Dr. Anurag Prakash Sunda

Assistant Professor, Chemistry
J. C. Bose University of Science and Technology, YMCA
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At Present

2020 **Assistant Professor**, *Chemistry* *(Feb. 03, 2020 - till date)*
J. C. Bose University of Science and Technology, YMCA, Faridabad 121006 INDIA.

Education

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

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 **Bachlor 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 (9+ years)

- DST INSPIRE Faculty (Research Grant - 21 Lakhs) (March 2015 - Feb 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 - March 2015)
- Project Assistant - II *(Supervisor: Dr. U. K. Kharul)*
  PSE Devision, National Chemical Laboratory, Pune (Aug. 2009 - Dec. 2009)

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***, A. Mondal, and S. Balasubramanian* Phys. Chem. Chem. Phys. **2015**, 17(6), 4625–4633.
- **A. P. Sunda** and A. Venkatnathan* J. Mater. Chem. A **2013**, 1(3), 557–569.

Teaching Experience (8+ years)

- —At J. C. Bose UST, YMCA: (16 hrs. per week)
  Physical Chemistry courses of PhD/BSc Chemistry (Hon's)/MSc Chemistry Programmes
- Designed Elective PG Course (—At CU, Rajasthan) : Advanced Computational Chemistry Credit: 04
- —At Central University, Rajasthan: (14 - 16 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

Personal Information:

Date of Birth: June 30, 1986 (Age ∼ 36 Years)
Skype ID: anurag.sunda

Nationality: Indian
Homepage: www.apsunda.com

Publications

2023 Atomistic Simulations of Hydrated Sulfonated Polybenzophenone Block Copolymer Membranes
A. P. Sunda*, Soni Singh, Sonia Yadav, Raman K Singh*
ChemPhysChem **2023**, Just Accepted DOI: 10.1002/cphc.202300104 . [IF - 3.52]

2020 Selenium coordinated palladium(II) trans-dichloride molecular rotor as catalyst for site selective annulation of 2-arylimidazo[1,2-a]pyridines
H. Joshi, N. Meena, S. Sharma, R. Bhatt, V. N. Shinde, **A. P. Sunda**, N Bhuvanesh and A. Kumar
Chem. Commun. **2020**, 56, 10223-10226. [IF - 6.06]

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 - 3.94]

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 - 8.31]

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 - 3.94]

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 - 14.51]

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 - 3.94]

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 - 3.46]

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 - 4.06]

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 - 14.51]

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 - 4.04]

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 - 2.34]

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 - 4.04]

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 - 3.6]

Book Chapter(s)

2021 Chapter Title: 'Advances in Environmental Applications of Metal-Organic Frameworks'
Book: 'Metal-Organic Frameworks for Environmental Remediation'
Author(s): **A. P. Sunda** and S. Yadav, 2021, Chapter 2 pp 25-52.
ACS Symposium Series Vol. 1395 DOI: 10.1021/bk-2021-1395.ch002

Sponsored/Research Projects

2023 **SERB Core Research Grant**: F. CRG-001938 (Ongoing)
Project Title: Microphase Separation .... Membrane Fuel Cell Applications Grant: **INR 32,14,464/-**
Awarded by: SERB New Delhi
Duration: 3-Years w.e.f. Jan 7, 2023

2022 **UGC BSR Start-up Grant**: F. 30/589-2021 (Ongoing)
Project Title: Polymeric Form of Ionic Liquids Grant: **INR 10,00,000/-**
Awarded by: University Grants Commission
Duration: 2-Years w.e.f. June 17, 2022

2021 **Research Seed Money Award** (Ongoing)
Project Title: Polymer Composite of ionic Liquids Grant: **INR 2,00,000/-**
Awarded by: J. C. Bose University of Science and Technology, YMCA
Duration: July 2021 to March 2023 (2-Years)

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/-**
2nd Year Review Grading: **Very Good**

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

2020-23 *J. C. Bose University of Science and Technology [PhD Supervision (Ongoing)]*

