

Mr. Sai Raj Ali



03-07-1993



Indian



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Hindi, English



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Research Interests

- Electrocatalysis for water splitting, specifically Hydrogen and Oxygen Evolution Reactions.
- Catalytic oxidation of carbon monoxide (CO) and reduction of carbon dioxide (CO₂).
- Exploring 2D materials like MXene and Transition Metal Dichalcogenides for diverse applications.
- Application of Density Functional Theory (DFT) in understanding and predicting material properties.
- Integrating DFT results with experimental synthesis techniques for a comprehensive study of 2D materials.



Skills

DFT Tools	Quantum ESPRESSO, PWTK, LOBSTER
Specialized DFT Calculations	AIMD, Phonon, FatBand, and COHP Analysis
Programming	Shell scripting, Python, Fortran
Graphics Tools	Blender, Inkscape, GIMP
Plotting Tools	Gnuplot, Matplotlib
Operating Systems	Linux, Windows
Miscellaneous	Vim, \LaTeX




Education

2017 – Present	Ph.D. in Material Science, Jamia Millia Islamia University, Delhi. Thesis title: : <i>Investigation of the Catalytic Role of Nanostructured Surfaces.</i> Supervisor: Prof. Lekha Nair Course Work CGPA : 8.6/10.0, First division.
2014 – 2016	M.Sc. Physics, Jamia Millia Islamia University, Delhi. Specialization in Theoretical Physics: General Relativity, Quantum Field Theory, Nuclear and Particle Physics. Project title: <i>Newman-Janis Algorithm for Black Hole.</i> CGPA: 8.9/10.0, First division.
2011 – 2014	B.Sc. (Hons.) Physics, Shivaji College, University of Delhi. Percentage: 72.7%, First division.
2011-2012	Higher Secondary, GBSSS, Rajouri Garden, Delhi. Percentage: 73.4%, First division.
2009-2010	Matriculation, GBSSS, Mohan Garden, Delhi. Percentage: 86.6%, First division.








Experience

- 2019  Worked as a **Teaching Assistant** for one semester in Electronics Lab B.Sc.(H) Physics, at the Department of Physics, Jamia Millia Islamia, New Delhi, January-June, 2019.
- 2018  Worked as a **Teaching Assistant** for one semester in Mechanics Lab, B.Sc.(H) Physics at the Department of Physics, Jamia Millia Islamia, New Delhi, July-December, 2018.




Invited Talks/Teaching Assistant

- 2023  Invited as **Teaching Assistant** in the workshop on "**Quantum Mechanical Modeling of Materials by Quantum ESPRESSO**" jointly organised by IEEE Nanocouncil PSIT Student Chapter, MRSI, Allahabad Chapter, and School of Basic Sciences, CSJM University, India, held during 15th - 19th March 2023.
- 2022  Invited as **Teaching Assistant** in the workshop on "**Mollywood to Molecular Nodes**" jointly organised by Gdańsk University of Technology, Poland, IRB Barcelona, Spain and Scidart Academy, India held during 8th - 11th September 2022.
- 2021  Invited as **Teaching Assistant** in Winter School on "**Advanced Molecular Dynamics simulation**" jointly organised by International School of Photonics, Cochin University of Science and Technology (CUSAT), India, Department of Physics and Green Club of thoughts, Kathmandu University, Nepal, held during 6th - 17th Sept, 2021.
-  Invited as **Teaching Assistant** in summer school on "**Advanced Molecular Dynamics simulation**" jointly organised by Department of Chemistry, IISER Pune, India, Department of Physics and Green Club of thoughts, Kathmandu University, Nepal, held during 5th - 16th July, 2021.

Awards and Achievements

- 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 9-11, 2022.
-  Qualified **CSIR Senior Research Fellowship** 2022-2023.
- 2020  **2nd position** on report submitted in the "*Winter School on Electronic Structure and Molecular Dynamics Simulations Using Open Source Software: From Theory to Practice*" jointly organized by Parvatibai Chowgule College of Arts and Science, Margao, Goa and Supercomputer Center, Kathmandu University, Nepal held during September 27- October 04, 2020.
-  "**Best poster**" award at Jamia Millia Islamia University National Symposium on "*Advances in Material Science and Theoretical Physics*" February 19-20, 2020.
- 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.
- 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.

Awards and Achievements (continued)

- 2009  **2nd position** in Zonal level “**Science quiz competition**” from GBSS School Rajouri Garden in 2009-10.
-  Scholarship for obtaining “**99 marks in Social-Science**” in class X.
- 2006  **1st position** in School level “**Science Quiz Competition**” in GBSS School Mohan Garden in 2006-07.










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 Ti₂CO₂ MXene decorated with Cu-cluster for Hydrogen evolution reaction. ” <i>Applied Surface Science</i> 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 ”	J. Energy Storage
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 Štanger, Iwona A. Rutkowska, Pavel Kulesza, Saim Emin, “ Phase transformation approach for the preparation of active Fe₂P catalyst for oxygen evolution ”	J. Chem. Eng.
3. Sai Raj Ali , Lekha Nair, Praveen Kumar, “ A Review of Electrochemical Water Splitting for Sustainable Hydrogen Production. ”	To be communicated

Schools, Workshops & Conferences

- March 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.
- November 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 on H₂&CO₂ virtual mode, organised by S&T Digital, India, held during 17th - 19th November, 2022.
- October 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.

Schools, Workshops & Conferences (continued)

- October 2020  One Week **National Certificate Program** on “Instrumental methods of analysis” virtual mode under MHRD Govt. of India held during 7th - 13th October, 2020.
- September 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.
- February 2020  **National Symposium** on “Advances in Material Science and Theoretical Physics” at JMI, New Delhi, India held during 19th - 20th February 2020.
- October 2019  **Winter School** on “Materials and Molecular Simulations using Open Source Softwares from theory to practice” at Department of Physics, Bishop Moore College, Mavelikara, Kerala, India held during 16th - 22nd October 2019.
- March 2019  **Workshop and Symposium** on “Advanced Simulation Methods: DFT, MD and Beyond” at IIT Delhi, India held during 6th - 10th March, 2019.
- October 2018  **International School** on “Ion Beams in Material Science” at Inter University Accelerator Centre (IUAC) New Delhi, India held during 3rd - 7th October, 2018.
- August 2018  The **GIAN course** Density Functional Theory for Heterogeneous Catalysis at IIT Guwahati, India held during 6th - 11th August, 2018.
- March 2016  The **GIAN course** on “Probing Large-Scale Structure of the Universe with Weak Lensing” at CTP, JMI, New Delhi, India held during March 07 - 12, 2016.
- February 2016  The **GIAN course** on “Cosmological and Theoretical applications of exact solutions of Einstein’s equations” at CTP, JMI, New Delhi, India held during February 12 - 23, 2016.

Referees

1. [Prof. Lekha Nair](#)

Relationship: **PhD Supervisor**
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2. [Dr. CS Praveen](#)

Relationship: **Collaborator**
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3. [Dr. Praveen Kumar](#)

Relationship: **Collaborator**
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