOURNAL REVIEWER:

- He is a reviewer of more than 15 International Journals, namely, Scientific Reports, ACS Nano, Soft Matter, The Journal of Physical Chemistry, Chemical Physics, Physical Chemistry Chemical Physics, etc.

REVIEW PANEL MEMBER:

- 2016 ASCR Leadership Computing Challenge

EXPERTISES:

- Methods: Coarse-grained, all atom classical, reactive, QM/MM and ab initio MD simulations, free energy methods, force field development, Free energy Methods, Machine Learning, electronics structure calculations
- Programming and Script Languages: FORTRAN, C++ , Python, bash, perl, TCL
- Molecular Modeling Packages: AMBER, NAMD, LAMMPS, Quantum Espresso, TeraChem, Gaussian09, GAMESS