- **Sonia Yadav** (20001901005)
  Polymer Composite Electrolytes for Fuel Cell Application
- **Parul** (22001901003)
  Electrolytes for Fuel Cell Application

Research guidance [PG Dissertations - 25]

2023 *J. C. Bose University of Science and Technology*

- Prachi Chandila (21001751033)
  Atomistic Simulation of Tetramethyl Ammonium Cation and bis(trifluromethanesulfonyl)imide Anions based Protic Organic Ionic Plastic Crystal
- Sweta Dagar (21001751057)
  Molecular Modeling of Acetamidium perchlorate Organic Ionic Plastic Crystal

2020-22 *J. C. Bose University of Science and Technology*

- Ajay Soni (20001751004)
  Atomistic simulations of Glycine and Serine Amino Acid based Biodegradable Ionic Liquids
- Jyotika (20001751023)
  Molecular Dynamics Simulations of Aliphatic Amino Acid Based Ionic Liquids
- Mehak Bhatiya (20001751029)
  Molecular Dynamics Simulations of Biodegradable Aromatic Amino-Acid Based Ionic Liquids
- Parul Sharma (19001751036)
  Molecular Dynamics Simulations of Ionic Liquid Doped Nafion as Anhydrous Fuel Cell Electrolyte
- Preeti Malviya (19001751042)
  Simulations of 1,2,4-triazole methanesulfonate Protic Ionic Liquid as High-Temperature Fuel Cell Electrolyte
- Anchal Gupta (18001751005)
  Molecular Dynamics Simulations of silicon-based pre-ceramic Poly(borosiloxane)s
- Gaurav (18001751010)
  Molecular Modelling of silicon-based preceramic poly(carbosilane)s Polymers
- Kritika Sehgal (18001751016)
  Molecular Dynamics Simulations of sulfonated polyarylene Ether Ketone as Low Temperature Polymer Electrolyte
- Munesh (18001751024)
  Molecular Modelling of Hydrated poly(arylene ether) Polymer Electrolyte for Fuel Cell Applications
- Preeti Kasana (18001751038)
  Atomistic Simulations of silicon-based Poly(methylsiloxane)s/ oxycarbide poly(carbosiloxane)s polymers
- Rachna Verma (18001751043)
  Molecular Modelling of Sulfonated polybenzophenone Polymer Electrolyte for Fuel Cell Applications

2017-19 *Central University of Rajasthan*

- Snehraj Gaur (2016IMSBCH013)
  Hydrophobic Interface Analysis of Amyloid $A\beta_{(1-42)}$ Peptide Plaque using Molecular Dynamics Simulations
- Kailash Mohar (2016IMSBCH015)
  Atomistic simulations of SO_2 Interactions with Amino-Acid based Bio-degradable Ionic Liquids
- Pradhuman Singh (2016IMSBCH020)
  Atomistic Simulations of Cholinium Cation and Amino-Acid based Ionic Liquids
- Yogita Gupta (2017MSCH009)
  CO_2 Sequestration using Atomistic Simulations of Cholinium based Ionic Liquids
- Srishti Gaur (2013IMSBCH023)
  Molecular Dynamic Simulation of Cholinium-Amino Acids based Ionic Liquid

2015-17 *Central University of Haryana*

- Sadhna Kaliramana (CU Haryana - 6164)
  Molecular Dynamics Simulations of Betaine-based Ionic Liquids for CO_2 Sequestration
- Amit Singh (CU Haryana - 6167)
  Atomistic Investigation of Ion-Transport in Aqueous betaine-based Ionic Liquids
- Jasveer Punia (CU Haryana - 6182)
  Effect of Anions in Ionic Liquids for the Application to SO_2 Capture
- Gaurav Panday (CU Haryana - 5174)
  Molecular Investigation of Ion-Transport in Aqueous Imidazolium-based Ionic Liquid
- Manjeet Kumar (CU Haryana - 5179)
  CO_2 Sequestration in 1-butyl-1-methyl-pyrolidium-based Ionic Liquids: A Molecular Dynamics Simulation Study
- Sonia Yadav (CU Haryana - 5189)
  Atomistic Simulations of butyl-pyridinium based Ionic Liquid: An Application to SO_2 Capture
- Ruchi Goyal (CU Haryana - 5582)
  Molecular Dynamics Simulations of CO_2 in 1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide IL

