

Sobitri Sen, PhD

Present Positions: 1. Postdoctoral Research Associate at [NIT Manipur, India](#).

2. Visiting Scientist, QuantAct Lab, IISER Kolkata

Past position: Visiting Faculty, Chemistry, Ideal Institute of Engineering (IIE), Kalyani (2024)

PhD: Theoretical and Computational Chemistry, IISER Kolkata, (2018-2024)

MSc: Chemistry, Lovely Professional University (LPU), Punjab, (2016-2018)

OBJECTIVE: Seeking a challenging career opportunity to fully utilize my training, while making a significant contribution to the success of the organization.



RESEARCH INTEREST

Catalysis, Metal-free N₂ activation, urea and NH₃ production, water-splitting reactions, HF/post-HF and DFT simulations, Organocatalysts, Charge transfer properties, Superconductivity, Solar Fuel.

MATERIALS of INTEREST

Cyclo[n]carbons, Zeolite, Graphene, Polynitrogen and gold clusters, HEDMS, Carbon based nano materials, Si-doped Carbon clusters.

FELLOWSHIPS and SCHOLARSHIPS

- NIT Manipur Postdoctoral Fellowship to pursue postdoc in India.
- INSPIRE-AORC Fellowship to pursue PhD in India.
- LPUNEST Scholarship to pursue MSc in Chemistry at LPU, India.

AWARDS and RECOGNITIONS

- **Invited Talk** at ACS Global Virtual Symposium- **In-silico Organic Chemistry**, Spring 2024, March 18, 2024.
- **Poster presentation** at Theoretical Chemistry Symposium (TCS), IIT Madras, India, Dec 07-10, 2023.
- **Best Poster award** at QSCP-XXVI: 26th International Workshop on Quantum Systems in Chemistry, Physics, and Biology, India, Oct 14-20, 2023.
- **University Gold Medal** and **First Rank Certificate** for securing the first position in MSc, LPU for the year 2016-18.
- **University Honor Roll**, LPU for the academic session of 2016-2017.
- **Third position** in Explorica-Exploring Young Talent, LPU, Nov 2017.
- **First position** in Explorica-Exploring Young Talent, LPU, Nov 2016.

ACHIEVEMENTS

- Job offer from AgNext, a smart AgroTech Company (2018).
- Job offer as Visiting Faculty, IIE Kalyani, (2024).

RESEARCH EXPERIENCE

- 6+ years of research in *simulations of catalysts and materials* relevant to renewable energy, drugs and useful chemicals using Si-based carbon structures and organocatalysts.
- 4+ months of **R&D experience** in NIR spectroscopy and data analysis, estimating active ingredients in agricultural products.
- Experienced simulation specialist working in the areas of cyclo[n]carbons, gold and polynitrogen nanoclusters, zeolites, graphene etc.
- 9+ months of postdoctoral (visiting scientist and research associateship) and 5+ years of doctoral research.
- MSc thesis under the joint supervision with Prof. Sourav Pal (IISER Kolkata) and Dr. Nupur Prasad (LPU), India.
- Experience in thermochemical analysis of surfactants on animal protein at IIT Bombay.

TECHNICAL EXPERIENCE

- **Scientific Softwares:** Gaussian, GAMESS, Multiwfn, MATLAB, Quantum Espresso etc.
- **Instrumental proficiency:** UV-IR, UV-thermal, Fluorescence NIR spectrophotometers, Flame photometer, TLC/Column chromatography, Digital pH meter, Moisture analyzer etc.
- **Important working tools:** MSOffice suites, GSuite programs, LaTeX, OverLeaf editors etc.
- **Picture editing tools:** XmGrace, XFig, GNUplot etc.
- **Databases and drawing tools:** ChemDraw, ChemSketch, Avogadro, GaussView, SciFinder, WebOfScience, Libgen, Materials Studio etc.
- **Programming Languages:** C, C++, Java, Python, R etc.

