

CURRICULUM VITAE

Agnibha Hanra (Graduate Assistant)

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PROFILE

With previous research experience in computational and theoretical chemistry, I am currently pursuing my Ph.D. that will fulfill my disposition to be a full-time researcher while maintaining my strong interest in the versatile and broad area of quantum chemistry.

EDUCATION

Ph.D. in Chemistry **August 2022 - Present**

Michigan State University, Michigan, U.S.A
Advisor: Professor Piotr Piecuch

M.Sc. in Chemistry **2021**

University of Hyderabad, Telangana, India
Advisor: Professor Susanta Mahapatra

B.Sc. in Chemistry **2019**

Narasinha Dutt College (Affiliated to University of Calcutta), West Bengal, India

Higher Secondary Education **2016**

Board: West Bengal Council of Higher Secondary Education
School: Santragachi Kedarnath Institution, West Bengal, India

Secondary Education **2014**

Board: West Bengal Board of Secondary Education
School: Santragachi Kedarnath Institution, West Bengal, India

PROFESSIONAL EXPERIENCE

Michigan State University (U.S.A) **August 2022 - Present**

Graduate Assistant: teaching freshmen-level general chemistry (CEM-141), while preparing for doctoral research in theoretical and computational chemistry.
Advisor: Professor Piotr Piecuch.

RESEARCH EXPERIENCE

1. University of Hyderabad | India **February 2021– July 2021**
Advisor: Professor Susanta Mahapatra

I studied the photo detachment spectrum of an open shell carbon doped boron cluster, CB_8^- . I performed geometry optimizations and frequency calculations using GAUSSIAN-09 software package, followed by the calculation of single-point energies using the *ab-initio* OVGF method in a particular distortion range. Also, I constructed potential energy surfaces based on this *ab-initio* method for four low-lying excited states of the neutral CB_8 via electronic detachment from HOMO and subsequent orbitals of the anionic reference state (CB_8^-) and applied the standard vibronic coupling theory to calculate the intrastate Hamiltonian parameters which are essential for understanding the nuclear dynamics and the subsequent explanation of photo detachment spectra.

2. University of Hyderabad | India

October 2021– February 2022

Advisor: Professor Susanta Mahapatra

I studied the photo detachment spectrum of another open shell carbon doped boron cluster, $C_2B_8^-$. After geometry optimizations and frequency calculations using GAUSSIAN-09 software package, I calculated the vertical detachment energies to determine the suitable active space which was later used to calculate the adiabatic energies of the electronic states employing the CASSCF-MRCI method present in the MOLPRO suite of program.

TECHNICAL SKILLS

- Programming language – FORTRAN.
- Software – GAUSSIAN-09, MOLPRO, MATHEMATICA.
- GUI – XMGRACE.

ORAL PRESENTATION

Let us think on the second law of thermodynamics – Nurturing Chemistry; Bonding and Beyond – The Bhawanipur Education Society College – 2017.

It was awarded “The Best Presentation”.

ACHIEVEMENTS

- Champion (**Agnibha Hanra**, Amit Dutta, and Arnab Dutta) at the prestigious 23rd National Chemquiz at Presidency University in 2019.
- Secured 3rd position (**Agnibha Hanra**, Anik Majila, and Sourin Ghosh) at Adamas Science Fair organized by Adamas Institute of Technology in 2015.

COMMUNICATION SKILLS

Professional efficiency in English (IELTS band – 7.5)