Anirban Mondal

Contact

Current Affiliation	Assistant Professor, Discipline of Chemistry, IIT Gandhinagar
Postal address	Academic Block 6, Room 337, Palaj, Gandhinagar, Gujarat, 382355, India
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Research interests

- Organic semiconductors, excited states, and optoelectronics
- Machine learning techniques to explore molecular chemical space
- Machine learning potentials for atomistic modeling of materials
- Materials for blue organic light-emitting diodes and organic solar cells
- Proton/ion transport in solid electrolytes

Employments

09/2021–present **Assistant Professor**, *Discipline of Chemistry, IIT Gandhinagar*, Gujarat, India

01/2021–08/2021 **Postdoctoral Researcher**, *University of Luxembourg*, Luxembourg
Advisor: Prof. Alexandre Tkatchenko

01/2019–12/2020 **Postdoctoral Research Associate**, *Princeton University*, Princeton, US
Advisor: Prof. Athanassios Z Panagiotopoulos

10/2016–12/2018 **Postdoctoral Fellow**, *Max Planck Institute for Polymer Research*, Mainz, Germany
Advisors: Prof. Denis Andrienko and Prof. Kurt Kremer

Education

06/2013–09/2016 **Ph.D.**, *Jawaharlal Nehru Centre for Advanced Scientific Research*, Bangalore, India
Thesis title: Computational Investigations of Ionic Liquids: Force Field development, Gas Solubility and Transport
Thesis advisor: Prof. Sundaram Balasubramanian
Degree awarded on: 16th May, 2017

08/2010–05/2013 **M.S.**, *Jawaharlal Nehru Centre for Advanced Scientific Research*, Bangalore, India
Subject: Materials Science
Thesis title: Computational Investigation of Complex Molecular Fluids
Thesis advisor: Prof. Sundaram Balasubramanian

08/2007–05/2010 **B.Sc.**, *Siksha Bhavana, Visva Bharati University*, Santiniketan, India
Subjects: Chemistry (Honours), Physics, and Mathematics

Awards and Grants

09/2019 Large-scale supercomputing facilities at the *Extreme Science and Engineering Discovery Environment* (XSEDE), National Science Foundation, USA
PI: Anirban Mondal; Co-PI: Prof. Athanassios Z Panagiotopoulos

12/2019 DOE Mission Science Allocation Award, *US Department of Energy*, USA
PI: Anirban Mondal; Co-PI: Prof. Athanassios Z Panagiotopoulos

2016 Max Planck Fellowship – *Max Planck Institute for Polymer Research*, Mainz, Germany

12/2014 Best Poster Award in *Theoretical Chemistry Symposium* at NCL, Pune, India

06/2014 Travel grant from the CECAM-HQ-EPFL, Lausanne, Switzerland to attend *Multiscale modelling of ionic liquids: from quantum methods to coarse-grained models*

06/2014 Best Poster Award in *Multiscale modelling of ionic liquids: from quantum methods to coarse-grained models* at CECAM-HQ-EPFL, Lausanne, Switzerland

12/2012 Best Poster Award in *Theoretical Chemistry Symposium* at IIT Guwahati, India

2010 Integrated Ph.D. fellowship; *Chemistry and Physics of Materials Unit*, JNCASR, India

Publications

2021 Molecular Library of OLED Host Materials—Evaluating the Multiscale Simulation Workflow **A. Mondal**, L. Paterson, J. Cho, K. Lin, B.v.d. Zee, G. A. H. Wetzelaer, A. Stankevych, A. Vakhnin, J. Kim, A. Kadashchuk, P. W. M. Blom, F. May, and D. Andrienko; *Chem. Phys. Rev.*, 2021, 2, 031304.

First-Principles Modeling of Transport Mechanisms in Carbonate-Hydroxide Electrolytes. **A. Mondal**, J. M. Young, G. Kiss, and A. Z. Panagiotopoulos; *J. Phys. Chem. C*, 2021, 125, 4412–4422.

2020 Genetic Algorithm Driven Force Field Parameterization for Molten Alkali-Metal Carbonate and Hydroxide Salts. **A. Mondal**, J. M. Young, T. Barckholtz, G. Kiss, L. Koziol and A. Z. Panagiotopoulos; *J. Chem. Theory Comput.*, 2020, 16, 5736-5746.

Predicting Chemical Reaction Equilibria in Molten Carbonate Fuel Cells via Molecular Simulations. J. M. Young, **A. Mondal***, T. Barckholtz, G. Kiss, L. Koziol and A. Z. Panagiotopoulos; *AIChE J.*, 2020, e16988. (*Equal contribution)

Transport and Interfacial Properties of Mixed Molten Carbonate/Hydroxide Electrolytes by Molecular Dynamics Simulations. **A. Mondal**, J. M. Young, T. Barckholtz, G. Kiss, L. Koziol and A. Z. Panagiotopoulos; *J. Phys. Chem. C*, 2020, 124, 23532-23540.

