

# Dr. Anurag Prakash Sunda

Assistant Professor, Chemistry,  
J C Bose University of Science and Technology, YMCA Faridabad, INDIA

☎ (91) 99825 60724  
✉ anurag.sunda@gmail.com



## AT PRESENT

2020 **Assistant Professor, Chemistry,** (Feb 03, 2020 - til date).  
Department of Chemistry,  
J C Bose University of Science and Technology, YMCA Faridabad, INDIA

## EDUCATION

2014 **PhD, Chemistry,** *Indian Institute of Science Education and Research (IISER), Pune.*  
*Atomistic Investigation of Polymer Electrolyte Membrane Nanostructure and Dynamics of Molecular Transport in Fuel Cells*  
2009 **MPhil, Energy (67.60%),** *Center for Non-conventional Energy Resources, University of Rajasthan, Jaipur.*  
2008 **MSc, Physical Chemistry (68.30%),** *Department of Chemistry, University of Rajasthan, Jaipur.*  
2006 **Bachelor in Science (78.08%),** *Shri Kalyan Govt. PG College (Sikar), University of Rajasthan, Jaipur.*  
2002 **High School (73.23%),** *Shri Kalyan Govt. Sr. Sec. School (Sikar), Board of Secondary Education, Ajmer.*  
2000 **Secondary (86.50%),** *AVM Sec. School (Sikar), Board of Secondary Education, Ajmer.*

## RESEARCH EXPERIENCE (~6 YEARS)

- **DST INSPIRE Faculty (Research Grant - 35 Lakhs)** (2015 - 2020)
  - Sharda University [Oct 2019 to Feb 2020]
  - Central University of Rajasthan [July 2017 to Oct 2019]
  - Central University of Haryana [July 2015 to July 2017]
  - PDU Shekhawati University [March 2015 to July 2015]
- **Postdoctoral Research Associate (Supervisor: Prof. Balasubramanian Sundaram)**  
*Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore* (Feb. 2014 - Mar. 2015)

## AWARDS/FELLOWSHIPS

2016 **SERB - International Travel Support,** *For EMN Meeting on Fuel Cells, Korea-Rok.*  
2014 **INSPIRE Faculty Award,** *Materials Sciences, by DST, New-Delhi.*  
2011 **Rajat Jayanti Vigyan Sancharak Fellowship,** *by NCSTC, DST, New-Delhi.*  
2010 **CSIR-UGC NET JRF,** *(Chemical Sciences) Rank 314 (2009).*  
2009 **GATE 2009,** *Chemical Sciences, 90.46 percentile score.*

## SELECTIVE PUBLICATIONS

- A. Mondal\* and A. P. Sunda\* **PHYS. CHEM. CHEM. PHYS.** **2018**, 20(28), 19268–19275.
- P. Roy\*, N. K. Uriel and A. P. Sunda\* **NANOSCALE** **2018**, 10(23), 11143–11149.
- A. P. Sunda\* **J. MATER. CHEM. A** **2015**, 3(24), 12905–12912.
- A. P. Sunda and A. Venkatnathan\* **J. MATER. CHEM. A** **2013**, 1(3), 557–569.
- A. P. Sunda and A. Venkatnathan\* **SOFT MATTER** **2012**, 8(42), 10827–10836.
- A. P. Sunda and A. Venkatnathan\* **J. COMPUT. CHEM.** **2011**, 32(15), 3319–3328. [Cover page article]

## TEACHING EXPERIENCE (5+ years)

- Designed Elective PG Course (—At CU, Rajasthan) : **ADVANCED COMPUTATIONAL CHEMISTRY** Credit: 04 [60 hrs.]
- —AT CENTRAL UNIVERSITY, RAJASTHAN: (10 - 12 hrs. per week)  
Physical Chemistry courses of PhD/Int. MSc/MSc/MSc-BEd Programmes
- —AT CENTRAL UNIVERSITY, HARYANA: (12 - 16 hrs. per week)  
Physical Chemistry core courses/Lab of PG Programmes

