SURAJIT NANDI

PERSONAL INFORMATION

Given Name	Surajit
Surname	Nandi
Date of Birth	9th November, 1988
Birth place	Panchmura, India

EDUCATION

PhD in Chemistry **December 2011 – October 2017**

Institute : Indian Institute of Technology Kharagpur, Kharagpur, India

Thesis Title : Computational Studies of Chemical Reactions: Manual Modelling and Development of Automated Methods

Master of Science in Chemistry **July 2009 – June 2011**

Institute : Indian Institute of Technology Kharagpur, Kharagpur, India

Master's Thesis Title : Studies on Coordination Driven Ligand Hydrolysis and Transition Metal Complexes of N,O Donor Ligands

GPA : 7.82 out of 10

Bachelor of Science in Chemistry with Honors **August 2006 – June 2009**

Institute : The University of Burdwan, West Bengal, India

Marks Obtained : 64.87 %

RESEARCH EXPERIENCE

- Indian Institute of Technology Indore, India

  Working as : Postdoctoral Fellow **December 2017 – September, 2018**

  Advisor : Dr. Biswarup Pathak

- Indian Institute of Technology Kharagpur, India

  Worked as : Research Scholar **December 2011 – October 2017**

  Advisor : Dr. Anoop Ayyappan

- Westfälische Wilhelms-Universität Münster, Germany

  Worked as : Guest student **1st May - 31st July, 2013**

  Advisor : Dr. Mark Paul Waller

- Implemented a **tabu-search** based algorithm for **automatically** predict chemical reactions.
- Published an opensource code at **https://github.com/anooplabiitkgp/PyAR**.
- Developed a method to **predict global minima** of molecular aggregates.
- **Cytochrome P450** catalysed oxetane formation in taxol biosynthesis.

- **Heterogeneous catalysis** by using periodic density functional theory.
- **Materials design**.
- **QTAIM** analysis.
- Oxygen reduction reaction.
- Studied **excited state** reactions using **TD-DFT** and **CASSCF** method.
- Studied **Pd-catalysed** cyclization reaction using DFT.
- Analysis of electronic structure using DFT.
- **DLPNO-CCSD(T)** method for electronic structure calculation.
- Applied **automated reaction** search method to solve a problem in **pre-biotic** chemistry.
- Use of unsupervised **machine learning** method to cluster molecular aggregates.
- ***Ab initio* molecular dynamics** simulation to analyse molecular stability.

COMPUTER SKILLS

Programming languages	Knowledge of C, Fortran, C++
Scripting languages	Experience in **Python**, **bash**, tclsh
Software packages used	VASP, ChemShell, Gaussian, Mopac, ORCA, TURBOMOLE, Modeller, Multiwfn, CHARMM, VMD, NAMD
Knowledge on database	Materials Project

TEACHING EXPERIENCE

Teaching Assistant, IIT Kharagpur, India **January 2012 – October 2017**

- Tutored sophomore students in Physical Chemistry Laboratory
- Tutored graduate students in Computational Chemistry Laboratory
- Taught Physical Chemistry to sophomore students
- Mentored undergraduate project students
- Mentored summer project students

HONORS AND AWARDS

- Qualified for Lectureship in National Eligibility Test carried out by Council of Scientific and Industrial Research-University Grant Commission
- Ranked 160 among 2585 students in Joint Admission Test to M. Sc. (JAM) in Chemistry - **2009**
- Ranked 386 among 10608 students in Graduate Aptitude Test in Engineering in Chemistry - **2011**

RESEARCH INTEREST

I am interested to involve in research on the origin of life on earth by using computational chemistry. Given my experience with reaction mechanism, algorithm implementation, I would like

to build a simulation model which can effectively mimic the pre-biotic condition and therefore give out the most probable path to the purine base formation. The shear amount of possible reaction paths to be explore in this process will demand to use computationally cheaper tools salong side DFT. Hence, I will learn new computational techniques which can qualitatively predict molecular structure without the expensive DFT calculation at least for the small molecules and hence help to achieve my goal.

PUBLICATIONS

1. *A Coordination-assisted General Approach to Nickel-based Nano Metallogels*; Santu Dey, D. Datta, K. Chakraborty, S. Nandi, A. Anoop, T. Pathak, *RSC Advances*, **2013**, *3*, 9163-9166.
2. *Viability of All-Pnictogen Anions*; S. Mandal, S. Nandi, A. Anoop, P. K. Chattaraj, *Physical Chemistry Chemical Physics*, **2016**, *18*, 11738-11745.
3. *A p-Hydroxyphenacyl–Benzothiazole–Chlorambucil Conjugate as a Real-Time-Monitoring Drug-Delivery System Assisted by Excited-State Intramolecular Proton Transfer*; S. Barman, S. K. Mukhopadhyay, S. Biswas, S. Nandi, M. Gangopadhyay, S. Dey, A. Anoop, N. D. P. Singh, *Angewandte Chemie*, **2016**, *128*, 4266-4270.
4. *Molecular Engineering of Triphenylamine Based Aggregation Enhanced Emissive Fluorophore: Structure Dependent Mechanochromism and Self-Reversible Fluorescence Switching*; P. S. Hariharan, V. K. prasad, S. Nandi, A. Anoop, D. Moon, S. Anthony, *Crystal Growth & Design*, **2017**, *17*, 146-155.
5. *Pd-Catalyzed Intramolecular Sequential Heck Cyclization and Oxidation Reactions: a Facile Pathway for the Synthesis of Substituted Cycloheptenone Evaluated Using Computational Studies*; J. K. Ray, S. Paul, P. Ray, R. Sinha, D. Y. Rao, S. Nandi, A. Anoop, *New Journal of Chemistry*, **2017**, *41*, 278-284.
6. A Tabu-Search Based Strategy For Modeling Molecular Aggregates And Binary Reactions; s. Nandi, S. R. McAnanama-Brereton, M. P. Waller, A. Anoop, *Computational and Theoretical Chemistry*, **2017**, *1111*, 69-81.
7. *Bis-Acetyl Carbazole: Photoremovable Protecting Group For Sequential Release Of Two Different Functional Groups And Its Application For Therapeutic Release;* P. Singh, Y. Venkatesh, S. Nandi, M. Shee, A. Anoop, *European Journal of Organic Chemistry,* **2017**, *2017*, 6121-6130.
8. *Esipt-Induced Fluorescent O-Hydroxycinnamate: Self-Monitoring Phototrigger For Prompt Image-Guided Uncaging Of Alcohols*; A. Paul, R. Mengji, O. Chandy, S. Nandi, M. Bera, A. Jana, A. Anoop, N. D. Pradeep Singh, *Accepted in Organic & Biomolecular Chemistry,* **2017**, *15*, 8544-8552.
9. *Prebiotic Chemistry of HCN Tetramerization by Automated Reaction Search*; S. Nandi, D. Bhattacharyya, A. Anoop, *Chemistry - A European Journal,* **2018**, *24*, 4885-4894.

SYMPOSIA ATTENDED

- Thirteen Theoretical Chemistry Symposium 2012, Organized at IIT Guwahati, India (Presented Poster).
- Fourteen Theoretical Chemistry Symposium 2014, Organized at CSIR-NCL, Pune, India (Presented Poster).
- **251st American Chemical Society National Meeting & Exposition**, Held at San Diego, California (Presented Poster).

- Computational Modelling of Molecules and Materials (CM3-2016), Held at Nainital, India (Presented Poster; **Best Poster Award**).

REFERENCES

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Associate Professor, Discipline of Chemistry,
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Indore – 453552, Madhya Pradesh, India
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