Aritra Roy

Theoretical Chemist

M.Sc. chemistry Student with a strong working knowledge of the **Chemical Information Science** and **Chemical Bonding Analysis**.

Interested in Theoretical Research of **Excited States, Quantum Effects, Light-matter Interaction, Electronic Structures, TD-DFT, MD Simulations, Programming** and **AI-ML.**

aritraroy24@gmail.com

+91 9851257150

Nadia, West Bengal, India

www.aritraroy.live

beacons.ai/aritraroy24

linkedin.com/in/aritraroy24

github.com/aritraroy24

aritraroy24.medium.com

SKILLS & TOOLS

Basic Computer Skills

MS Office (Excel, Word, PowerPoint) Knowledge | Windows 10 | Linux (Debian-based Distro) | Touch Typing | Terminal (Bash, cmd, PowerShell | Troubleshoot | Graphic Design (Ps, Canva) | Googling

Chemistry Skills & Tools

- Physical Chemistry | Inorganic Chemistry | Organic Chemistry | Theoretical | Computational Chemistry | Semiconductors | Nanomaterials | Surface Chemistry | Basis Set | Potential Energy Surface | DOS | PDOS | Band Structure | Dirac Cone | Phonon Dispersion | Chemical Bonding | Borophene | TD-DFT | Electronic Structures | Excited States
- Gaussian 16 | GaussView 6.0 | Spartan '14 | WinCACAO | ChemDraw Professional | Origin 2018 | Materials Studio 2017 | Avogadro | Math Editor | EndNote X9 | Multiwfn | VMD

Programming Skills & Tools

- Python 3.x | SciPy | NumPy | Matplotlib | MATLAB | C Programming | Java | HTML5 | CSS3 | JavaScript | React | React Native | SASS
- GitHub | Git Version Control | Visual Studio Code | Node Package Manager (npm) | Yarn | Firebase | Expo CLI | Chrome DevTools | Netlify Deploy | GitHub Pages

EDUCATION

- **M.Sc. in Chemistry** from **Pondicherry University (3rd Position)** — *CGPA 8.88 | July, 2019-Aug, 2021*
- **B.Sc. in Chemistry** from **Ramakrishna Mission Vivekananda Centenary College, Rahara** — *CGPA 7.34 | July, 2016-May, 2019*

- **10+2 Board Exam** from **Nabadwip Bakultala High School** *89.2% | May, 2015-June, 2016*
- **Madhyamik Board Exam** from **Nabadwip Bakultala High School** *90% | July, 2016-May, 2019*

CHEMISTRY PROJECTS

- **DFT study for selective amino acid (L-Cysteine) sensing by a Cu(II)**
  DOI: NA **(Ongoing Project)** *Dec, 2022 – Present*

  Dr. Biswa Nath Ghosh (NIT Silchar, India): Collaborator

  Finding different binding modes of Cysteine amino acid with Cu(II) metal-ligand complex due to its crucial significance in various biological processes, such as energy transduction, protein regulation, and cell signalling.

- **Tuning the Optoelectronic Properties by End-capped Group Modification for Efficient Organic Solar Cells**
  DOI: NA **(Ongoing Project)** *Sep, 2022 – Present*

  Faheem Abbas (Tsinghua University, China): Collaborator

  Finding the impact of side-chain engineering for organic molecules with donor and acceptor site for efficient organic solar cells and photovoltaic performance.

- **Surface Adsorption and Encapsulated Storage of H_2 in a Cage-like $(MO)_x$ Cluster**
  DOI: NA **(Ongoing Project)** *Aug, 2022 – Present*

  Dr. Saeedeh Kamalinahad (Arak University, Iran): Collaborator

  We will investigate the surface adsorption and encapsulated storage of H_2 molecules in a cage-like metal-oxide cluster. This is completely a theoretical project collaborating with Dr. Saeedeh and Dr. Felipe from Kent University.

- **Electronic Structure and Reactivity of an Allyl-Like Trialuminium Compound**
  DOI: NA **(Ongoing Project)** *Jun, 2022 – Present*

  Felipe Fantuzzi Group (Kent University, UK): Guest Researcher

  Our main objective is to find the reason behind the abnormal C-C activation in a allyl-like trialuminium compound and its reactivity using DFT calculations to support the experimental work (theoretical+experimental collaborative project). The experimental group is led by Prof. Dr. Holger Braunschweig from University of Würzburg.

- **First-Principles Study of CO Gas Sensing on Elite Metal-Oxides**
  DOI: 10.2139/ssrn.4166227 **(Preprint)** *Nov, 2021 – May, 2022*

  Chemical Information Science Laboratory (Pondicherry University, India)

  Our main target was to benchmark CO sensing performances based on the selectivity, sensitivity, adsorption energy, and response time calculations on different hybrid metal-oxides using DFT calculations.

  Achievements

  - **Studied the sensing mechanism of CO** on SnO_2 [110], ZnO [0002], ZnO/SnO_2, CuO/SnO_2, AgO/SnO_2, and CdO/SnO_2 surface.
  - Computed results showed that the **CO reacts with the pre-adsorbed oxygen site** on the MOs and MOs/SnO_2 lattice.
  - We explained the improved sensing performance based on the **selectivity, sensitivity, adsorption energy, and response time** calculations.
  - **Heterojunction-based thin-film sensors** are found to be highly sensitive and could be utilized for CO gas sensing applications.

