Shreyas Ramachandran

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Research Interests

Computational Materials Science, Energy Materials, Functional Materials

Academic Background

University of Edinburgh — Edinburgh, UK
PhD in Condensed Matter Physics — *Nov. 2023 – Present*
- Supervised by **Dr Elton Santos**

Imperial College London — London, UK
Master of Science in Advanced Materials Science and Engineering — *Oct. 2022 – Oct. 2023*
- Graduated with **Distinction** (Mark: 74.25%)
- **Student Representative** of the MSc Cohort

Birla Institute of Technology and Science — Hyderabad, India
Bachelor of Engineering in Mechanical Engineering; CGPA: 9.33/10.0 — *Aug. 2017 – July 2021*
Minor in Materials Science and Engineering; Minor GPA: 9.84/10.0
- **Meritorious Student** of the Class of 2021

Research Experience

Masters Dissertation — June 2023 – Oct. 2023
Materials Department, Imperial College London, UK — *Mentor: Prof Johannes Lischner*
Title: ***Modelling Plasmonic Nanoparticles for Solar Energy Conversion***
- Using in-house developed tight-binding model to study hot carrier generation by plasmonic nanoparticles
- Modifying the model to determine the feasibility of alloy nanoparticles for hot carrier generation

Research Assistant — July 2021 – August 2022
Materials Modelling Division, Institute of Materials Science, TU Darmstadt, Germany — *Mentor: Prof Karsten Albe*
Title: ***Understanding the Thermodynamics of Mixing of Lithium in Sodium Niobate***
- Used DFT to study the effect of Lithium substitution in $NaNbO_3$
- Performed Cluster Expansion and Monte Carlo simulations to study mixing properties

Bachelor's Thesis — Jan. 2021 – June 2021
Materials Modelling Division, Institute of Materials Science, TU Darmstadt, Germany — *Supervisor: Prof Karsten Albe*
Title: ***Monte-Carlo Simulations of Pore Formation in Lithium Metal Anodes***
- Analysed pore filling phenomenon of Ionic Liquid interlayer on Li anode using KMC
- Modified in-house existing KMC code using Python3 to study modified Li—IL—LLZO interface

Research Project Lead — July 2020 – Feb. 2021
Department of Mechanical Engineering, BITS Pilani Hyderabad Campus, India — *Mentor: Dr Sujith R*
Title: ***Hydrogen Adsorption Studies on Phosphorene***
- Computational study of H_2 adsorption on modified phosphorene surfaces using DFT
- Decorated pristine and defective phosphorene with Ni to improve adsorption energy of system

Undergraduate Research Assistant — July 2020 – Dec. 2020
Department of Mechanical Engineering, BITS Pilani Hyderabad Campus, India — *Mentor: Prof K Sumithra*
Title: ***Investigation of Doped Bilayer Graphene***
- Using DFT to study properties of Bilayer and Doped Bilayer Graphene
- Analyzing adsorption of small gas molecules on doped bilayer graphene

Undergraduate Research Assistant — March 2019 – March 2020
Department of Mechanical Engineering, BITS Pilani Hyderabad Campus, India — *Mentor: Dr Sujith R*
Title: ***Anodes for Lithium Ion Batteries***
- Worked on synthesis and analysis of SiOC-based and Nano Si-based anodes
- Reviewed literature on solid state electrolytes and its applications

Publications

[1] S. Srinivasan K V, A. Seth, D. Mohapatra, **S. Ramachandran**, and R. Sujith, "Iron decorated defective phosphorene as a viable hydrogen storage medium – a dft study", *International Journal of Hydrogen Energy*, 2022, ISSN: 0360-3199. DOI: 10.1016/j.ijhydene.2022.08.074.

[2] **S. Ramachandran**, K. Sai Srinivasan, and R. Sujith, "Nickel-decorated single vacancy phosphorene – a favourable candidate for hydrogen storage", *International Journal of Hydrogen Energy*, vol. 46, no. 54, pp. 27 597–27 611, Aug. 2021, ISSN: 03603199. DOI: 10.1016/j.ijhydene.2021.05.206.

[3] J. Gangadhar, **S. Ramachandran**, and S. Ravindran, "Study on effect of structure and surface/ physical characteristics of a silicon oxycarbide by hydrofluoric acid etching", *Advances in Materials and Processing Technologies*, vol. 6, no. 2, pp. 301–309, 2020. DOI: 10.1080/2374068X.2020.1728991.

Relevant Coursework - Masters

- Characterisation of the Structure of Materials
- Theory and Simulation
- Modelling Materials with Density Functional Theory
- Optoelectronic Materials
- Surfaces and Interfaces
- Electroceramics

Technical Skills

Programming Languages: Python, Julia, FORTRAN 90, MATLAB *[Additional - Experience with HPCs]*
Simulation Packages: Quantum Espresso, VASP, VAMPIRE

Miscellaneous

- **MSc Student Representative**, Imperial College London [2022-2023]
- **Meritorious Student** (Undergraduate); Ranked in the top 2% of the Class of 2021, comprising of 1058 students
- **Association Treasurer**, Mechanical and Manufacturing Engineering Association, BITS Hyderabad [2019-2020]
- **Core Committee**, Mechanical and Manufacturing Engineering Association, BITS Hyderabad [2017-2021]