

Aritra Roy

Computational Chemist

PhD Student at **London South Bank University**. Researching Ferroelectric Domain Walls manipulation using ML-AI.

Interested in Theoretical Research of **Semiconductor, Defects, Ferroelectric Materials, Electronic Structures, TD-DFT, MD Simulations, Programming** and AI-ML.



g R⁶ id

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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
- VASP VESTA Gaussian 16 GaussView 6.0 Spartan '14 ChemDraw Multiwfn VMD
Materials Studio 2017 Avogadro Math Editor Origin 2018 Zotero

Programming Skills & Tools

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

RESEARCH

- Doctoral Researcher at London South Bank University, UK *Sep, 2023 - Present*
- Visiting Researcher at King's College London, UK *Mar, 2024 - Present*
- Guest Researcher at Fantuzzi Group, University of Kent, UK *Jun, 2022 - Present*

EDUCATION

- M.Sc. in Chemistry from Pondicherry University (3rd Position) CGPA 8.88 | Jul, 2019 – Aug, 2021
- B.Sc. in Chemistry from Ramakrishna Mission Vivekananda Centenary College, Rahara CGPA 7.34 | Jul, 2016 – May, 2019
- 10+2 Board Exam from Nabadwip Bakultala High School 89.2% | May, 2015 – Jun, 2016
- Madhyamik Board Exam from Nabadwip Bakultala High School 90% | Jul, 2016 – May, 2019

CHEMISTRY PROJECTS

- **Piezoelectric Materials Prediction Using Text-mined Data and Deep Learning**
DOI: NA (Ongoing PhD Project) Jul, 2023 – Present
 Dr. John Buckeridge (LSBU, UK): Doctoral Researcher
We are focusing for using text-mined journal article data for piezoelectric materials to find novel piezoelectric materials with higher dielectric properties.
- **Exploring the Frontier: LLMs for Molecular and Materials Design, Automation, and Scientific Discovery**
DOI: 10.48550/arXiv.2411.15221 (Preprint)  May, 2024 – Present
 Ben Blaiszik (University of Chicago, US): Collaborator
Analyzing diverse applications of LLMs in chemistry, both molecular and materials design, automation etc. through a hackathon where 34 total projects were developed.
- **Surface Adsorption and Encapsulated Storage of H₂ in a Cage-like (MO)_x Cluster**
DOI: NA (Final Draft) Aug, 2022 – Present
 Dr. Pablo Gamallo (University of Barcelona, Spain): Collaborator
We will investigate the surface adsorption and encapsulated storage of H₂ molecules in a cage-like metal-oxide cluster. This is completely a theoretical project collaborating with Dr. Pablo Gamallo and Dr. Felipe Fantuzzi.
- **A Discrete Trialane with a Near-Linear Al₃ Axis**
DOI: 10.1021/jacs.4c10967  Jun, 2022 – Nov, 2024
Journal of American Chemical Society (Gold Open Access)
 Felipe Fantuzzi Group (Kent University, UK): Guest Researcher
Finding 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 led by Prof. Dr. Holger Braunschweig from University of Würzburg.
- **A Copper Complex Receptor for Nanomolar Sulfide Sensing and Applications in DNA/BSA Binding**
DOI: 10.1016/j.jphotochem.2024.116154  Dec, 2023 – Nov, 2024
RSC Sensors & Diagnostics (Gold Open Access)
 Dr. Biswa Nath Ghosh (NIT Silchar, India): Collaborator
Understanding the sulfide sensing for a copper complex receptor using DFT and TD-DFT calculations. The receptor also exhibits strong binding interactions with CT-DNA and bovine serum albumin (BSA).

- **A Simple Copper(II) Dpppy-Based Receptor for Sensing of L-Cysteine and L-Histidine in Aqueous Acetonitrile Medium**

DOI: 10.1039/D3SD00183K 

Dec, 2022 – Oct, 2023

RSC Sensors & Diagnostics (Gold Open Access)

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.

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 | • Theoretical |
| • DFT Calculations | • MD Simulations |
| • Semiconductors | • Electronic Structures |
| • Defects | • Ferroelectric Materials |
| • Energy Materials | • Programming |
| • 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 [↗](#)
- Oh-My-Posh V3 is Out in the Market [↗](#)
- Personal Website: Why You Should Have One Right Now and How? [↗](#)

YOUTUBE TUTORIALS

- How to Build High-Quality MEP Surface Using Multiwfn & VMD from Gaussian CheckPoint File? [↗](#)
- Do This: Gaussian 16 Linux Version on Windows 10/11 Using WSL in 15 Minutes! [↗](#)
- Best Materials Studio Tutorial: How to Build Any Structure from Scratch? [↗](#)

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

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

ADDRESS

Permanent: Pirtala, Nabadwip, Nadia, West Bengal, India - 741302

Present: Department of Chemical and Energy Engineering, London South Bank University, London SE1 0AA, UK