CURRICULUM VITAE

PERSONAL INFORMATION

SWATI SNIGDHA PRIYADARSINI

Michigan State University

East Lansing, Michigan, USA

priyada2@msu.edu snigdhaswati04@gmail.com

Gender Female | Date of birth 10 April 1998 | Nationality Indian

EDUCATION

August 2021 – Present

Graduate Student in the Department of Chemistry

Pursuing Ph.D. in Theoretical and Computational Chemistry

Research Advisor: Prof. Piotr Piecuch

Michigan State University, USA

August 2016 – August 2021

Master of Science (5 Year Integrated) - Chemistry

National Institute of Science Education and Research (NISER) Bhubaneswar

Cummulative Grade Points Average (CGPA): 8.97/10

ACADEMIC ACHIEVEMENTS

Fellowships

- Summer Undergraduate Research Fellowship in Computational and Theoretical Chemistry (SURF-CTC), University of Minnesota, 2020 (cancelled due to COVID-19)
- Indian Academy of Sciences Summer Project Fellow, 2019
- Indian Academy of Sciences Summer Project Fellow, 2018
- Qualified Kishore Vygyanik Protsahan Yojna (KVPY), SB Stream Fellowship, All India Rank 2
- Department of Science and Technology - Innovation in Science Pursuit for Inspired Research (DST-INSPIRE) Fellow, 2016-17

Awards

- Academic Excellence Award, School of Chemical Sciences, NISER, 2019-20 and 2020-21
- First position, Prof. M. K. Rout Memorial Essay Competition, Orissa Chemical Society, 2018
- Qualified National Entrance Screening Test (NEST) for undergraduate admission to NISER Bhubaneswar
- **School Rank 1** with 95.2% in Class 12 and received certificate of merit from the Ministry of Human Research Development (MHRD), Government of India

RESEARCH INTERESTS

- Theoretical and Computational Chemistry
- Electronic Structure Theory
- Reaction Mechanism and Dynamics

RESEARCH EXPERIENCE

M.Sc. Thesis (2019 – 2021)
Dynamics of Automerization of Cyclooctatetraene and Ring Opening in Bicyclo[4.2.0]octa-2,4,7-triene under External Force
Project Supervisor: Dr. U. Lourderaj, NISER Bhubaneswar, India

Summer 2019
Stabilization of Cr-Cr Quintuple Bond using (2.1.2.1) Porphyrinoid Based Ligand : A Computational Study
Project Supervisor: Prof. P. K. Chattaraj, IIT Kharagpur, India

Summer 2018
Study of Li-Be Bonding with N-heterocyclic carbene and N-heterocyclic boryl Ligands.
Project Supervisor: Prof. P. K. Chattaraj, IIT Kharagpur, India

Summer 2017
Study of Lanthanide (Europium and Terbium) Doped Hydroxyapatite Nanotubes.
Project Supervisor: Prof. D. Khushalani, TIFR, Mumbai, India

PUBLICATIONS

Dynamics of Ring Inversion and Double Bond Shift in Cyclooctatetraene
Swati Snigdha Priyadarsini and Upakarasamy Lourderaj
(To be submitted to *J. Phys. Chem. A*)

PARTICIPATION IN WORKSHOPS

- VIJYOSHI (National Science Camp) organised by Indian Institute of Science Bengaluru, 2017
- National Initiative for Undergraduate Sciences (NIUS) camp in Chemistry organized by HBCSE, Tata Institute of Fundamental Research (TIFR), December 2016
- INSPIRE Science Camp, KIIT University, Odisha, 2013
- National Adventures Camp organised by Bharat Scouts and Guides, 2012

COMPUTER SKILLS

Operating Systems	Windows, Linux
Languages	C, C++, Fortran, Python, Bash Shell Scripting
Scientific Software	Gaussian, Molpro, NWChem, VENUS, CHARMM
Data Analysis	Molden, Avogadro, VMD, Chemcraft, Chemdraw, Gnuplot
Word Processing	LaTeX, Microsoft Office, LibreOffice

LANGUAGES

- Odia (Mother tongue)
- Hindi
- English

RESEARCH ABSTRACT

M.Sc. Thesis (2019 – Present) — Dynamics of Automerization of Cyclooctatetraene and Ring opening in Bicyclo[4.2.0]octa-2,4,7-triene under External Force

Abstract Cyclooctatetraene (COT) is known to undergo automerization reactions, viz., ring inversion (RI) and double bond shift (DBS) under thermal and photochemical conditions. In this project, the mechanisms and dynamics of the thermal automerization of COT was investigated computationally. The potential energy surface for the RI and DBS isomerization reactions were mapped using multi-reference wavefunction (CASSCF(8,8)) methods and the dynamics was studied using *ab initio* classical trajectory simulations. The reactions were found to avoid the minimum energy paths and exhibit non-statistical dynamics.

In the next part of the project, the force-induced ring opening of bicyclo[4.2.0]octa-2,4,7-triene, a valence isomer of COT was investigated. The potential energy profiles for the force-induced reactions were mapped using the constrained geometries simulate external force (CoGEF) method. This work is in progress.

Summer 2019 — Stabilization of Cr–Cr Quintuple Bond using (2.1.2.1) Porphyrinoid Based Ligands: A Computational Study

Abstract Stabilization of Cr(I)–Cr(I) quintuple bond is of fundamental interest in chemical bonding. In this project, density functional theory based computations (BLYP/def2-TZVP) were carried out to study the structure, stability, and nature of bonding in Cr(I)–Cr(I) dimer with (2.1.2.1) porphyrin based frameworks as the ligands. The thermodynamic stability of the systems were studied by considering the various dissociation channels. The dissociation reactions were found to be non-spontaneous and hence these complexes are expected to be stable at 298.15 K and 1 atm pressure.

Summer 2018 — Study of Li–Be Bonding with N-heterocyclic carbene and N-heterocyclic boryl Ligands

Abstract In this work, the nature of bonding in Li–Be units stabilized by N-heterocyclic carbene and N-heterocyclic boryl ligands was investigated by quantum chemical methods. The complexes involved the formation of bonds between four consecutive elements of the second period, viz., B–Li–Be–C and C–Li–Be–B. The nature of metal-metal and metal-ligand bonds was explored through the natural bond orbital and electron density analyses within the atoms-in-molecule approach.

Summer 2017 — Study of Lanthanide (Europium and Terbium) Doped Hydroxyapatite Nanotubes

Abstract Hydroxyapatite (HAp), $Ca_{10}(PO_4)_6(OH)_2$ is the main component of vertebrate bone and teeth with Ca:P mole ratio of 1:0.67. It exhibits excellent biodegradability, biocompatibility, and ability to penetrate the cell membrane which makes it a potential biomaterial. Hence, extensive research work is being carried out to use HAp for the purpose of bioimaging, but HAp is not fluoroscent. So, if doped with atoms having fluoroscent property, it can be used as a probe. In this work, HAp was doped with Eu and Tb as that have fluoroscent property. Eu^{3+} and Tb^{3+} have an ionic radii similar to that of Ca^{2+} (Ca^{2+}:114pm; Eu^{3+}:108.7pm; Tb^{3+}:106.3pm) which satisfies the necessary condition for doping.The lanthanide doped HAp nanorods were synthesized using sol-gel method. The nanorods were characterized using various techniques like XRD, SEM, TEM, and EDAX.