Santanu Roy

Chemical Sciences Division
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Education

University of Groningen, The Netherlands	Ph.D.	2012	Natural Science
University of Pune, India	M.Sc.	2006	Physics
University of Calcutta, India	B.Sc.	2004	Physics (HONS), Chemistry, Mathematics

Research and Professional Experience

2020 – Present Research and Development Associate, Carbon and Composite Group, Chemical Sciences Division, Oak Ridge National Laboratory, USA
2017 – 2019 Postdoctoral Research Associate, Chemical Separations Group, Chemical Sciences Division, Oak Ridge National Laboratory, USA
2014 – 2017 Postdoctoral Research Associate, Chemical Physics and Analysis Group, Physical Sciences Division, Pacific Northwest National Laboratory, USA
2012 – 2014 Postdoctoral Research Associate, Department of Chemistry, University of Wisconsin, Madison, Wisconsin, USA

Predoctoral Research Experience

2008 Guest Researcher, Mathematics Department, Free University-Berlin, Germany
2007 – 2008 Project Student, Jawaharlal Nehru Center for Advanced Scientific Research, India
2006 – 2007 Junior Research Fellow, Bioinformatics Center, University of Pune, India

Research Expertise Electronic Structure Calculations, *Ab Initio* and Force Field-Based Molecular Dynamics Simulations, Statistical Mechanics (Rare-Event Theory), Computational Nonlinear Spectroscopy (Modeling Light-Matter Interactions for Condensed Phase Systems)

Research Topics
(a) Structure, dynamics, and chemistry of molten salts, rare-earth minerals, carbon-based materials, and biological systems such as membranes, proteins, and polymers
(b) Clean water and water in energy: Investigating ion solvation, ion-pairing, and ion transport in aqueous environment

Synergistic Activities

2009-current 15 oral presentation (including 5 invited seminar) and 9 poster presentation
2012-current Served as a reviewer for Nature Communication, Journal of Chemical Physics, Journal of Physical Chemistry, Journal of Molecular Liquid, ACS Catalysis, International Journal of Molecular Sciences, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy
2019 Won poster prize in the Critical Material Institute Meeting, Colorado School of Mines, Golden, Colorado, "Development of Computational Tools for Beneficiation of Rare-Earth Elements"
2018-2019 Served as an Early Career Network (ECN) Representative of *Molten Salt in Extreme Environment*, a DOE EFRC center
2018-2019 Organized mini-symposium, webinar, and diversity and inclusion workshop
2010 Won poster prize in *Theory and Spectroscopy* in "Scientific meeting on

Chemistry Related to Physics and Material Science", Veldhoven, The Netherlands.
2009 Won poster prize in *We Heraeus Summer School* at Jacobs University, Bremen, Germany.

Selected Publications

1. **S. Roy**, D. Skoff, D. Perroni, J. Mondal, A. Yethiraj, M. K. Mahanthappa, M. T. Zanni, and J. L. Skinner, "Water dynamics in the gyroid phases of gemini surfactants", *J. Am. Chem. Soc.* 138, 2472 (**2016)**
2. J. Lessing, **S. Roy**, M. Reppert, M. Baer, D. Marx, T. L. C. Jansen, J. Knoester, and A. Tokmakoff, "Identifying Residual Structure in Intrinsically Disordered Systems: A 2DIR Spectroscopic Study of the GVGXPGVG Peptide", *J. Am. Chem. Soc.* 134, 5032 (**2012**)
3. **S. Roy**, M. S. Pshenichnikov, and T. L. C. Jansen "Analysis of 2D CS Spectra for Systems with Non-Gaussian Dynamics", *J. Phys. Chem.* B 115, 5431 (**2011**)
4. **S. Roy**, J. Lessing, G. Meisl, Z. Ganim, A. Tokmakoff, J. Knoester, and T. L. C. Jansen, "Solvent and conformation dependence of amide-I vibrations in peptides and proteins containing proline", *J. Chem. Phys.* 135, 234507 (**2011**)
5. **S. Roy**, S. M. Gruenbaum, and J. L. Skinner, "Theoretical vibrational sum-frequency generation spectroscopy of water near lipid and surfactant monolayer interfaces", *J. Chem. Phys.* 141, 18C502 (**2014**)
6. **S. Roy**, M. D Baer, C. J. Mundy, and G. K. Schenter, "Marcus Theory of Ion-Pairing", *J. Chem. Theory. Comput.* 13, 3470 (**2017**)
7. **S. Roy**, M. Galib, G. K. Schenter, and C. J. Mundy, "On the relation between Marcus theory and ultrafast spectroscopy of solvation kinetics", *Chem. Phys. Lett. (Frontiers Article)* 692, 407 (**2018**)
8. F. Wu, **S. Roy**, A. S. Ivanov, S. K. Gill, M. Topsakal, E. Dooryhee, M. Abeykoon, G. Kwon, L. C. Gallington, P. Halstenberg, B. Layne, Y. Ishii, S. M. Mahurin, S. Dai, V. S. Bryantsev, and C. J. Margulis, "Elucidating Ionic Correlations Beyond Simple Charge Alternation in Molten $MgCl_2$-KCl Mixtures", *J. Phys. Chem. Lett.* 10, 7603 (**2019**)
9. **S. Roy**, L. Wu, S. Goverapet Srinivasan, A. G. Stack, A. Navrotsky, and V. S. Bryantsev, "Hydration structure and water exchange kinetics at xenotime–water interfaces: implications for rare earth minerals separation", *Phys. Chem. Chem. Phys.* DOI: https://doi.org/10.1039/d0cp00087f (**2020**)
10. J. E. Sutton, **S. Roy**, A. U. Chowdhury, L. Wu, A. K. Wanhalam, N. De Silva, S. Jansone-Popova, B. P. Hay, M. C. Cheshire, T. L. Windus, A. G Stack, A. Navrotsky, B. A. Moyer, B. Doughty and V. S. Bryantsev, "Molecular recognition at mineral interfaces: Implications for the beneficiation of rare earth ores", *ACS. Appl. Mater. Interfaces*, DOI: https://doi.org/10.1021/acsami.9b22902 (**2020**)

Collaborators

Ganim, Z. (Yale University), Tokmakoff, A. (University of Chicago), Zanni, M. T. (University of Wisconsin-Madison), Mundy, C. J. (Pacific Northwest National Laboratory), Markland, T. E. (Stanford University), Frenkel, A., Gill, S., and Wishart, J. (Brookhaven National Laboratory), Margulis, C. J. (University of Iowa), Maginn, E. J. (University of Notre Dame)

Doctoral Advisors

Jansen, T. L. C. and Knoester, J. (University of Groningen)

Postdoctoral Supervisors

Skinner, J. L. (University of Wisconsin-Madison, now in University of Chicago)
Schenter, G. (Pacific Northwest National Laboratory)
Moyer, B. and Bryantsev, V (Oak Ridge National Laboratory)