


Dr. Sai Raj Ali

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 Hindi, English



Research Interests

- Electrocatalysis for water splitting, focusing on Hydrogen and Oxygen Evolution Reactions.
- Exploring 2D materials like MXene and Transition Metal Dichalcogenides for diverse applications.
- Applying Density Functional Theory (DFT) and Machine Learning (ML) to understand and predict material properties.
- Integrating DFT results with experimental synthesis techniques for a comprehensive study of 2D materials.

Skills

DFT Tools	■ Quantum ESPRESSO, PWTK, LOBSTER.
Advanced DFT	■ AIMD, FatBand, COHP Analysis, and Oxidation state calculation.
Lab Mastery	■ 2D-TMD synthesis, XRD, Raman, FTIR, SEM, TEM analysis.
Coding Proficiency	■ Shell scripting, Python, Fortran, GitHub, VirtualBox.
Data Science & Analysis	■ ASE, pandas, NumPy, SciPy, Jupyter Lab.
Visualization/Plotting	■ Blender, Inkscape, GIMP, Gnuplot, Matplotlib.
Productivity & OS	■ MS Office, Google Suite, Slack, Linux and Windows
Technical Proficiency	■ Linux, Vim, L ^A T _E X, HPC on CPU/GPU platforms.
AI/ML Fundamentals	■ Basic understanding of machine learning algorithms and frameworks.
Scientific Writing	■ Mendeley and self-written Python scripts for citation management.
Soft Skills	■ Critical thinking, teamwork, adaptability, leadership.

Experience

- 01/2019 – 06/2019 ■ **University Teaching Assistant, Electronics Lab**, B.Sc.(H) Physics, Department of Physics, Jamia Millia Islamia, New Delhi
- Developed lab manuals with faculty, improving course content.
 - Ensured equipment functionality and lab safety.
- 07/2018 – 12/2018 ■ **University Teaching Assistant, Mechanics Lab**, B.Sc.(H) Physics, Department of Physics, Jamia Millia Islamia, New Delhi
- Prepared lab manuals and guided 35+ students.
 - Provided technical support and troubleshooting.

Education

12/2017 – Current

■ **Ph.D. in Material Science, Jamia Millia Islamia University, Delhi.**

Thesis title: *Investigation of the Catalytic Role of Nanostructured Surfaces.*

Supervisor: Prof. Lekha Nair

Course Work CGPA: 8.6/10.0, First division.

- Gained hands-on experience working with UHV systems at Inter University Accelerator Centre, Delhi under Prof. Lekha Nair.
- Acquired expertise in 2D-TMD and quantum dot synthesis at Indian Association for the Cultivation of Science, Kolkata under the guidance of Dr. Praveen Kumar.
- Developed proficiency in Density Functional Theory (DFT) at Cochin University of Science and Technology, Kochi under the guidance of Dr. C.S. Praveen.

07/2014 – 07/2016

■ **M.Sc. Physics, Jamia Millia Islamia University, Delhi.**

Specialization in Theoretical Physics: General Relativity, Quantum Field Theory, Nuclear and Particle Physics.

CGPA: 8.9/10.0, First division.

- **Project-1:** *Newman-Janis Algorithm for Black Hole.*
- **Supervisor:** Prof. Sushant G. Gosh, Centre for Theoretical Physics-JMI, Delhi.
- **Project-2:** *Gamma Ray Detection and Variation in Energy Resolutions with Different Scintillation Detectors.*
- **Supervisor:** Dr. Akhil Jhingan, Inter University Accelerator Centre, Delhi.

07/2011 – 06/2014

■ **B.Sc. (Hons.) Physics, Shivaji College, University of Delhi.**

Percentage: 72.7%, First division.

Invited Talks/Teaching Assistant/Resource Person

07/2024

■ Invited as a **Teaching Assistant** for the "INDO-POLISH Workshop on Electronic Structure Calculations and Visualization with Molecular Nodes", jointly organized by the Indian Institute of Petroleum and Energy, Visakhapatnam, AP, India, and Gdańsk University of Technology, Poland, held from the 30th of July to the 3rd of August 2024.



03/2023

■ Invited as a **Teaching Assistant** for the workshop on "Quantum Mechanical Modelling of Materials by Quantum ESPRESSO", organized by IEEE Nanocouncil PSIT Student Chapter, MRSI, Allahabad Chapter, and School of Basic Sciences, CSJM University, India, held from the 15th to the 19th of March 2023.



09/2022

■ Invited as a **Teaching Assistant** for the workshop on "Molywood to Molecular Nodes" organized by Gdańsk University of Technology, Poland, IRB Barcelona, Spain, and Scidart Academy, India, held from September 8th to 11th, 2022.




Invited Talks/Teaching Assistant/Resource Person (continued)

- 09/2021  Invited as a **Teaching Assistant** for the Winter School on "**Advanced Molecular Dynamics Simulation**" jointly organized by the International School of Photonics, Cochin University of Science and Technology (CUSAT), India, the Department of Physics, and Green Club of Thoughts, Kathmandu University, Nepal, held from September 6th to 17th, 2021.
- 07/2021  Invited as a **Teaching Assistant** for the Summer School on "**Advanced Molecular Dynamics Simulation**" jointly organized by the Department of Chemistry, IISER Pune, India, the Department of Physics, and Green Club of Thoughts, Kathmandu University, Nepal, held from July 5th to 16th, 2021.





