

# RAM MUNDE


Senior Undergraduate (B.Tech)  
Materials Science and Engineering

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## ACADEMIC QUALIFICATIONS

Degree	Institute	Year of Completion	CPI/%
B.Tech, MSE	Indian Institute of Technology Delhi	2024	8.2/10



## PUBLICATIONS AND PATENTS


- **Patent: “ Eco-friendly Stapling Material and Device ” - Ram Munde and Amitendra Singh** *Indian Patent Application No- 202221043097 USA Patent Application No -63438506 CPA - Dr. Alan Wolf, Cooper Union Edu. New York , USA*
- **Undergraduate Thesis : Computational Insights into Modulating the Performance of MXene-Based Electrocatalysts for Hydrogen Evolution Reaction (HER)** Ram Munde<sup>1</sup> Supervisor: Prof. Dibyajyoti G AU : Indian Institute of Technology, Delhi 

## INTERNSHIPS

- **United Phosphorus Limited, Bangalore, India -Research Internship (Data Scientist)** *May-Jul '23*
  - A robust machine learning model was constructed to predict the feasibility of chemical compounds for agro-chemical applications, employing density functional theory for the computation of energy of formation. Received letter of appreciation from Manager, United Phosphorus Ltd 
- **Cooper Union Edu. New York - Invention Internship** *Product Prototyped at IITGN May-July '22*
  - Synthesized a polymer clay that serves as an adhesive for paper binding, contributing to the enhancement of paper recycling processes. I successfully patented a binding device with material invention in both the United States and India, and I had the honor of presenting this innovation at the prestigious **Lemelson Student Prize event at MIT, USA**, demonstrating my dedication to advancing the field of materials science.
- **The University of New South Wales, Sydney- Research Internship** *Dec '21 - April '22*  
*Prof. Jiaojiao Jiang, UNSW Computing Lab *
  - Developed a robust framework called Input-Output Network Embedding (IONE) to capture network heterogeneity by preserving structural proximity, aligning anchor nodes, and incorporating structural diversity. It utilized mathematical objective functions and optimization techniques for accurate network representation.

## RESEARCH EXPERIENCE

- **Computational Insights into Modulating the Performance of Mxene-Based Electrocatalysts**  
*Senior Thesis: Heterostructure Electrocatalysts Prof. Dibyajyoti Ghosh, IIT Delhi  Jul - Dec '23*
  - Performed computational simulations to determine the  $\Delta G_h$  of various potential active sites on MXenes using Density Functional Theory (DFT). Our objective was to discover the most reactive site and most suitable surface functionalization of MXene for the HER . Structural and electronic properties analysed using DFT on VASP using high-performance computing.
  - The MXenes considered in this study are those that have been modified with halogen functional groups, specifically  $Ti_3C_2F_2$ ,  $Ti_3C_2Cl_2$ ,  $Ti_3C_2Br_2$ , and  $Ti_3C_2I_2$ . The efficiency of MXene as an electrocatalyst has been improved through modifications like defect formation, single-atom catalysis, and mixing of functional groups.
  - All calculations are done using pseudo-potential potpaw-PBE-54, KPOINTS generated from vaspkit (9 x 9 x1) for SCF and (4 x 4 x 1) for force optimisation, and DFT-D3 for vDW corrections.
- **Fabrication of Large-Area Blade-Coated Perovskite Solar Cells**  
*Mitacs Globallink Research Internship, Prof. Vivek Maheshwari, University of Waterloo Nov '22- Jan '23*
  - Manufactured plain and 1 wt% polystyrene -  $MAPbI_3$  solar cells with an active area of  $1cm^2$  under ambient conditions using the blade-coating technique.
  - Optimised the key parameters such as the annealing temperature and duration, spin coating speed, active layer thickness, electrode deposition technique, and surface treatment technique to achieve a power conversion efficiency of 4.59%.
- **A Deep Learning Approach to Estimate Stress Distribution on Aorta**  
*Course MLL213, Computational Materials Science Prof. S.Vikrant Karra, IIT Delhi  Jul- Nov '22*

