Aritra Roy

Computational Materials Science | PhD Researcher

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PhD researcher developing ComProScanner, a multi-agent text-mining framework for piezoelectric materials discovery. Expertise in LLMs, RAG systems, fine-tuning, AI agents, DFT/VASP calculations, and deep learning for materials informatics. Published researcher with a strong Python programming and computational chemistry background.

EDUCATION

- 2023 – Present ◇ **Ph.D., London South Bank University, UK** in Chemical Engineering
  Thesis title: *Text Mining and Deep Learning for Piezoelectric Materials Discovery*.
- 2019 – 2021 ◇ **M.Sc. Chemistry, Pondicherry University, India** in Computational Chemistry
  Thesis title: *Finding a More Stable Semiconductor Borophene Using the Theoretical Approach*.
- 2016 – 2019 ◇ **B.Sc. Chemistry, RKM Vivekananda Centenary College, India** in Chemistry Honours

RESEARCH EXPERIENCE

- 2023 – Present ◇ **Doctoral Researcher,** London South Bank University, UK.
  • Developed ComProScanner: generalisable multi-agent platform for automated materials composition-property database construction using LLM agents and RAG
  • Demonstrated ComProScanner's capability by extracting piezoelectric materials data from 10,000+ scientific papers across 4 major publishers
  • Built high-throughput VASP DFT framework performing ∼2,000 piezoelectric property calculations on doped ZnO supercells
- 2024 – Present ◇ **Visiting Researcher,** King's College London, UK.
  • Cross-institutional collaboration on advanced materials characterisation
  • Contributing to computational modelling of piezoelectric system under the supervision of *Dr Chiara Gattinoni*
- 2022 – Present ◇ **Guest Researcher,** Fantuzzi Group, University of Kent, UK.
  • Performed DFT calculations supporting experimental works on main-group chemistry and organometallic chemistry
  • Resulted in five co-authored publications including one *JACS* with *Dr Felipe Fantuzzi*

RESEARCH PUBLICATIONS

PhD Research

1. A. Roy, E. Grisan, J. Buckeridge, and C. Gattinoni, "Comproscanner: A multi-agent based framework for composition-property structured data extraction from scientific literature," *arXiv preprint*, 2025.

Collaborative Research (Selected)

1. D. Das et al., "A copper complex receptor for nanomolar sulfide sensing and applications in dna/bsa binding," *Journal of Photochemistry and Photobiology A: Chemistry*, vol. 461, p. 116 154, 2025.
2. S. Kamalinahad, A. Roy, P. Gamallo, and F. Fantuzzi, "Engineering high-capacity hydrogen storage in pristine Ca12O12 nanocages via cooperative adsorption," *New Journal of Chemistry*, 2025.
3. D. Dhara et al., "A discrete trialane with a near-linear al3 axis," *Journal of the American Chemical Society*, vol. 146, no. 49, pp. 33 536–33 542, 2024.

Workshop/Hackathon Contribution

1. Y. Zimmermann et al., "32 examples of LLM applications in materials science and chemistry: Towards automation, assistants, agents, and accelerated scientific discovery," *Mach. Learn. Sci. Technol.*, vol. 6, no. 3, p. 030 701, 2025.

TECHNICAL SKILLS

Machine Learning & AI	◇ PyTorch, TensorFlow, scikit-learn, LangChain, LangGraph, CrewAI, Hugging Face Transformers, Unsloth AI, NumPy, Pandas, NLP, Data Science, Prompt engineering, Fine-tuning (Gemma, Llama 3), RAG, AI Agents
Programming	◇ Python 3.x, Bash/Shell, C, JavaScript, SQL, HTML/CSS, PHP, LaTeX
Computational Chemistry	◇ VASP, Gaussian 16, ORCA, VESTA, Phonopy, GaussView, Chemcraft, Multiwfn, SLURM
Development Tools	◇ VS Code, Jupyter Notebook, Git/GitHub, Docker, Anaconda, MongoDB, Postman, Netlify, Hostinger
Web Technologies	◇ React, Astro, Bootstrap, Tailwind CSS, jQuery, Node.js, Laravel

AWARDS, ACHIEVEMENTS & TRAINING

Awards & Achievements

2025 ◇ **Winter School: Robotics & AI for Materials Chemistry**, AIChemy, University of Liverpool. Selected as 1 of 30 students internationally for intensive hands-on workshop (Dec 8–12, 2025).

2024 ◇ **Top 5 Team – Devpost Hackathon**, MOFMaster Project. Developed AI-powered tool for MOFid generation and CH_4/N_2 gas separation prediction. Fine-tuned Llama-3-8B model and implemented MOF-GRU architecture for property prediction.

2021 ◇ **3^{rd} Position in M.Sc. Chemistry**, Pondicherry University (CGPA: 8.88/10).

Technical Training

2025 ◇ **PyTorch 101 Crash Course For Beginners** (Daniel Bourke).

2024 ◇ **Deep Learning for Molecules & Materials** (Assoc. Prof. Andrew D. White, University of Rochester) **Materials Informatics** (Prof. Taylor Sparks, University of Utah).

2023 ◇ **Machine Learning A-Z** (Udemy, SuperDataScience Team).

TECHNICAL BLOG ARTICLES (Selected)

- ◇ AI-ML Powered Materials Design Breakthrough: Is the Colorful Future of Materials Science Near?
- ◇ How to Make Your Chemical Synthesis Absolutely Easier Using AI Advantage
- ◇ Fascinating Power of Googling in Computational Chemistry
- ◇ Introduction To Computational Chemistry Calculations: PES and Saddle Point

LANGUAGES

■ **English:** Fluent (IELTS Academic: 7.0, CEFR Level C1) ■ **Bengali:** Native ■ **Hindi:** Conversational

REFERENCES

- ◇ Available upon request from: Dr John Buckeridge (London South Bank University, UK), Dr Chiara Gattinoni (King's College London, UK), Dr Felipe Fantuzzi (University of Kent, UK).