Sipra Mohapatra

Ph.D. Scholar
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Indian Institute of Technology Jodhpur
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Research Interest

My research work primarily focuses on the investigation of ion transport mechanisms and the structural properties of different types of solid polymer electrolytes using molecular dynamics simulations. The main goal is to achieve a fundamental understanding of the ion transport mechanisms, the relaxation phenomenon, and their correlations in battery electrolytes and electrode-electrolyte interfaces at the molecular level.

Education

2019–Ongoing **Ph.D.**, *Indian Institute of Technology Jodhpur*, India, *8.75/10 (Course Work CGPA)*
Supervisor- Dr. Santosh Mogurampelly,
Thesis Title: "Molecular Mechanisms of Ion Transport in Polymer Electrolytes"
Polymer Electrolytes and Materials Group,
Department of Physics, Indian Institute of Technology Jodhpur, India

2016–2018 **M. Sc.**, *Berhampur University*, Odisha, India, *7.75/10 (CGPA)*
M. Sc. in Physics with specialisaton in Condensed Matter Physics.

2013–2016 **B. Sc. (Hons. with Distinction)**, *Utkal University*, Odisha, India, *7.1/10 (CGPA)*
Physics (Hons.), Chemistry, Mathematics

2011–2013 **CHSE (12^{th})**, *Angul Govt. (Auto) College*, Odisha, India, *64 %*
(Physics, Chemistry, Mathematics, Geography)

2011 **CHSE (10^{th})**, *Angul Govt. High School*, Angul, Odisha India, *78.5 %*

Publications

2024 **Mohapatra, S.**; Teherpuria, H.; Chowdhury, S. S. P.; Ansari, S. J.; Jaiswal, P. K.; Netz, R. R.; Mogurampelly, S. "Ion Transport Mechanisms in Pectin-Containing EC-LiTFSI Electrolytes", *Nanoscale*, 2024, **16**, 3144 - 3159. (IF: 8.307)

2024 Ansari, S.J.; Haider, S.; **Mohapatra, S.**; Varanasi, S.R.; Mogurampelly, S. "Effects of pectin and temperature on the diffusion of ions and water in saltwater membranes", *J. Mol. Liq.* 2024, **396**, 124045. (IF: 6.633)

2024 Kumari, P; **Mohapatra, S.**; Halder S.; Mogurampelly S. "Viscosity of Pectin-[BMIM][PF_6] Electrolytes and the Interplay of Ion-ion Interactions", *J. Mol. Liq.*, 2024, **397**, 124159. (IF: 6.633)

2023 **Mohapatra, S.**; Halder, S.; Chaudhari, S. R.; Netz, R. R.; Mogurampelly, S. "Insights into the Structure and Ion Transport of Pectin-[BMIM][PF_6] Electrolytes", *J. Chem. Phys.* 2023, **159**, 154902. (IF: 4.304)

2022 **Mohapatra, S.**; Sharma, S.; Sriperumbuduru, A.; Varanasi, S. R.; Mogurampelly, S. "Effect of Succinonitrile on Ion Transport in PEO-Based Lithium-Ion Battery Electrolytes". *J. Chem. Phys.* 2022, **156**(21), 214903. (IF: 4.304)

2021 Prasad, D.; Praveen, A.; **Mahapatra, S.**; Mogurampelly, S.; Chaudhari, S. R. "Existence of β-Diketone Form of Curcuminoids Revealed by NMR Spectroscopy", *Food Chem.*, 2021, 360, 130000. (IF: 9.231)

Submitted Manuscript

2024 Teherpuria, H.; Yadav, H.; Mohapatra, S.; and Mogurampelly, S.; "Polymer alignment induced changes in ion solvation structure in EC-LiTFSI electrolytes", 2024

2024 **Mohapatra, S.**; and Mogurampelly S.; Kannam S. S., "Ionic flow through partially blocked nanopores", 2024

2024 **Mohapatra, S.**; Mogurampelly, S. "Molecular Dynamics Study of Bovine Serum Albumin (BSA) Based Biocompatible Solid Polymer Electrolyte". 2024.

