

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
Programming	■ Python, Fortran, Shell scripting
Graphics Tools	■ Blender, Inkscape, GIMP
Plotting Tools	■ Gnuplot, Matplotlib
Operating Systems	■ Linux, Windows
Miscellaneous	■ Vim, L ^A T _E X

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 Co-Supervisor: Dr. Praveen Kumar, IACS, Kolkata. Course Work CGPA : 8.6, 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, 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 "**Molywood 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 Štangaar, 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
4. Sai Raj Ali , Sivaprasad Surendran [†] , Sruthy Sajeevkumar [†] , Lekha Nair, KC Bhamu, Praveen Kumar, CS Praveen, “ Enhancing Hydrogen Evolution in Mo₂CO₂ MXene through Transition Metal Doping and Atomic-Level Modulation ”	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 H_2 & CO_2 virtual mode, organised by S&T Digital, India, held during 17th - 19th November, 2022.

Schools, Workshops & Conferences (continued)

- 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.
- 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**
Department of Physics,
Jamia Millia Islamia University,
New Delhi-110025, India.
Phone : +91 98100 32194
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2. **Dr. Praveen Kumar**

Relationship: **PhD Co-supervisor**
School of Material Science,
Indian Association for the
Cultivation of Science
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3. **Dr. CS Praveen**

Relationship: **Collaborator**
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Photonics, Cochin University of
Science and Technology,
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