Fellowships/Grants/Academic Honors

- 01/2022  Qualified **CSIR Senior Research Fellowship** 2021-2022.
- 12/2016  Qualified **National Eligibility Test (NET)** examination for lectureship conducted by *Council of Scientific and Industrial Research (CSIR)*: Eligible for a Junior Research Fellowship in India. **All India rank-92**, in the December 2016 exam.

Awards and Achievements (Selected)

- 10/2022  "**Best Oral Presentation**" award at CSIR-CSIO Chandigarh "*1st IEEE-NTC AcSIR-CSI International Conference on Emerging Materials for Sustainable Development (EMSD-2022)*" October 9th - 11th, 2022.
- 02/2020  "**Best poster**" award at Jamia Millia Islamia University National Symposium on "*Advances in Material Science and Theoretical Physics*" February 19th - 20th, 2020.
- 03/2014  1st **position** in "**Powerpoint Presentation**" organised by Physics Society (Invenio 2014) at Shivaji College, University of Delhi.
-  2nd **position** in "**Science Quiz Competition**" organised by Physics Society (Invenio 2014) in Shivaji College, University of Delhi.

Schools, Workshops & Conferences (Selected)

- 02/2024  3rd **International Conference** on "Materials Genome (ICMG-III)" organised by Organized by SRM University AP, under the Asian Consortium on Computational Materials Science (ACCMS) theme meeting, held during 22th - 24th February, 2024.
-  **Workshop** on "Computational Design of Electrocatalyst (CDE 2024)" organised by Organized by SRM University AP, held during 18th - 20th February, 2024.
- 03/2023  Online 2nd **International Conference** on "Advanced Functional Materials and Devices (AFMD-2023)" organised by Organized by IQAC & Physics Department of Atma Ram Sanatan Dharma College, Delhi, held during 13th - 15th March, 2023.
-  **International Materials Conclave (IMC-2023)** & 33rd Annual Foundation Day, organised by Centre for Materials for Electronics Technology (C-MET), Pune, held during 8th - 10th March, 2023.

Schools, Workshops & Conferences (Selected) (continued)

- 11/2022  **International Conference** on Nanotechnology: Opportunities and Challenges (ICNOC-2022) virtual mode, organised by JMI University, Delhi, held during 28th - 30th November, 2022.
-  **International Conference** on H_2 & CO_2 virtual mode, organised by S&T Digital, India, held during 17th - 19th November, 2022.
- 10/2022  1st IEEE AcSIR-CSIO **International Conference** on Emerging Materials for Sustainable Development (EMSD-2022) virtual mode, organised by CSIR-CSIO, Chandigarh, held during 9th - 11th October, 2022.
- 09/2020  One Week **National Faculty Development Program** on “Research Ethics and Characterisation Techniques in Materials Science” virtual mode under MHRD Govt. of India held during 9th - 15th September, 2020.
- 02/2020  **National Symposium** on “Advances in Material Science and Theoretical Physics” at JMI, New Delhi, India held during 19th - 20th February 2020.

Research Publications

Published/Accepted

Impact Factor

1. **Sai Raj Ali**, CS Praveen, Sung Gu Kang, Lekha Nair, KC Bhamu, Praveen Kumar, “Exploring the catalytic properties of Ti_2CO_2 MXene decorated with Cu-cluster for Hydrogen evolution reaction.” *Applied Surface Science* 641(2023) : 158439

6.7

Under Review/Preparation

Journal

1. Javeesh Alex, S. Rajkumar[†], **Sai Raj Ali**[†], J.Princy Merlin, Arun Aravind, D. Sajan, C. S. Praveen, “Enhanced Pseudocapacitance Performance of NiO and Ce-Doped NiO Synthesized via Modified Combustion Technique” *Manuscript Number: CERI-D-24-03497*
2. Takwa Chouki, Sreejith P. Nandan, Romana Cerc-Korošec, Georgi Tyuliev, **Sai Raj Ali**, CS Praveen, Manel Machreki, Dominik Eder, Alexey S. Cherevan, Urška Lavrenčič Štangaar, Iwona A. Rutkowska, Pavel Kulesza, Saim Emin, “Phase transformation approach for the preparation of active Fe_2P catalyst for oxygen evolution” *Manuscript Number: POWER-D-24-01173*
3. **Sai Raj Ali**, Jose Antony VJ, KC Bhamu, Sung Gu Kang, Lekha Nair, CS Praveen, “Comparative Analysis of Single Copper Atom and Copper Cluster Effects on Enhancing Hydrogen Evolution in Mo_2CO_2 MXene” *About to Submit*
4. Jose Antony VJ, Maneesha M, **Sai Raj Ali**, CS Praveen, “Exploring Cu_3 -Decorated MXene Materials as Promising Catalysts for Hydrogen Evolution Reaction” *Under Preparation*

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J.
Power
Sources

Peer Review Activities

Reviewer Responsibilities

Impact Factor

1. Sai Raj Ali, "Reviewer for *Sustainable Energy Technologies and Assessments*" 7.1

Referees

1. **Prof. Lekha Nair**
Relationship: **PhD Supervisor**
Department of Physics,
Jamia Millia Islamia University,
New Delhi-110025, India.
Phone : +91 98100 32194
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2. **Dr. CS Praveen**
Relationship: **DFT Collaborator**
International School of
Photonics, Cochin University of
Science and Technology,
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3. **Dr. Praveen Kumar**
Relationship: **Expt. Collaborator**
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Indian Association for the
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