Raj Roy

Curriculum Vitae

Mangal Bari, Malda-732142, West Bengal, India
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rr4398@nyu.edu
https://github.com/rr4398

RESEARCH EXPERIENCE

CURRENT, FROM FEB 2023 (FT)

NYU Shanghai, Dept. of Chemistry

My current project aims at modeling the dynamics of DNA strand breaking by low-energy electrons through the FlexiBLE scheme, a novel constrained QM/MM embedding approach.

Supervisor: Prof. William J. Glover

SEPT 2020 – SEPT 2022 (FT)

Indian Institute of Science Education and Research Kolkata (IISER-K), Dept. of Chemical Sciences

My research aimed at overcoming the challenges faced by conventional Time Dependent(TD)-Density Functional Theory(DFT). Within the DFT paradigm, I adopted a simple ΔSCF method to compute optical gap and charge-transfer excitation energy. The focus was to extend the domain of ΔSCF method in areas where conventional methods have limitations.

Expertise: I can very well handle **GAMESS, Gaussian** and **Q-Chem** software.

JAN 2018 – JUNE 2018

University of Gour Banga, Dept. of Physics

As my postgarduate dissertation I worked on "Saturated Absorption Spectroscopy" under the supervision of Prof. Chanchal Chaudhuri. The objective was to calculate the hyperfine constant of rubidium(^{87}Rb) for; $5^2S_{1/2}$ and $5^2P_{3/2}$ state. As a part of my dissertation, I also presented an oral presentation of my work to my professors and external members.

Thesis Title: Investigation of Rubidium by Saturated Absorption Spectroscopy

NOV 2018 – SEPT 2020 (PT)

University of Gour Banga, Dept. of Physics

After completing my masters, I worked with a team led by Dr. Ankur Sen Sharma. My task was to assist the graduate students with coding and in literature survey. During this period, I have enhance my computational skills and learned many numerical methods.

RESEARCH INTERESTS

- To study excited state properties through DFT
- Theoretical modeling of condense phase system
- Theoretical studies of impurities and defects in crystalline materials
- DFT-based molecular dynamics simulation

PUBLICATIONS

Published:

Raj Roy, Abhisek Ghosal and Amlan K. Roy; "A Simple Effective ΔSCF Method for Computing Optical Gaps in Organic Chromophores". *Chem Asian J.*, **2021**, 16, 2729–2739.

COURSES AT IISER-K

Advance Quantum Chemistry
Prof. Sourav Pal and Dr. Sangita Sen

Computational Physics
Prof. Amit Ghosal, Dr. Ananda Dasgupta, Dr. Anandamohan Ghosh and Prof. Rangeet Bhattacharyya

Introduction to DFT
Prof. Amlan K. Roy

EDUCATION

2023–PRESENT **PhD in Computational Chemistry**
Department of Chemistry
NYU Shanghai

2016–2018 **Master of Science (Physics)**
MARKS OBTAINED: 83.6%
Department of Physics
University of Gour Banga

2013–2016 **Bachelor of Science (Physics Hons.)**
MARKS OBTAINED: 60.80%
Department of Physics
Malda College, University of Gour Banga

2011–2013 **ISC (Higher Secondary Examination)**
MARKS OBTAINED: 83%
The St. Xavier's School, Malda

2011 **ICSE (Secondary Examination)**
MARKS OBTAINED: 89%
North Point English Academy, Malda

AWARDS

2017 **Swami Vivekananda Merit Cum Mean Scholarship**
University of Gour Banga

2018 **Gold Medal in M.Sc. (Physics)**
University of Gour Banga

2020 **Qualified GATE examination in Physics**
Organized by IIT Delhi

2020 **Certificate for "From the Big Bang to Dark Energy"**
Online non-credit course offered through Coursera
Authorized by The University of Tokyo

COMPUTER SKILLS

PROG. LANGUAGE: Fortran(expertise) and Python
OPERATING SYSTEM: Windows and Ubuntu
MISC. PROGRAMS: LaTeX, Vim, GNU plot

Raj Roy, Abhisek Ghosal and Amlan K. Roy; "Charge-Transfer Excitation within a Hybrid-(G)KS Framework through Cartesian Grid DFT". *J. Phys. Chem. A*, **2022**, 126, 8, 1448–1457.

In Preparation:
Raj Roy and Abhisek Ghosal; "Relevance of high lying excited state, core excitation and conical intersection through Becke exciton model".

Publications by DOI

2021 **doi:https://doi.org/10.1002/asia.202100692**

2022 **doi:https://doi.org/10.1021/acs.jpca.1c10593**

CURRENT (AND PREVIOUS) POSITION

NYU Shanghai

PhD Student in **Glover Group**

Current Project: "Modeling DNA strand breaking by low-energy electrons"

Supervisor: Prof. William J. Glover

Indian Institute of Science Education and Research Kolkata

Junior Research Fellow (Project) in the Dept. of Chemical Sciences

Project Title: "Design of appropriate DFT method to mimic pressure effect on atoms and molecules confined in various environments (SERB)"

Funding Support: DST SERB (sanction order: CRG/2019/000293)

CONFERENCES

INTERNATIONAL 17th Theoretical Chemistry Symposium (TCS-2021), organized by IISER-K, IACS Kolkata, Kalyani University and S.N Bose National Centre for Basic Sciences Kolkata

NATIONAL Oral presentation on *Departmental day of Chemical Sciences* at IISER Kolkata–9th April,

POSTERS Poster presentation at the 17th Theoretical Chemistry Symposium–2021

REFERENCES

Prof. William J. Glover

POSITION Asistant Professor
EMPLOYER Department of Chemistry, *NYU Shanghai*
EMAIL william.glover@nyu.edu

Prof. Chanchal Chaudhuri

POSITION Professor
EMPLOYER Department of Physics, *University of Gour Banga*
EMAIL cchanchal@yahoo.com

Dr. Atul Bandyopadhyay

POSITION Associate Professor
EMPLOYER Department of Physics, *University of Gour Banga*
EMAIL atulbandyopadhyay@yahoo.com