Molecular Simulation of Liquid-Vapor Coexistence for NaCl: Full-Charge Versus Scaled-Charge Interaction Models. D. Kussainova, **A. Mondal**, J. M. Young, S. Yue and A. Z. Panagiotopoulos; *J. Chem. Phys.*, 2020, 153, 024501.

2019 A Window to Trap-free Charge Transport in Organic Semiconducting Thin Films. N. B. Kotadiya, **A. Mondal**, D. Andrienko, P. W. M. Blom and G. A. H. Wetzelaer; *Nat. Mater.*, 2019, 18, 1182-1186.

Perspectives of Unicoloured Phosphor-sensitised Fluorescence (UPSF): A Computer Simulation Study. L. Paterson, **A. Mondal**, P. Heimel, R. Lovrincic, F. May, C. Lennartz, D. Andrienko; *Adv. Electron. Mater.*, 2019, 1900646.

Electron Trapping in Conjugated Polymers. D. Abbaszadeh, A. Kunz, N. B. Kotadiya, **A. Mondal**, D. Andrienko, J. J. Michels, G. A. H. Wetzelaer, P. W. M. Blom; *Chem. Mater.*, 2019, 6380.

Self-organization and Charge Transport Properties of Selenium and Tellurium Analogues of Polythiophene. Sh. Ye, L. Janasz, W. Zajaczkowski, J. G. Manion, **A. Mondal**, T. Marszalek, D. Andrienko, K. Muellen, W. Pisula, D. S. Seferos; *Macromol. Rapid Commun.*, 2019, 1800596.

The Influence of Impurities on the Charge Carrier Mobility of Small Molecule Organic Semiconductors. P. Friederich, A. Fediai, J. Li, **A. Mondal**, N. Kotadiya, G. D'Avino, F. Symalla, G. A. H. Wetzelaer, D. Andrienko, D. Beljonne, P. Blom, J-L, Bredas, W. Wenzel. *arXiv preprint*, 2019

2018 Unicolored Phosphor-Sensitized Fluorescence for Efficient and Stable Blue OLEDs. P. Heimel, **A. Mondal**, F. May, W. Kowalsky, C. Lennartz, D. Andrienko and R. Lovrincic; *Nat. Commun.*, 2018, 4990.

Rigorous Characterization of Hole Transport in Amorphous Organic Semiconductors. N. B. Kotadiya, **A. Mondal***, H. Lu, D. Andrienko, P. W. M. Blom and G. A. H. Wetzelaer; *Adv. Electron. Mater.*, 2018, 1800366. (*Equal Contribution)

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. (*Corresponding author)

Charge Environment and Hydrogen Bond Dynamics in Binary Ionic Liquid Mixtures: A Computational Study. N. Avula, **A. Mondal** and S. Balasubramanian; *J. Phys. Chem. Lett.*, 2018, 9, 3511 - 3516.

Universal Strategy for Ohmic Hole Injection into Organic Semiconductors with High Ionization Energies. N. B. Kotadiya, H. Lu, **A. Mondal**, Y. Le, D. Andrienko, P. W. M. Blom and G. A. H. Wetzelaer; *Nat. Mater.*, 2018, 17, 329 - 334.

2017 Recent Advances in Modeling Green Solvents. S. Das, **A. Mondal** and S. Balasubramanian; *Curr. Opin. Green Sustainable Chem.*, 2017, 5, 37 - 43.

2016 Molecular Dynamics Investigation of Efficient SO_2 Absorption by Anion-Functionalized Ionic Liquids. **A. Mondal** and S. Balasubramanian; *J. Chem. Sci.*, 2016, 129, 859 - 872.

Proton Hopping Mechanism in a Protic Organic Ionic Plastic Crystal. **A. Mondal** and S. Balasubramanian; *J. Phys. Chem. C*, 2016, 120, 22903 - 22909.

Understanding SO_2 Capture by Ionic Liquids. **A. Mondal** and S. Balasubramanian; *J. Phys. Chem. B*, 2016, 120, 4457 - 4466.

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, 2047 - 2053.

2015 A Refined All-Atom Potential for Imidazolium-Based Room Temperature Ionic Liquids: Acetate, Dicyanamide and Thiocyanate Anions. **A. Mondal** and S. Balasubramanian; *J. Phys. Chem. B*, 2015, 119, 11041 - 11051.

Vibrational Signatures of Cation-Anion Hydrogen Bonding in Ionic Liquids: A Periodic Density Functional Theory and Molecular Dynamics Study. **A. Mondal** and S. Balasubramanian; *J. Phys. Chem. B*, 2015, 119, 1994 - 2002.

