

Dr. Anurag Prakash Sunda

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EDUCATION

- 2010 - 2014 **PhD, Chemistry.**
Indian Institute of Science Education and Research (IISER), Pune
Title: Atomistic Investigation of Polymer Electrolyte Membrane Nanostructure and Dynamics of Molecular Transport in Fuel Cells [Supervisor: Dr. Arun Venkatnathan]
- 2008 - 2009 **MPhil, Energy.**
Center for Non-conventional Energy Resources, University of Rajasthan, Jaipur
- 2006 - 2008 **MSc, Physical Chemistry.**
Dept. of Chemistry, University of Rajasthan, Jaipur
- 2003 - 2006 **BSc, Chemistry.**
University of Rajasthan, Jaipur

EXPERIENCE

- At Present **DST INSPIRE Faculty,** (06.07.2015 - Present).
Central University of Haryana, Haryana
- 2015 **DST INSPIRE Faculty,** (11.03.2015 - 03.07.2015).
Pandit Deendayal Upadhyay Shekhawati University, Rajasthan
- 2014 **Postdoctoral Research Associate,** (03.02.2014 - 10.03.2015).
Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore
Supervisor: Prof. Balasubramanian Sundaram
- 2009 **Project Assistant,** (26.08.2009 - 16.12.2009).
PSE Division, National Chemical Laboratory-Pune

AWARDS/FELLOWSHIPS

- 2016 **SERB - International Travel Support.**
EMN MEETING ON FUEL CELLS held at Jeju, KOREA-ROK.
- 2015 **INSPIRE Faculty Award, Materials Science - July'14.**
by Ministry of Science and Technology, DST, New-Delhi
- 2011 **Rajat Jayanti Science Communication Award.**
by NCSTC, Department of Science and Technology, New-Delhi
- 2010 **UGC-Junior/Senior Research Fellowship.**
Chemical Sciences, CSIR-UGC NET JRF Rank 314
- 2009 **GATE 2009.**
Chemical Sciences, 90.46 percentile score

PUBLICATIONS

- 2016 Thermal Phase Behavior and Ion Hopping in 1,2,4-Triazolium Perfluorobutanesulfonate Protic Organic Ionic Plastic Crystal
A. Mondal, **A. P. Sunda** and S. Balasubramanian
PHYS. CHEM. CHEM. PHYS. **2016**, 18(3), 2047-2053. [IF - 4.45]
- 2015 Ammonium-based Protic Ionic Liquid Doped Nafion Membrane as Anhydrous Fuel Cell Electrolyte
A. P. Sunda
J. MATER. CHEM. A **2015**, 3(24), 12905–12912. [IF - 8.26]
- Atomistic Simulations of Ammonium-based Protic Ionic Liquids: Steric Effects on Structure, Low Frequency Vibrational Modes and Electrical Conductivity
A. P. Sunda, A. Mondal, and S. Balasubramanian
PHYS. CHEM. CHEM. PHYS. **2015**, 17(6), 4625–4633. [IF - 4.45]
- 2014 Structure and Dynamics of Benzyl-NX₃ (X=Me, Et) Trifluoromethanesulfonate Ionic Liquids
A. P. Sunda, V. M. Dhavale, K. Sreekumar and A. Venkatnathan
J. PHYS. CHEM. B **2014**, 118(7), 1831-1838. [IF - 3.18]
- Polymer Chain Length, Phosphoric Acid Doping and Temperature Dependence on Structure and Dynamics of ABPBI [poly(2,5-benzimidazole)] Polymer Electrolyte Membrane
M. More, **A. P. Sunda** and A. Venkatnathan
RSC ADVANCES **2014**, 4(38), 19746-19755. [IF - 3.28]
- 2013 Molecular Dynamics Simulations of Side Chain Pendant of PFSA Polymer Electrolyte Membranes
A. P. Sunda and A. Venkatnathan
J. MATER. CHEM. A **2013**, 1(3), 557–569. [IF - 8.26]
- A Molecular Investigation of Structure and Dynamics of the Phosphoric/Triflic Acid Blends of ABPBI (2,5-Benzimidazole) Polymer Electrolyte Membrane
A. P. Sunda, M. More and A. Venkatnathan
SOFT MATTER **2013**, 9(4), 1122–1131. [IF - 3.79]
- Parametric Dependence on Shear Viscosity of SPC/E Water from Equilibrium and Non-equilibrium Molecular Dynamics Simulations
A. P. Sunda and A. Venkatnathan
MOLECULAR SIMULATION **2013**, 39(9), 728–733. [IF - 1.67]
- 2012 Atomistic Simulations of Structure and Dynamics of Hydrated Aciplex Polymer Electrolyte Membrane
A. P. Sunda and A. Venkatnathan
SOFT MATTER **2012**, 8(42), 10827–10836. [IF - 3.79]

- 2011 Molecular Dynamics Simulations of Triflic Acid and Triflate/water Mixture: A Potential Electrolyte in Fuel Cells
A. P. Sunda and A. Venkatnathan
J. COMPUT. CHEM. **2011**, 32(15), 3319–3328. [On Cover] [IF - 3.64]