Academic activities

Aug - 2022 **Convener** of the Panel Discussion of the Institution Innovation Council Q-4 Activity held on August 18, 2022.
Invited Speakers: Dr. Vishal (CSIR-CECRI) & Mr Alkesh from Central University of Rajasthan
Topic: Innovation and Start-up: Electric Vehicles Challenges.

Nov - 2021 **Convener** of the Webinar of the Institution Innovation Council Q-1 Activity held on November 17, 2021.
Invited Speaker: Dr. Anuj K Sharma, from Central University of Rajasthan
Topic: Coordination Chemistry & Alzheimer's Disease: Innovations & Challenges.

Dec - 2020 **Convener** of the Webinar on the theme 'To innovate and integrate' held on December 14, 2020.
Invited Speaker: Dr. Vishal M Dhavale, Scientist from CSIR-CECRI
Topic: Fuel Cells - The challenges and advancement in Indigenous Technology.

Nov - 2020 **Convener** of one-week **National e-Workshop** cum value added course on 'Hands-On Training & Practices in Computational Chemistry' held from Nov 23-27, 2020. (Click here for Flyer & Report)

May - 2020 Organized One Week Online Faculty Development Program (OFDP) as Observer on the 'Spectroscopy Techniques and Applications'.

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.

Workshop, Seminar and Conferences

Invited Lectures

March - 2022 International Conference on 'Emerging Trends in Science and Technology' (ICETST-2022) Vedanta PG Girls College, Sikar from March 29-31, 2022.

July - 2021 International Conference (Virtual) ICRACS-2021, JCBose UST, YMCA Faridabad from July 14-16, 2021.

Feb - 2020 Vikram Sarabhai Space Centre (VSSC), Thiruvananthapuram (The lead Centre of ISRO).

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^{th} CRSI-RSC Symposium, IIT BHU-Varanasi.

Oral presentations

Feb - 2022 APA Nanoforum-2022, Nanomaterials & Nanoengineering (Feb. 24-26, 2022). (International e-Conference)

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 1st Indo-US Research Fellowship Conclave at Pune.

Memberships

2021 Life Time Member of Asian Polymer Association (APA) [L 623]

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

Additional Responsibilities

@J. C. Bose University of Science and Technology

- **Incharge** - *University Guest House* *(Since July 2022)*
- **Incharge** - *University Old Guest House* *(Since July 2022)*
- Coordinator -*Research & Development* *(Since Aug. 2021)*
- Coordinator -*IQAC: NAAC Criteria-1* *(Since Nov. 2022)*
- Coordinator -*CSIR Fellowships (Maker)* *(July 2021 to Sept. 2022)*
- Co-Coordinator -*Sports (Eklavya Club under office of Student Welfare)* *(Since Aug. 2020)*
- Nodal Officer -*Fit-India Programme* *(Since Sept. 2020)*
- Coordinator -*PhD Program in Chemistry* *(Since April 2020)*
- Deputy Centre Supdt.: NTA CET Exam 2022 *(November 5-6, 2022)*
- Member (Activity Coordinator) -*Institute Innovation(s) Council* *(Since Oct. 2020)*
- Member - Research Advisory Council *(Since Jan. 2023)*
- Member - HSHEC UG Chemistry Model Curriculum Design *(2021-2022)*
- Member of Board of Studies (BOS) Chemistry, JCBoseUST, YMCA. *(w.e.f. Feb 09, 2021)*
- Member of Board of Faculty (BOF) Sciences, JCBoseUST, YMCA *(July 28, 2020 to July 27, 2022)*

Other (Misc.)

Election Duty

- Duty Megistrate : Haryana Panchayat Election 2022 - Faridabad Block *(November 22 & 25, 2022)*

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