2024 **Mohapatra, S.**; Halder S.; Kumari, P; Mogurampelly, S. "Ionic Diffusion and Glass Transition Temperature of Pectin-[BMIM][PF6] Electroles", 2024

Manuscripts Under Preparation

2024 Authors and Mogurampelly S., "Effect of FEC on Ionic Conductivity Mechanisms at SEI in Graphite Electrode system", 2024

2024 Authors and Mogurampelly S., "Effect of Molecular Weight on Ionic Transport Mechanisms in PEO-NaPF6 system", 2024

2024 Authors and Mogurampelly S., "Ionic Conductivity Mechanisms in PEO-NaPF6 Electrolytes", 2024

2024 Authors and Mogurampelly S.; Kannam S. S., "Translocation of Proteins in Nanopores: A Coarse-Grained Brownian Dynamics Study", 2023

2024 Authors and Mogurampelly S, "Friction in nanoscale for graphene-Ionic liquid system", 2023

Conference Proceedings

2024 Teherpuria, H.; Chowdhury, S. S. P.; **Mohapatra, S.**; Jaiswal, P. K.; Mogurampelly, S. "Diffusion and ion-ion correlations in EC-LiTFSI electrolytes", *Conference proceeding in A Springer book series Advances in Sustainability Science and Technology*, 2024

2024 **Mohapatra, S.**; Mogurampelly, S., "Ionic Conductivity and the Correlation with Viscosity in Pectin Ionic Liquid Electrolytes", AIP Proceedings, *Under Review.*

Workshops/ Conferences

2024 MD@60 at JNCASR, Bangalore, India during February 25-29, 2024

2023 CompFlu 2023 at the Indian Institute of Technology Madras, Chennai, India during December 18-20, 2023

2023 Structure and Dynamics of Chemical and Biomolecular Systems (SDCBS23), IIT Kanpur, Kanpur, India, Oct 26-28, 2023.

2023 *Poster on* "Insights into the Structure and Transport Mechanisms in Pectin-EC-LiTFSI Electrolytes" at Seventh International Symposium Frontiers in Polymer Science, Gothenburg, Sweden, 29 May – 1 June 2023

2022 *Presented on* "Molecular Dynamics Study of Bovine Serum Albumin (BSA) Based Biocompatible Solid Polymer Electrolyte" at international conference Supercaps & Batteries – India 2022

2021 *Presented Poster on* "Structure and Ionic Diffusivity Studies in Novel Biocompatible Polymer Electrolytes" at CMDAYS2021 Organised by Department of Physics Central University of Jharkhand, Ranchi 835205, Jharkhand, India

2021 *Attended* MolSSI Workshop on HPC in Computational Chemistry and Materials Science, December 13-15 2021

2021 *Presented Poster on "Effect of Succinonitrile on Transportation of Ions in PEO-based Battery Electrolytes"* at the Soft Matter: Young Investigators e-Meet 2021 (e-SMYIM 2021) Organized by IIT Bombay

Future Workshops/ Conferences

2024 MRS sping meeting 2024

2024 ACS Fall meetings 2024

Mentorship and Teaching Experience

- Mentored 6 Masters Students and 2 Ph.D. students for individual Projects
- Got invitation to Review 2 journal articles
- Teachinh Assistance at IIT Jodhpur for B. Tech. Students in Electromagnetism and Optics course, Physics Lab.
- Teachinh Assistance at IIT Jodhpur for M. Sc./P.h.D. Students in Computational Physics, Computational materials science, Soft Matter Physics.

Skills

Theory and concept	Expertise in Atomistic molecular dynamics simulations, Density functional theory, Soft matter Physics, Polymer science.
Programming Languages	FORTRAN, Basics of Python, bash scripting, Shell scripting
Scientific Softwares	GROMACS, VMD, GNUPlot, XMGrace, PACKMOL, Quantum ESPRESSO, MATLAB, TRAVIS, GaussView 6, Avogadro
Others	LaTeX

Awards and Achievements

- Graduate Aptitude Test 2019 in Engineering(GATE) Paper : PH-Physics, All India Rank:2095
- Received International Travel Scheme From Science and Engineering Research Board (SERB), Government of India.

Languages Known

- Odia, Hindi, English

Referees

- **Prof. Santosh Mogurampelly**
  Associate Professor, Department of Physics
  Indian Institute of Technology Jodhpur, Rajasthan, India
  E-mail: santosh@iitj.ac.in
  Tel : 0291-280-1613
  URL: *http://home.iitj.ac.in/∼santosh/index.html*

- **Prof. Roland R Netz**
  Professor, Department of Physics
  Freie Universität Berlin, Germany
  E-mail: rnetz@physik.fu-berlin.de
  Tel : +49 30 838 55737
  URL:*https://www.physik.fuberlin.de/en/einrichtungen/ag/ag-netz/group-members/professor/netz-roland/index.html*

- **Prof. Prabhat Jaiswal**
  Associate Professor, Department of Physics
  Indian Institute of Technology Jodhpur, Rajasthan, India
  E-mail: prabhat.jaiswal@iitj.ac.in
  Tel : 0291-280-1612
  URL: *https://sites.google.com/site/prabhatjaiswal/*

- **Prof. Ananya Debnath**
  Professor, Department of Chemistry
  Indian Institute of Technology Jodhpur, Rajasthan, India
  E-mail: ananya@iitj.ac.in
  Tel : 0291-280-1307
  URL: *http://home.iitj.ac.in/∼ananya/*