**SUMAN BHAUMIK**

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| 218, SOH 1, Jatni Campus,  National Institute of Science Education and Research,  P.O.: Bhimpur-Padanpur, Jatni,  Dist.: Khordha, Odisha, India. PIN 752050.  Email: [suman.bhaumik@niser.ac.in](mailto:suman.bhaumik@niser.ac.in) |  |

EDUCATION

**5 - Year Integrated MSc in Chemistry** 2014 – May 2019 (Expected)

National Institute of Science Education and Research (NISER), Bhubaneswar **Current CGPA = 9.06/10.0**

### All India Senior School Certificate Examination 2014

Ramakrishna Mission Vidyalaya, Viveknagar **Percentage-92.6%**

### All India Secondary School Examination 2012

Ramakrishna Mission Vidyalaya, Viveknagar **CGPA-10.0/10.0 (A1 in all)**

RESEARCH INTEREST

Computational Chemistry, Computational Biology, Cheminformatics, Bioinformatics, Theoretical Chemistry, Density Functional Theory, Reaction Dynamics, Molecular Dynamics, Spectroscopy, etc.

## EXPERIENCES



**Master’s Thesis**

**School of Chemical Sciences, NISER, Bhubaneswar July 2017- Ongoing**

Mentor: Dr. Himansu Sekhar Biswal, Reader-F.

Topic: Computational study of unusual noncovalent interactions in proteins.

* *Carbon Bonds as Ubiquitous Hydrophobic Interactions in Proteins.(Completed)*
  + Built in codes were written in Python providing specific geometrical criterias for the search of the above mentioned unique type of sigma hole interactions in proteins.
  + Positive results aided in the development of model systems for the study of this unique type of interaction both computationally and experimentally.
  + NBO, AIM, NCI and MESP calculations revealed the interaction to be the same as conventional carbon bond.
  + Similar results were obtained through the help of experimentalists in our group.
  + Detailed secondary structure analysis of the donor and acceptor pairs of the enlisted interactions were done using a combined platform of STRIDE, DSSP and built in python codes that helped us unravel in depth preferences of the protein structures for each other.

(*Manuscript currently under preparation for publication. Preprint available [here](https://github.com/sumanbhaumik/sumanbhaumik.github.io/blob/master/docs/CARBON_BONDING.pdf).*)

* *Geometrical Characterization of sulfur and selenium containing hydrogen bonds.(Ongoing)*
  + Addition of hydrogen coordinates to the PDB files with the help of REDUCE-H.
  + Python codes for finding different sulfur and selenium centred hydrogen bonds.
  + Distance and angular distributions of the enlisted interactions.
  + Secondary structural analysis of the donor-acceptor interactions.
* *Software development based on python for finding any kind of noncovalent interactions in proteins based on geometrical parameters.(Ongoing)*

**Summer Internship**

**Solid State and Structural Chemistry Unit,**

**Indian Institute of Science, Bangalore. May 2018 – Ongoing**

Mentor: Prof. Gautam R. Desiraju

### Topic: Cambridge Structural Database (CSD) and Computational Analysis of noncovalent interactions in pnicogen series.

* Extensive CSD search for specific noncovalent interactions involving pnicogens.
* Distance and angular distributions of the respective interactions.
* Model systems to be designed for computational study of specific type of noncovalent interaction.
* NBO, AIM, NCI and MESP calculations to confirm the interaction and specify its type.

**Short project**

**School of Chemical Sciences, NISER, Bhubaneswar January 2018 – February 2018**

Mentor: Dr. Himansu Sekhar Biswal, Reader-F.

Topic: Electron transfer dissociation of synthetic and natural peptides containing lanthionine/methyllanthionine bridges.

* Performed the computational studies on radical‐mediated side‐chain cleavage of the MeLan bridges.
* Performed the geometry optimizations and frequency calculations of the reactants and the products using Turbomole quantum chemistry package.
* Performed the single point energy calculations done using higher basis sets as that of geometry and frequency calculations.
* Devised pathways of fragmentation with the aid of convenient quantum chemistry calculations.

(*Work published at Rapid Communications in Mass Spectrometry. Publication available [here](https://github.com/sumanbhaumik/sumanbhaumik.github.io/blob/master/docs/mass_spectrometry.pdf).*)

**Summer Internship**

**Department of Chemistry,Indian Institute of Technology, Kharagpur** **June 2017 – July 2017**

Mentor: Prof. Pratim Kumar Chattaraj

Topic: Check of Size Consistency in Electronic Structure Calculations at Different Levels of Theory.

* Understood the concepts of size consistency and size extensivity through Einstein-Podolsky-Rosen Paradox, Bell’s inequality, etc.
* Verified the size consistency criterion for hydrogen, fluorine and hydrogen fluoride molecules by generating respective graphs of potential energy profiles.
* Performed the work using methods like Hartree-Fock, B3LYP, B3PW91, BPV86, MP2, CCSD, etc and basis sets like 3-21G, 6-31G, 6-31G(d,p), 6-31G++(2d,p), cc-pVTZ, Def2-TZVP, etc.
* Obtained the energy-distance scans and single point calculations using Gaussian 09 and plotted the same using Origin- Pro8.

(*Work is available [here](https://github.com/sumanbhaumik/sumanbhaumik.github.io/blob/master/docs/SizeConsistency.pdf).)*

**Summer Internship**

**Inorganic and Physical Chemistry,**

**Indian Institute of Science, Bangalore. May 2017 – June 2017**

Mentor: Dr. Atanu Bhattacharya, Assistant Professor.

