Dr. Anurag Prakash Sunda

Assistant Professor (DST INSPIRE Faculty)
School of Chemical Sciences & Pharmacy
Central University of Rajasthan
Kishangarh, Ajmer PIN - 305817 INDIA

(91) 99825 60724
anurag.sunda@gmail.com
www.apsunda.com

Education

2010 - 2014 **Ph. D.**, *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 (Award date: May 09, 2014)
Supervisor: Dr. Arun Venkatnathan

2008 - 2009 **M. Phil.**, *Energy (67.60%)*.
Center for Non-conventional Energy Resources, University of Rajasthan, Jaipur

2006 - 2008 **M. Sc.**, *Physical Chemistry (68.30%)*.
Deptartment of Chemistry, University of Rajasthan, Jaipur

2004 - 2006 **B. Sc.**, *Chemistry (78.08%)*.
University of Rajasthan, Jaipur

Experience

2015 - 2017 **DST INSPIRE Faculty**, (06.07.2015 - 17.07.2017).
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 (Chair, CPMU)

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**, *Material Sciences - Jan'15*.
by Ministry of Science and Technology, DST, New-Delhi

2011 **Rajat Jayanti Vigyan Sancharak Fellowship**.
by NCSTC, Department of Science and Technology, New-Delhi

2010 **UGC-Junior/Senior Research Fellowship**.
Chemical Sciences, CSIR-UGC NET JRF Rank 314 (2009)

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-NX_3 (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/-
Host 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/-
Host Institute: IISER, Pune

Teaching Experience

2015/16 M. Sc.: Physical Chemistry-I (Fall) [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 Acitvity

2016/17 M. Sc.: Physical Chemistry-II (Spring) [4 hrs per week]
- Chemical Kinetics: Order of Reaction, Rate Laws, Arrhenius Equation
- SSA, Theory of Unimolecular Reaction and Enzyme Kinetics
- Quantum Mechanics, Rigid Rotator and Approximation Methods
- Group Theory and Symmetry: Symmetry operations, Element, Character Tables and Group

2015/16 M. Sc.: Physical Chemistry-III (Fall) [4 hrs per week]
- Solid State: Conductor, Semi-Conductors and Superconductivity
- Quantum Chemistry: Molecular Orbital Theory and its applications

2015/16 M. Sc.: Physical Chemistry-IV (Fall) [4 hrs per week]
- Kinetics of polymerization and polymer in solutions
- Polymer structure, crystalline arrangement of polymers, morphology and viscoelastic behaviour
- Langmuir Isotherm, BET Theory and Surface area determination

2015/16/17 M. Sc.: Physical Chemistry Laboratory Practicals (Spring) [8 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 7^{th} 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

Jan - 2017 INSPIRE Faculty Interaction Meet, KIIT University, Bhubaneswar, Odisha.

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 1^{st} Indo-US Research Fellowship Conclave at Pune.

Academic activities

Sept - 2016 Organized One Day National Symposium on "Recent Trends on Eco-friendly Chemistry' as a member at CUH.

Feb - 2016 Organized National Science Day as a member of organizing committee on 28-02-2016/17 in the coordination with all science departments at CUH.

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 at CUH.

Research guidance

M. Sc. Project Dissertation (Spring 2017)

- Sadhna Kaliramana (CUH - 6164)
  Title: Molecular Dynamics Simulations of Betaine-based Ionic Liquids for CO_2 Sequestration
- Amit Singh (CUH - 6167)
  Title: Atomistic Investigation of Ion-Transport in Aqueous betaine-based Ionic Liquids
- Jasveer Punia (CUH - 6182)
  Title: Effect of Anions in Ionic Liquids for the Application to SO_2 Capture

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: CO_2 Sequestration in 1-butyl-1-methyl-pyrolidium-based Ionic Liquids: A Molecular Dynamics Simulation Study
- Sonia Yadav (CUH - 5189)
  Title: Atomistic Simulations of butyl-pyridinium based Ionic Liquid: An Application to SO_2 Capture
- Ruchi Goyal (CUH - 5582)
  Title: Molecular Dynamics Simulations of CO_2 in 1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide Ionic Liquid

Memberships

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

Residential Address: Piprali Road, Sikar, Rajasthan PIN 332001 INDIA
Email: anurag.sunda@gmail.com, Tel: +91 1572 258944
Webpage: www.apsunda.com