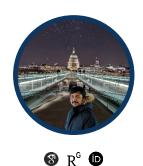
Aritra Roy

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.



Chemical Bonding

contact@aritraroy.live +44 73930 62351 London, United Kingdom www.aritrarov.live * beacons.ai/aritraroy24 linkedin.com/in/aritraroy24 in github.com/aritraroy24 aritraroy24.medium.com

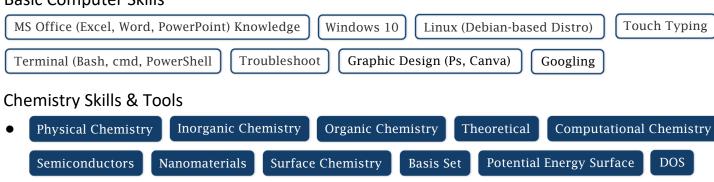
Borophene

TD-DFT

SKILLS & TOOLS

Basic Computer Skills

PDOS



Excited States Electronic Structures VASP VESTA Gaussian 16 GaussView 6.0 Spartan '14 ChemDraw Multiwfn VMD

Phonon Dispersion

Materials Studio 2017 Avogadro Math Editor Origin 2018 Zotero

Dirac Cone

Programming Skills & Tools

Band Structure

Java HTML5 CSS3 Matplotlib MATLAB C Programming Python 3.x NumPy SciPv JavaScript **React Native** Bash LaTeX React **SASS** Git Version Control Node Package Manager (npm) Yarn GitHub Visual Studio Code 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 H_2 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) Dppy-Based Receptor for Sensing of L-Cysteine and L-Histidine in Aqueous Acetonitrile Medium		
<i>DOI:</i> 10.1039/D3SD00183K ☐	Dec, 2022 - Oct, 2023	
RSC Sensors & Diagnostics (Gold Open Access)		
Dr. Biswa Nath Ghosh (NIT Silchar, India): Collabora	ator	
Finding different binding modes of Cysteine amino acid with Cu(II) meta biological processes, such as energy transduction, protein regulation, an		
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**
- Semiconductors
- Defects
- **Energy Materials**
- AI-ML

- Theoretical
- **MD Simulations**
- **Electronic Structures**
- Ferroelectric Materials
- **Programming**

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)
B	LOGS
•	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?
Y	OUTUBE 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?
S	YMPOSIUMS
	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
R	ECOMMENDATIONS
•	Dr. Felipe Fantuzzi - <u>f.fantuzzi@kent.ac.uk</u> (+44 (0)1227 82 3462) [University of Kent]
•	Dr. M. M. Balakrishnarajan - <u>mmbkr.che@pondiuni.edu.in</u> (+91 98943 60048) [Pondicherry University]

• Dr. Sougata Sarkar - <u>sougata.sarkar81@gmail.com</u> (+91 94774 02759) [RKMVC College]

Dr. Biswa Nath Ghosh - <u>bnghosh@che.nits.ac.in</u> (+91 80181 23682) [NIT Silchar]

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
 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