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 **Materials Designing, Nanomaterials, Electronic Structures, Spectroscopy, Energy Storage, DFT Calculations, Programming and AI-ML**

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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 | Astro Build | 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 **(Submitted for review)** *Dec, 2022 – July, 2023*

  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 signaling.

- **Tuning the Optoelectronic Properties by End-capped Group Modification for Efficient Organic Solar Cells**
  DOI: NA **(Submitted for review)** *Sep, 2022 – July, 2023*

  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 **(Submitted for review)** *Nov, 2021 – Sept, 2022*

  Chemical Information Science Laboratory (Pondicherry University, India)

  Our main target was to benchmark CO sensing performances based on the selectivity, sensitivity, and adsorption energy 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, and adsorption energy** 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 purpose 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
- Materials Design
- Spectroscopic Analysis
- Programming and Development
- Theoretical
- MD Simulations
- Nanomaterials
- Energy Materials
- 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
  - Julia Language for Computational Chemists
  - CSIR-Central Electrochemical Research Institute Skill Development Training Programme
- ## 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. Biswa Nath Ghosh – ***bnghosh@che.nits.ac.in*** *(+91 80181 23682)* **[NIT Silchar]**
- Dr. Sougata Sarkar – ***sougata.sarkar81@gmail.com*** *(+91 94774 02759)* **[RKMVC College]**

LANGUAGES

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

- International English Language Testing System (IELTS Academic): **7.0 (Minimum 6.0 in Each Module) ⇒ CEFR Level: C1**

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

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N.B.

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