Adithya Maurya K R

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Education

UM–DAE–Centre for Excellence in Basic Sciences, Mumbai, India Aug. 2022 – 2027 (Expected)
CGPA: 8.56/10
Currently: 4th year Int-M.Sc. Chemical Sciences *1st Rank in Chemical Sciences Major*

Research Experience

International Institute of Information Technology (CCNSB)
Hyderabad, Telangana | Supervisor: Prof. U. Deva Priyakumar May 2025 – Present

- Designed, implemented, and trained Graph Neural Network architectures for adsorption energy predictions of MOF – CO_2 systems using the ODAC23 Dataset.
- Trained and adapted existing machine learning models on the MNSolv dataset for a better capture of solute–solvent interactions.

Centre for High Computing, CSIR-CLRI (Council of Scientific & Industrial Research)
Chennai, Tamil Nadu | Supervisor: Dr. Mudit Dixit May 2024 – Aug. 2024

- Understanding fundamentals of First-Principles DFT & Machine Learning Interatomic Potentials (MLIPs)
- Developed innovative pipeline accelerating material screening using MLIPs prior to in-depth DFT calculations
- Spearheaded the development of PACE (Precise & Accurate Configuration Evaluation) to determine low-energy adsorption sites using pre-trained MLIPs

KLE Technological University
Karnatka, India | Supervisor: Dr. Ashok Sajjan May 2023 – Dec. 2023

- Fabrication of Flexible Supercapacitor and electrolytes for Voltage Regulated Lead Acid Batteries
- Process optimization and synthesis of high-performance electrode materials
- Examined various electrolytes using electroanalytical techniques such as EIS, GCD, and CV.

Karnatak University
Karnatka, India | Supervisor: Prof. Ravindra R Kamble Nov. 2022 – Dec. 2022

- Analyzed Sorrel leaves constituents as a potential reagent for the synthesis of Copper and Silver nanoparticles. Characterized the synthesized Cu nanoparticles, anticipating applications in optics, anti-cancer, and antibacterial activities

Publications

4. Kumar, S., **KR, Adithya. Maurya.**, Dixit, M. (2025, October 17). Unravelling the catalytic activity of Dual-Metal doped N6-Graphene for sulfur reduction via Machine Learning-Accelerated First-Principles calculations. arXiv.org. https://arxiv.org/abs/2510.15397
3. Singh, P., **KR, Adithya. Maurya.**, Dixit, M.* (2024). Unraveling the Contribution of Cationic and Anionic Redox in Na-Rich Cathode Materials through First-Principles Calculations. ACS Applied Electronic Materials. https://doi.org/10.1021/acsaelm.4c01199
2. Chikkatti, B. S., **KR, Adithya. Maurya.**, Sajjan, A. M.*, Banapurmath, N. R. (2024). Elucidating the electrochemical performance of poly(methyl methacrylate) embracing manganese dioxide membranes for supercapacitors. New Journal of Chemistry 48, 14548-14555. https://doi.org/10.1039/d4nj02854f
1. **KR, Adithya. Maurya.**, Chikkatti, B. S., Sajjan, A. M.*, Banapurmath, N. R., Khan, T. Y., Saleel, C. A. (2024). Facile development of flexible cellulose acetate-lead dioxide membrane electrodes for supercapacitor applications. Next Energy, 5, 100178. https://doi.org/10.1016/j.nxener.2024.100178

Awards and Fellowships

DAE–DISHA Fellowship | *Issued by Dept. of Atomic Energy, Govt. of India* Aug. 2022 – Present

- Department of Atomic Energy offers this fellowship to meritious UM DAE CEBS and NISER students.

Skills

Languages & Tools: Python, Git, Linux, LaTeX
Libraries & Frameworks: PyTorch, ASE, Pymatgen, Scikit-learn, Fairchem, PyTorch-geometric, RDKit
Concepts: DFT, MLIPs, GNNs, Transformers, Machine Learning and Deep Learning Algorithms.

Referees

Dr. Mudit Dixit | **muditdixit@clri.res.in**
Center for High Computing Advanced Materials Lab, CSIR-Central Leather Research Institute, Chennai, Tamil Nadu, India

Prof. Neeraj A | **na@cbs.ac.in**
Head, School of Chemical Sciences, UM DAE CEBS, Mumbai, Maharastra, India