PROJECTS

- 2015 INSPIRE Faculty Project – DST (Ongoing)
Title: Ab Initio Molecular Dynamics simulation of Ionic Liquid doped Polymer Electrolyte Membranes and Platinum Electrode Interface
No. DST/INSPIRE/04/2014/015731 INR 35,00,000/-
Institute: Central University, Haryana
- 2011 Rajat Jayanti Vigyan Sancharak Fellowship – NCSTC, DST (Completed)
Title: Molecular Modeling in Design and Development of Novel Materials for Renewable Energy
No. CO/S/TR/F09/2012 INR 2,29,000/-
Institute: IISER, Pune

TEACHING EXPERIENCE

- 2016 M. Sc.: **Physical Chemistry-II** [4 hrs per week]
○ Chemical Kinetics: Order of Reaction, Rate Laws, Arrhenius Equation
○ SSA, Theory of Unimolecular Reaction and Enzyme Kinetics
- 2016 M. Sc.: **Physical Chemistry-IV** [4 hrs per week]
○ Solid State: Conductor, Semi-Conductors and Superconductivity
○ Quantum Chemistry: Molecular Orbital Theory and its applications
- 2016 M. Sc.: **Polymer Chemistry-IV** [3 hrs per week]
○ Kinetics of polymerization and polymer in solutions
○ Polymer structure, crystalline arrangement of polymers, morphology and viscoelastic behaviour
- 2015 M. Sc.: **Physical Chemistry-I** [4 hrs per week]
○ Electrochemistry: Electrochemistry of solutions, Debye Hückel Theory, Inter/Intra ionic interactions
○ Classical Thermodynamics: Law of thermodynamics, Partial Molar Properties, Fugacity and Acitivity
- 2015 M. Sc.: **Physical Chemistry-III** [3 hrs per week]
○ Chemical Kinetics: Order of Reaction, Rate Laws, Arrhenius Equation, Unimolecular Theory and Enzyme Kinetics
○ Group Theory and Symmetry: Symmetry operations, Element, Character Tables and Group
○ Langmuir Isotherm, BET Theory and Surface area determination

- 2015/2016 M. Sc.: **Physical Chemistry Laboratory Practicals** [6/3 hrs per week]
A manual has been prepared with 7 different experiments which cover various physical chemistry concept related to Chemical Kinetics, Electrochemistry, Liquids Phases, Photochemistry/Spectroscopy and Thermodynamics.

WORKSHOP, SEMINAR AND CONFERENCES

INVITED LECTURES

- June - 2016 Indian Institute of Science Education and Research (IISER), Mohali.
May - 2016 EMN Meeting on Fuel Cells (May 23-27), Jeju Island, KOREA-ROK.
Sep - 2013 One Day Awareness workshop on Science Communication (organized by DST, New-Delhi), Visvaniketan's IMEET-Mumbai.
Jan - 2013 7th CRSI-RSC Symposium, IIT BHU-Varanasi.

ORAL PRESENTATIONS

- Nov - 2014 NFM-2014, BITS-Pilani.
(A National Conference)
Sep - 2012 Chemical Constellation Cheminar-2012, NIT-Jalandhar.
(An International Conference)
Dec - 2010 3rd Polymer Science Congress MACRO, IIT New-Delhi.
(An International Conference)

POSTER PRESENTATIONS

- Mar - 2016 Emerging Trends in Applied Chemical Sciences, A National Symposium, Central University of Rajasthan.
Aug - 2014 MD@50, An International Conference, JNCASR-Bengaluru.
Dec - 2012 Theoretical Chemistry Symposium, IIT-Guwahati.
Mar - 2011 International Symposium on Material Education, Yashada-Pune.
Sep - 2010 RSC West India Ph.D. Symposium, University of Goa.

HONORARY WORK AND WORKSHOPS

- Aug - 2014 Volunteer in MD@50, International Conference, JNCASR-Bengaluru.
Mar - 2013 Volunteer in 1st Indo-US Research Fellowship Conclave at Pune.

ACADEMIC ACTIVITIES

- Feb - 2016 Organized National Science Day as a member of organizing committee on 28-02-2016 in the coordination with all science departments, Central University of Haryana.
Oct - 2015 Visited 'Jawaharlal Nehru University (JNU)' and 'Inter University Acceleration Centre (IUAC)', Delhi on 24.09.2015 as a representative of the University, for the establishment of Center of High-Performance Computing (C-HPC) and submitted proposal for the same to the University/UGC.

Aug - 2015 Organized three day Workshop on 'Thin Film and Vacuum Technology' as a member of organizing committee from 22-09-2015 to 24-09-2015 at Department of Chemistry in the coordination with Department of Physics, Central University of Haryana.

RESEARCH GUIDANCE

M. SC. PROJECT DISSERTATION (SPRING 2016)

- Gaurav Panday (CUH - 5174)
Title: Molecular Investigation of Ion-Transport in Aqueous Imidazolium-based Ionic Liquid
- Manjeet Kumar (CUH - 5179)
Title: CO₂ Sequestration in 1-butyl-1-methyl-pyrrolidinium-based Ionic Liquids: A Molecular Dynamics Simulation Study
- Sonia Yadav (CUH - 5191)
Title: Atomistic Simulations of butyl-pyridinium based Ionic Liquid: An Application to SO₂ Capture
- Ruchi Goyal (CUH - 5582)
Title: Molecular Dynamics Simulations of CO₂ in 1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide Ionic Liquid

MEMBERSHIPS

2015 Life Time Member of Chemical Research Society of India (CRSI)
[LM 1847]

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