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, 4625 - 4633. (*Equal Contribution)

Dissolution of Cellulose in Room Temperature Ionic Liquids: Anion Dependence. R. S. Payal, Karteek K. Bejagam, **A. Mondal** and S. Balasubramanian; *J. Phys. Chem. B*, 2015, 119, 1654 - 1659.

2014 A Molecular Dynamics Study of Collective Transport Properties of Imidazolium Based Room Temperature Ionic Liquids. **A. Mondal** and S. Balasubramanian; *J. Chem. Eng. Data*, 2014, 59, 3061 - 3068.

Intermolecular Structure in tri-*n*-butyl phosphate/*n*-octane Mixtures: A Molecular Dynamics Simulation Study. **A. Mondal** and S. Balasubramanian; *Current Science*, 2014, 106, 1235 - 1242.

Quantitative Prediction of Physical Properties of Imidazolium based Room Temperature Ionic Liquids Through Determination of Condensed Phase Site Charges: A Refined Force Field. **A. Mondal** and S. Balasubramanian; *J. Phys. Chem. B*, 2014, 118, 3409 - 3422.

Scientific programming skills

Languages	C++, Python, FORTRAN 90, Bash, LaTeX, Tcl, MATLAB
Software packages	LAMMPS, GROMACS, Gaussian 03/09/16, CPMD, CP2K, VOTCA, Turbomole, ASE, FHI-Aims, DFTB+
Others	Scipy, Numpy, Matplotlib, Git, VMD, Mercury, Molden, JMOL, Avogadro, XmGrace, Gnuplot, Inkscape, Msketch, ChemBioDraw, Origin, QtiPlot, GIMP
OS	Linux, macOS, Windows

Selected conferences, workshops, and seminars talks

02/2021	Invited Talk, School of Chemistry, Indian Institute of Science Education and Research, Thiruvananthapuram, India
02/2021	Invited Talk, Discipline of Chemistry, Indian Institute of Technology, Gandhinagar, India
12/2020	Invited Talk, Discipline of Chemistry, Indian Institute of Technology, Palakkad, India
10/2020	Invited Talk, Department of Chemistry, Indian Institute of Technology, Delhi, India
08/2020	Invited Talk, Department of Materials Science and Metallurgical Engineering, Indian Institute of Technology, Hyderabad, India
07/2020	Invited Talk, Department of Metallurgical and Materials Engineering, Indian Institute of Technology, Roorkee, India
03/2020	Invited Talk, Department of Chemistry, Indian Institute of Technology, Chennai, India
08/2019	Contributed Talk, ACS National meeting, Chemistry and Water, San Diego, US
08/2019	Poster presentation: GRC, Chemistry and Physics of Liquids, New Hampshire, US
03/2018	Contributed Talk, DPG Spring Meeting, Berlin, Germany
02/2018	Contributed Talk, InterPhase Project Meeting, Heidelberg, Germany
09/2017	Contributed Talk, Multiscale Modelling of Organic Semiconductors: from Elementary Processes to Devices, CECAM Workshop, Grenoble, France
07/2017	Poster presentation: Interface Properties in Organic Electronics: Key Challenges, Cergy Pontoise, France
07/2017	Contributed Talk, SoMaS Summer School, Mittelwihr, France
11/2015	Contributed Talk, In-House Symposium, JNCASR, Bangalore, India
01/2015	Poster presentation: School on Materials and Processes for Applications in Energy and Environment, JNCASR, India
12/2014	Poster presentation: Theoretical Chemistry Symposium, NCL Pune, India
11/2014	Poster presentation: In-House Symposium, JNCASR, Bangalore, India
08/2014	Poster presentation: MD@50, an International Conference, JNCASR, Bangalore, India
06/2014	Poster presentation: Multiscale Modelling of Ionic Liquids: from Quantum Methods to Coarse-grained Models, CECAM-HQ-EPFL, Lausanne, Switzerland

11/2013 Poster presentation: In-House Symposium, JNCASR, Bangalore, India

11/2012 Poster presentation: Theoretical Chemistry Symposium, IIT Guwahati, India

09/2012 Intel Cluster Software Tools (Workshop), JNCASR, Bangalore, India

09/2012 Exploring Materials using Spallation Neutron Source, Indo-US (Workshop), JNCASR, Bangalore, India

05/2012 Essentials for Scientific Computing (Workshop), JNCASR, Bangalore, India

Teaching

Spring 2019 **Co-Lecturer**, Chemical & Biological Engineering, Princeton University, Princeton, US
Introduction to Molecular Modeling

2015 **Teaching Assistant**, Thematic Unit of Excellence in Computational Material Science, JNCASR, India
–**Teaching discussion sections — Introduction to FORTRAN Programming**

2013-2014 **Teaching Assistant**, Thematic Unit of Excellence in Computational Material Science, JNCASR, India
–**Teaching discussion sections — Computational Laboratory — I & II**

Academic References

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Updated in: September 7, 2021