SOFT SKILLS

- Excellent proposal writing skills for financial grant. Received DST-INSPIRE-AORC fellowship (2019). Submitted proposals for Tea analysis in R&D (2018) and DST-WISE-PDF funding (2024) for research.
- Experienced in drafting articles, reviews, and reports, with 4 first-author publications in high-impact journals and 2 under review.
- Proficient with ScholarOne™, Editorial Manager®, and other tools for manuscript processing.
- Excellent oratory and presentation skills.
- Skilled in building professional networks through strong communication and improving efficiency by identifying issues and streamlining processes.

TEACHING and MENTORING EXPERIENCE

Taught chemistry to B.Tech students, focusing on conceptual and analytical skills through rigorous coursework. Mentored MSc and PhD students in organic synthesis and spectroscopy, blending theory with practical expertise.

MANAGEMENT SKILLS

- Experience of 6+ years of managing own research projects.
- Experience in managing 2 different financial grants during doctoral and postdoctoral training.
- Presently responsible of managing 2 research projects in NIT Manipur.

PERSONAL DETAILS

- Nationality: Indian
- Date of Birth: 29th August 1993
- Gender: Female
- Marital Status: Unmarried
- Languages: English, Hindi and Bengali

CONTACT INFORMATION



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<https://scholar.google.com/citations?user=y78xhYIAAAAJ&hl=en&oi=ao>



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PUBLICATIONS

1. Sen, S.; Bag, A.; Pal, S. Genesis of Polynitrogen Compounds employing Silicon Substituted Cyclo[18]Carbon: A DFT Investigation, *ChemPhysChem* **2024**, e202400535.
2. Sen, S.; Bag, A.; Pal, S. Mechanistic Inquisition on the Reduction of C₁₇Si(NH₂)₂ to NH₃: A DFT Study, *ChemPhysChem* **2024**, e202300723.
3. Sen, S.; Bag, A.; Pal, S. Activation and Conversion of Molecular Nitrogen to the Precursor of Ammonia on Silicon Substituted Cyclo[18]Carbon: A DFT Design, *ChemPhysChem* **2023**, 24, e202200627.
4. Sobitri, Sen., Abhrajit, Bag., and Arijit, Bag. Justicia adhatoda - A Proven Medicine for COVID-19: Clinical Survey Report. *Acta Scientific Clinical Case Reports*. **2021**, 2, 25-29.
5. Sen, S.; Bag, S.; Dinda, M.; Bag, A. The Magic Molecule- Cyclo[18]Carbon: A Detailed Review. *(Communicated)*
6. Sen, S.; Bag, A. Water-splitting reactions on doped Au₇-cluster: A First Principle Mechanistic Approach. *(Communicated)*

SUBJECT AREAS of INTEREST

- **Physical Chemistry:** Quantum Chemistry, Thermodynamics, Chemical Kinetics and Equilibria, Solid States, Kinetic Theory, and Spectroscopy.
- **Organic Chemistry:** Stereochemistry, IUPAC Nomenclatures, Synthesis, Name Reactions.
- **Inorganic Chemistry:** Catalysis, Main Group and Coordination Chemistry, Chemical Bonding.
- **Interdisciplinary Chemical Sciences:** Environmental Chemistry, Industrial Chemistry, Biophysical Chemistry, Macromolecules and Polymer Chemistry, Computer Programming and its Applications in Chemistry, Legal Compliances and Industry Standards in Chemistry.

PhD Supervisor

Prof. Sourav Pal

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Former Director, IISER Kolkata
Head, Department of Chemistry,
Ashoka University, India.

Postdoc Supervisor

Prof. Chandi Charan Malakar

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Associate Professor, Department of
Chemistry, NIT Manipur, India.

Research Collaborator and Mentor

Prof. Debashis Chakraborty

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Professor, Department of
Chemistry, IIT Madras, India.

I HEREBY DECLARE THAT THE ABOVE PARTICULARS ARE
TRUE TO THE BEST OF MY KNOWLEDGE AND BELIEF

Sobitri Sen

Dr. Sobitri Sen