## MEMBERSHIPS

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

## PERSONAL INFORMATION:

Date of Birth: June 30, 1986 (Age ~ 33 Years)  
Skype ID: apsunda

Nationality: Indian  
Homepage: www.apsunda.com

## PUBLICATIONS

- 2018 Molecular Dynamics Simulations of Ammonium/Phosphonium-based Protic Ionic Liquids: Influence of Alkyl to Aryl group  
A. Mondal\* and **A. P. Sunda\***  
*PHYS. CHEM. CHEM. PHYS.* **2018**, 20, 19268-19275. [IF - 3.9]
- Nanoscale Defolding Influence of Polypeptide in Charge Transfer Process through Organic-Inorganic Nano Hybrid System  
P. Roy\*, N. K. Uriel and **A. P. Sunda\***  
*NANOSCALE* **2018**, 10(23), 11143-11149 . [IF - 7.2]
- 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 - 3.9]
- 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 - 10.77]
- 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 - 3.9]
- 2014 Structure and Dynamics of Benzyl-NX<sub>3</sub> (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 - 3.1]
- 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 - 3.1]
- 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 - 10.77]
- 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 - 3.8]
- 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 - 1.9]
- 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 - 3.8]
- 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 - 3.2]

## SPONSORED PROJECTS

- 2015 **DST INSPIRE Faculty:** DST/INSPIRE/04/2014/015731 [IFA14-MS31] (Completed)  
*Project Title: Ab Initio Molecular Dynamics simulation of Ionic Liquid doped Polymer Electrolyte Membranes and Platinum Electrode Interface*  
Awarded by: Department of Science and Technology, Delhi  
Duration: March 2015 to Feb 2020 (5-Years) Grant: **INR 35,00,000/-**
- 2011 **Rajat Jayanti Vigyan Sancharak Fellowship:**CO/S/TR/F09/2012 (Completed)  
*Project Title: Molecular Modeling in Design and Development of Novel Materials for Renewable Energy*  
Awarded by: National Council of Science & Technology, DST, New-Delhi.  
Duration: Jan 2013 to Dec 2013 (1-Year) Grant: **INR 2,29,000/-**  
Host Institute: Indian Institute of Science Education and Research (IISER), Pune

## RESEARCH GUIDANCE [PG DISSERTATIONS - 12]

- 2019 **Snehraj Gaur** (CU Rajasthan - 2016IMSBCH013)  
*Title: Hydrophobic Interface Analysis of Amyloid A $\beta$ <sub>(1-42)</sub> Peptide Plaque using Molecular Dynamics Simulations*
- Kailash Mohar** (CU Rajasthan - 2016IMSBCH015)  
*Title: Atomistic simulations of SO<sub>2</sub> Interactions with Amino-Acid based Bio-degradable Ionic Liquids*
- Pradhuman Singh** (CU Rajasthan - 2016IMSBCH020)  
*Title: Atomistic Simulations of Cholinium Cation and Amino-Acid based Ionic Liquids*
- Yogita Gupta** (CU Rajasthan - 2017MSCH009)  
*Title: CO<sub>2</sub> Sequestration using Atomistic Simulations of Cholinium based Ionic Liquids*
- 2018 **Srishti Gaur** (CU Rajasthan - 2013IMSBCH023)  
*Title: Molecular Dynamic Simulation of Cholinium-Amino Acids based Ionic Liquid*
- 2017 **Sadhna Kaliramana** (CU Haryana - 6164)  
*Title: Molecular Dynamics Simulations of Betaine-based Ionic Liquids for CO<sub>2</sub> Sequestration*
- Amit Singh** (CU Haryana - 6167)  
*Title: Atomistic Investigation of Ion-Transport in Aqueous betaine-based Ionic Liquids*
- Jasveer Punia** (CU Haryana - 6182)  
*Title: Effect of Anions in Ionic Liquids for the Application to SO<sub>2</sub> Capture*
- 2016 **Gaurav Panday** (CU Haryana - 5174)  
*Title: Molecular Investigation of Ion-Transport in Aqueous Imidazolium-based Ionic Liquid*
- Manjeet Kumar** (CU Haryana - 5179)  
*Title: CO<sub>2</sub> Sequestration in 1-butyl-1-methyl-pyrrolidinium-based Ionic Liquids: A Molecular Dynamics Simulation Study*
- Sonia Yadav** (CU Haryana - 5189)  
*Title: Atomistic Simulations of butyl-pyridinium based Ionic Liquid: An Application to SO<sub>2</sub> Capture*
- Ruchi Goyal** (CU Haryana - 5582)  
*Title: Molecular Dynamics Simulations of CO<sub>2</sub> in 1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide Ionic Liquid*

## WORKSHOP, SEMINAR AND CONFERENCES

### INVITED LECTURES

- March - 2019 National Conference: Energy and Environment (NCEE-2019) JNVU Jodhpur.
- 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<sup>th</sup> 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

Feb - 2019 Theoretical Chemistry Symposium, BITS Pilani.

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<sup>st</sup> 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.

- \* - \* - \* -