

# 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 (CO<sub>2</sub>).
- 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, $\text{\LaTeX}$




## Education

2017 – Present	■ <b>Ph.D. in Material Science, Jamia Millia Islamia University, Delhi.</b> 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 : 8.6/10.0, First division.
2014 – 2016	■ <b>M.Sc. Physics, Jamia Millia Islamia University, Delhi.</b> 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>B.Sc. (Hons.) Physics, Shivaji College, University of Delhi.</b> Percentage: 72.7%, First division.
2011-2012	■ <b>Higher Secondary, GBSSS, Rajouri Garden, Delhi.</b> Percentage: 73.4%, First division.
2009-2010	■ <b>Matriculation, GBSSS, Mohan Garden, Delhi.</b> 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 15<sup>th</sup> - 19<sup>th</sup> 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 8<sup>th</sup> - 11<sup>th</sup> 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 6<sup>th</sup> - 17<sup>th</sup> 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 5<sup>th</sup> - 16<sup>th</sup> July, 2021.

## Awards and Achievements

- 2022  "**Best Oral Presentation**" award at CSIR-CSIO Chandigarh "*1<sup>st</sup> 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  **2<sup>nd</sup> 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  **1<sup>st</sup> position** in "**Powerpoint Presentation**" organised by Physics Society (Invenio 2014) at Shivaji College, University of Delhi.
-  **2<sup>nd</sup> position** in "**Science Quiz Competition**" organised by Physics Society (Invenio 2014) in Shivaji College, University of Delhi.

## Awards and Achievements (continued)

- 2009      **2<sup>nd</sup> 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      **1<sup>st</sup> position** in School level “**Science Quiz Competition**” in GBSS School Mohan Garden in 2006-07.










## Research Publications

Published/Accepted	Impact Factor
1. <b>Sai Raj Ali</b> , CS Praveen, Sung Gu Kang, Lekha Nair, KC Bhamu, Praveen Kumar, “ <b>Exploring the catalytic properties of Ti<sub>2</sub>CO<sub>2</sub> MXene decorated with Cu-cluster for Hydrogen evolution reaction.</b> ” <i>Applied Surface Science</i> 641 (2023): 158439	6.7
Under Review/Preparation	Journal
1. Javeesh Alex, S. Rajkumar <sup>†</sup> , <b>Sai Raj Ali</b> <sup>†</sup> , J.Princy Merlin, Arun Aravind, D. Sajan, C. S. Praveen, “ <b>Enhanced Pseudocapacitance Performance of NiO and Ce-Doped NiO Synthesized via Modified Combustion Technique</b> ”	J. Energy Storage
2. Takwa Chouki, Sreejith P. Nandan, Romana Cerc-Korošec, Georgi Tyuliev, <b>Sai Raj Ali</b> , CS Praveen, Manel Machreki, Dominik Eder, Alexey S. Cherevan, Urška Lavrenčič Štanger, Iwona A. Rutkowska, Pavel Kulesza, Saim Emin, “ <b>Phase transformation approach for the preparation of active Fe<sub>2</sub>P catalyst for oxygen evolution</b> ”	J. Chem. Eng.
3. <b>Sai Raj Ali</b> , Lekha Nair, Praveen Kumar, “ <b>A Review of Electrochemical Water Splitting for Sustainable Hydrogen Production.</b> ”	To be communicated

## Schools, Workshops & Conferences

- March 2023      Online **2<sup>nd</sup> 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 13<sup>th</sup> - 15<sup>th</sup> March, 2023.
-  **International Materials Conclave (IMC-2023)** & 33<sup>rd</sup> Annual Foundation Day, organised by Centre for Materials for Electronics Technology (C-MET), Pune, held during 8<sup>th</sup> - 10<sup>th</sup> March, 2023.
- November 2022      **International Conference** on Nanotechnology: Opportunities and Challenges (ICNOC-2022) virtual mode, organised by JMI University, Delhi, held during 28<sup>th</sup> - 30<sup>th</sup> November, 2022.
-  **International Conference** on on  $H_2$ & $CO_2$  virtual mode, organised by S&T Digital, India, held during 17<sup>th</sup> - 19<sup>th</sup> November, 2022.
- October 2022      **1<sup>st</sup> IEEE AcSIR-CSIO International Conference** on Emerging Materials for Sustainable Development (EMSD-2022) virtual mode, organised by CSIR-CSIO, Chandigarh, held during 9<sup>th</sup> - 11<sup>th</sup> 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 7<sup>th</sup> - 13<sup>th</sup> 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 9<sup>th</sup> - 15<sup>th</sup> September, 2020.
- February 2020     **National Symposium** on “Advances in Material Science and Theoretical Physics” at JMI, New Delhi, India held during 19<sup>th</sup> - 20<sup>th</sup> 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 16<sup>th</sup> - 22<sup>nd</sup> October 2019.
- March 2019     **Workshop and Symposium** on “Advanced Simulation Methods: DFT, MD and Beyond” at IIT Delhi, India held during 6<sup>th</sup> - 10<sup>th</sup> March, 2019.
- October 2018     **International School** on “Ion Beams in Material Science” at Inter University Accelerator Centre (IUAC) New Delhi, India held during 3<sup>rd</sup> - 7<sup>th</sup> October, 2018.
- August 2018     The **GIAN course** Density Functional Theory for Heterogeneous Catalysis at IIT Guwahati, India held during 6<sup>th</sup> - 11<sup>th</sup> 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,  
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3. **Dr. CS Praveen**

Relationship: **Collaborator**  
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