### Topic: Comparison of Internal Conversion Dynamics of Azo and Azoxy Energetic Moieties through the (S1/S0) Conical Intersection

* Performed a nonadiabatic molecular dynamics study of the nonradiative decay of photoexcited cis-trans isomers of azomethane as well as azoxymethane
* Performed molecular dynamics study using the ab initio multiple spawning (AIMS) program that has been interfaced with the General Atomic and Molecular Electronic Structure System (GAMESS) quantum chemistry package for on-the-fly electronic structure evaluation.
* Carried out the AIMS-GAMESS simulations of the nonadiabatic decay of the n−π\* excited state using the state averaged (SA)-complete active space self- consistent field (CASSCF) method with an active space of six electrons in four orbitals, denoted CASSCF(6,4).

(*Currently under review at the Chemical Physics - Journal - Elsevier. Preprint available [here](https://github.com/sumanbhaumik/sumanbhaumik.github.io/blob/master/docs/iisc_paper_chemphys.pdf).*)

FELLOWSHIPS AND ACHIEVEMENTS

* Received silver medal in Chess at Inter IISER Sports Meet (IISM) held at Indian Institute of Science Education and Research (IISER), Kolkata. (*2016*)
* Selected for the prestigious **Indian Academy of Sciences Summer Research Fellowship**

**Programme** to work at Indian Institute of Technology (IIT), Delhi. (*2016*)

* Received the **semester topper (3rd semester)** prize in my parent institute. (*2016*)
* Qualified the **Regional Mathematics Olympiad (RMO)** and appeared for the **Indian National Mathematical Olympiad (INMO).** (*2012*, *2013* and *2014*)
* Received the **Innovation in Science Pursuit and Inspired Research Fellowship (INSPIRE)**

Grant from **Department of Science and Technology (DST)**, Government of India.

(*August, 2014 – ongoing*)

SEMINARS & CONFERENCES

* The **22nd Biennial Indian Photobiology Society (IPS) Conference on Bimolecular Dynamics- Experimental**

**and Theoretical Perspectives** held at National Institute of Technology (NIT) Rourkela from December 18-20, 2017.

It comprised of talks from eminent researchers across India.

* The **CV Raman memorial talk** given by Nobel laureate and renowned astrophysicist **Prof. Brian Schmidt** at Indian Institute of Science (IISc) Bangalore on 2nd June, 2017.
* The 30th **Annual Conference of Orissa Chemical Society** held at Kalinga Institute of Social Sciences Auditorium, Bhubaneswar from December 24–25, 2016. It comprised of talks from eminent researchers across India.

RELEVANT COURSEWORKS



**Chemistry Core Theory Courses**

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| * **BASIC INORGANIC CHEMISTRY** | * **CHEMICAL THERMODYNAMICS** |
| * **REACTION MECHANISMS IN ORGANIC CHEMISTRY** | * **REAGENTS IN ORGANIC SYNTHESES** |
| * **MAIN GROUP AND ORGANOMETALLIC CHEMISTRY** | * **QUANTUM CHEMISTRY I** |
| * **PHYSICAL ORGANIC CHEMISTRY** | * **MOLECULAR SPECTROSCOPY AND GROUP THEORY** |
| * **STATISTICAL MECHANICS** | * **COORDINATION CHEMISTRY** |
| * **CHEMICAL BINDING** | * **PHYSICAL METHODS IN CHEMISTRY I** |
| * **PHYSICAL METHODS IN CHEMISTRY II** | * **CHEMISTRY OF HETEROCYCLES AND NATURAL PRODUCTS** |
| * **CHEMICAL RATE PROCESS** |  |

**Chemistry Core Laboratory Courses**

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| * **CHEMISTRY LAB III** | * **ELECTRONICS LAB** |
| * **PHYSICAL CHEMISTRY LAB I** | * **BIOMOLECULAR CHEMISTRY LAB** |
| * **ORGANIC CHEMISTRY LAB I** | * **INORGANIC CHEMISTRY LAB I** |
| * **PHYSICAL CHEMISTRY LAB II** | * **ORGANIC CHEMISTRY LAB II** |

**Biology and Chemistry Electives**

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| * **BIOCHEMISTRY** | * **GENETICS** |
| * **PRINCIPLES OF DRUG DESIGN** | * **ECOLOGY** |
| * **NUCLEAR MAGNETIC RESONANCE** | * **MOLECULAR MODELLING** |
| * **ADVANCED BIO-INORGANIC CHEMISTRY** |  |

TECHNICAL SKILLS

**Programming Languages: Other Packages:** Gnuplot, Latex, Origin, **Gaussian09**,

Python, C++, Java **GAMESS, TURBOMOLE, AMBER, MOLPRO, etc.**

# Operating Systems:

## Linux, Windows.

EXTRA CIRRICULAR ACTIVITIES



*Activities and Positions of Responsibility*

* **Admin of Science Activities Club** of NISER, Bhubaneswar (July 2016 – ongoing) - Responsible for organizing talks and events especially in the fields of chemistry. The activities of the club includes public colloquia, open days and public demonstration and guided laboratory tours for school students.
* **Trained Cricketer** and participated in many club tournaments during early school days.
* **Chess player** and won several competitions starting from the age of 6 years.
* **Singer** and have interest in country music, folk songs, pop songs, melody songs, etc.

*Social Activities*

### Member of the outreach committee of a social organization named “Zaariya”.