- Estimated stress on materials using supervised learning demonstrating its feasibility over **FEA** approach. Deployed CNN with Prewitt Operator to calculate strain to satisfy static equilibrium analysis of stress. Encoded and decoded data by implementing unsupervised learning using PCA and SVD to reduce computation costs. Achieved remarkable AME and AE values of approximately 1.8 and 1.6 and generated a comprehensive report using LaTeX. 
- Molecular Dynamics Simulations of  $WS_2$  Using SW Potential**  
*Collaborative Project Prof. Alexander Shluger, University College London* July '23 - Sept '23
  - Tested the performance of the Stillinger - Weber (SW) potential in modeling the properties of  $WS_2$  by conducting Molecular Dynamics simulations using LAMMPS.
  - Calculated the geometric properties, cohesive energy, Young's modulus, and poisson ratio for two system sizes and compared them with known experimental and DFT calculations.
  - Visualized and analyzed the tensile deformation simulation results using Ovito.
- Superhydrophobic Brass Surface with Fabricated via Micro-Etching**  
*Winter Research Project: Advancing Superhydrophobicity Prof. Lakshmi Narayana, IIT Delhi* Nov - Dec '21
  - Made a superhydrophobic brass surface using solution immersion & chemical leaching method. The increase in the contact angle of the brass substrate was achieved by fabrication via micro-etching followed by modifications using **STA**. The resulting contact angle was  $155^\circ$  which is superhydrophobic in nature.
  - Using SEM, analyzed the morphological micro-nanostructure of the substrate. The CAs for water were measured using the sessile drop method. The chemical composition was analyzed using XPS and XRD (Bruke D8 Advance).

## RELEVANT COURSES

Electromagnetic Waves and Quantum Mechanics (PYL101)	Deep Learning in Solid Mechanics (APL405)
Numerical Methods and Computation (MTL107)	Thermodynamics of Materials (MLL103)
Characterization of Materials (MLL104)	Math. Methods in Materials Eng (MLL212)
Corrosion and Degradation of Materials (MLL452)	Materials Modeling (MLL213)
Nanostructures and Nanomaterials (MLL740)	Transport Phenomenon (CLL110)

## LEADERSHIP EXPERIENCE

- Technical Overall Coordinator, Offices of Career Services, IITD** (Sept 2021–Present):
  - Managing a team of 4 staff, 2 coordinators, 2 technical members, & 3 executives to develop the OCS portal, which is currently being used by **10000+** students and **1000+** recruiters.
  - Awarded **Best Contribution (2022)** and **Significant Contribution (2023)** by Senate.*
- Convener : Department of Materials Science & Engineering** (March 2023 - Present):
  - Managing academic administrative concerns for 120+ students. Actively addressed potential issues within the branch, collaborating with faculty and students to develop effective solutions.
- Coordinator, Board of Sports Activities** (May 2022–April 2023):
  - Led a 3-tier team with 20+ executives. Spearheaded the organization of the sports fest (**INTER-IIT**) spanning over 15 days, with all 13 sports being played after a gap of many years.
- Academic Mentor, Board for Student Welfare** (May 2022 - Dec 2022):
  - Mentoring **20+ freshmen** in their classes to help them adjust to the new IIT academic culture.

## TECHNICAL SKILLS

- Experimental:** Spin Coating, Blade coating, UV-vis spectroscopy, Glovebox, XRD, SEM, FTIR
- Computational:** VASP, LAMMPS, Linux, HPC, Ovito, VESTA, COMOSOL Multiphysics
- Languages:** Python, C++, Bash, SML, SQL, Node.js, Matlab, Java, Latex
- ML/AI Libraries:** PyTorch, Tensorflow, Keras, Matplotlib, Numpy, Flask

## EXTRA CURRICULAR ACTIVITIES

- Aquatics Captain** (Jun 2022–May 2023): Managed swim team activities, coordinated training sessions, and represented the team in competitions and events. **The team achieved the silver position in the INTER-IIT under my captaincy..**
- Athletics Vice Captain** (June 2021–May 2022)
  - Won **Silver Medal in 200m** event in Sportech the Institute Annual Sports Fest (August 2022)
  - Won **gold medal in 100m** event in Athletics Premium League (Jun 2021)
  - Won **gold medal in 4\*4 100m relay** in Athletics Premium League (Jun 2021)
  - Participation in 400m and 800m events in the Annual Sports Fest Sportech 2022 IIT Delhi
- NXP Semiconductors, Netherlands: Fellowship for 4 Years of Undergraduate Study**
- 1st Place Winner, Micron Semiconductor Hackathon: Champion of Memory Optimisation**