- **Finding a More Stable Semiconductor Borophene Using the Theoretical Approach**

  DOI: 10.13140/RG.2.2.18066.32965 **(M.Sc. Thesis)** ***Dec, 2020 – Jul, 2021***

  Chemical Information Science Laboratory (Pondicherry University, India)

  The basic pupose of this project was finding a kinetically stable semiconductor borophene for application purposes using Quantum Calculations like DFT.

  ### *Achievements*

  - Learned the usage of **Gaussian 09W**, **GaussView 6.0**, **Materials Studio** and **CASTEP** Module.
  - Studied different structures to get a **Potentially Stable Semiconductor Borophene**.
  - **One semiconductor identified**, but later studies found that it is not dynamically stable.
  - Studied over **13** different structures.

  Contact: Dr. Musiri M. Balakrishnarajan (*mmbkr.che@pondiuni.edu.in)* – Project Supervisor

PROGRAMMING PROJECTS

- **Google Contacts Using Gmail API** ***Three Days***

  A python program to get the contacts associated with Google Account. Python3.x and Gmail API is used to get all the contacts. Also a blog has been written based on this project on Medium platform.

  ### *Achievements*

  - This one is my **first python project** and also I've written my **first blog** based on this project.
  - **Gmail API gives us the permission to get all the contacts** stored in Google Contacts.
  - Without Gmail API **maximum 30 contacts** can be fetched from Google Contacts.
  - The blog based on this project was published under one of the well-known Analytics and Data Science Company **Analytics Vidhya**.

- **CompChemNews Bot Using Python & Tweepy** ***One Week***

  A Twitter Bot made using python tweepy and beautifulsoup4 module for automatically getting latest news in the field of Computational Chemistry.

  ### *Achievements*

  - The Twitter Bot is made using **python3.x** programming language.
  - Learned two new python modules **tweepy** and **beautifulsoup4 (bs4)**.
  - Also learned to host a python program online and schedule the script to run per day using **WayScript Time Trigger**.

RESEARCH INTERESTS

- Computational
- DFT Calculations
- Excited States
- Light-matter Interactions
- Quantum Effects
- Programming
- Theoretical
- MD Simulations
- Electronic Structures
- Photophysical Properties
- Radiation / Decay Process
- AI-ML

COURSES & CERTIFICATES

- ## Chemistry Courses
  - Computational Quantum Mechanics of Molecular and Extended Systems (MIT OpenCourseWare)
  - Fundamentals of Macroscopic and Microscopic Thermodynamics
  - Nanotechnology and Nanosensors
- ## Programming Courses
  - State Govt. Python Programming Course (90%-100%)
  - State Govt. Java Programming Course (80%-90%)
  - State Govt. C Programming Course (80%-90%)
  - Front-End Web Development with React (Coursera Course with Honors)

BLOGS

- ## Chemistry Articles
  - Fascinating Power of Googling in Computational Chemistry
  - How to Make Your Chemical Synthesis Process Absolutely Easier Using AI Advantage
  - Basic Introduction to Computational Chemistry Tools: Spartan
  - Introduction to Computational Chemistry Calculations: PES and Saddle Point
- ## Programming Articles
  - Retrieving Email and Phone No. for a Desktop App from Google Contacts Using Python and Gmail API
  - Customize Your Windows PowerShell With oh-my-posh & posh-git
  - How to Tweet Daily Update by Active Twitter-Bot Made Using Tweepy and Python

SYMPOSIUMS

- ## Chemistry Seminars
  - CSIR-Central Electrochemical Research Institute Skill Development Training Programme
  - International Virtual Symposium on Advances in Chemical Sciences, RSC
- ## Programming Seminars
  - Microsoft AI Classroom Series, Microsoft
  - Machine Learning | Lyrics Generation, Coding Blocks

RECOMMENDATIONS

- Dr. Felipe Fantuzzi – ***f.fantuzzi@kent.ac.uk*** *(+44 (0)1227 82 3462)* **[University of Kent]**
- Dr. M. M. Balakrishnarajan – ***mmbkr.che@pondiuni.edu.in*** *(+91 98943 60048)* **[Pondicherry University]**
- Dr. Sougata Sarkar – ***sougata.sarkar81@gmail.com*** *(+91 94774 02759)* **[RKMVC College]**
- Dr. Bidhu Bhusan Das – ***bidhubnds@gmail.com*** *(cell : 91-413-2654413(O))* **[Pondicherry University]**

LANGUAGES

English ◉ ***Bengali*** ● ***Hindi*** ◉

- International English Language Testing System (IELTS Academic): **6.5 (Minimum 6.0 in Each Module) ⇒ CEFR Level: B2**

EXTRACURRICULAR ACTIVITIES

- Participated in Relief Works under Ramakrishna Mission: 2016-2019
- NSS (National Service Scheme) Volunteer for 2 Years: 2016-2018
- 3rd Year Completion Certificate with Distinction in Drawing: 2015
- 1st Prize in State Level Essay Competition: October 2012
- 'A' Certificate of N.C.C. under 54 Bengal Bn, Kalna: March 2013
- Participated in District Level 'Youth Mock Parliament' competition: 2013

HOBBIES

- Drawing
- Travelling
- Violin (Indian Classical Music)
- Story Books
- Drama
- NGO

ADDRESS

512, Pirtala, Poramatala Road, Nabadwip, Nadia, West Bengal, India - 741302

N.B.

All the programming skills learned on my own interest. No academic (chemistry) projects have been done using those so far.