Santanu Roy, R & D Staff

Chemical Sciences Division, ORNL
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Education

2008–2012 **PhD. in Natural Science,** Center for Theoretical Physics and Zernike Institute for Advanced Materials, **University of Groningen, The Netherlands.**

Research topic Development and application of computational 2DIR spectroscopy for resolving structure, dynamics, and folding of proteins

Advisor Prof. Thomas la Cour Jansen and Prof. Jasper Knoester

2004–2006 **M.Sc. in Physics**, **University of Pune, India.**

Thesis title Formulation of path-integral in the presence of magnetic field

Advisor Prof. Anil D. Gangal

2001–2004 **B.Sc. in Physics (HONS)**, **Chemistry, Mathematics, University of Calcutta, India.**

Research and Professional Experience

2020–Current **R & D Staff (2023), R & D Associate (2020), Chemical Sciences Division, ORNL, USA.** Investigating time-dependent molecular events through the development of rate theory, non-linear vibrational and EXAFS spectroscopic modeling, machine learning, and *ab initio*/classical molecular dynamics simulations: (1) direct air capture of CO_2, (2) structure, dynamics, and properties of molten salts for nuclear energy applications (3) reactivity and charge transport in PAN-based polymer (4) superior properties of carbon-based molecules/materials (5) separation of critical elements (6) mineral nucleation

2017–2020 **Postdoctoral Associate, Chemical Sciences Division, ORNL, USA**

Investigating interfacial structure and dynamics of rare-earth minerals and chemistry of molten salts in extreme environments by employing density functional theory, *ab initio* molecular dynamics, and rate theory.

Supervisor Dr. Vyacheslav Bryantsev and Dr. Bruce Moyer

2014–2017 **Postdoctoral Associate, Physical Sciences Division, PNNL, USA**

Development of rate theory, classical and *ab initio* molecular dynamics, ion pairing, ion and proton solvation, and solvent exchange dynamics

Supervisor Dr. Gregory K. Schenter and Christopher J. Mundy

2012–2014 **Postdoctoral Associate, University of Wisconsin-Madison, Chemistry Dept.**

Investigating the structure and dynamics of water confined by self-assembled lipids and surfactants with computational IR, SFG, 2DIR and 2DSFG spectroscopy

Supervisor Prof. James L. Skinner

Predoctoral Research Experience

2008 **Guest Researcher, Fee University, Mathematics Dept., Berlin, Germany**
Microsolvation of peptides: Density functional theory-based study

2007– 2008 **Project Student**, **JNCASR, Bangalore, India.**
Study on proton transfer in F0-F1 ATP Synthase.

2006– 2007 **Junior Research Fellow**, **Bioinformatics Centre, University of Pune, India.**
Quantum mechanical/molecular mechanical study on Metalloproteins

Achievements: Grants, Awards, News

2022 Contributed as a **PI** to a successful renewal of an **EFRC-DOE grant awarded to the *Molten Salts in Extreme Environment (MSEE)* center**

2021 Contributed as **co-PI** to a successful **BES-DOE grant on Direct Air Capture**.

2021 Contributed as **co-PI** to a successful **NEUP-DOE grant on development of machine learning potentials for molten salts**.

2018 **Elected Early Career Network Representative of MSEE** within the DOE Basic Energy Science EFRC centers and Energy Innovation Hubs. **Organized mini-symposium, webinar, and diversity and inclusion workshop**.

2019 **Poster prize** in the Critical Material Institute Meeting, Colorado School of Mines, Golden, Colorado, "Development of Computational Tools for Beneficiation of Rare-Earth Elements"

2012 **Doctoral work** was selected for publication in the news paper of University of Groningen (http://issuu.com/universiteitskrant/docs/universiteitskrant04-jg42/7#print).

2010 **Poster prize** in the Theory and Spectroscopy section in "Scientific meeting on Chemistry Related to Physics and Material Science" ,Veldhoven, The Netherlands.

2009 **Poster prize** in We Heraeus Summer School at Jacobs University, Bremen, Germany.

Mentoring Experience

2020-current **Mentoring several ORNL postdocs** in BES/EERE projects.

2011 **Teaching Assistant**, Zernike Institute for Advanced Materials, University of Groningen, The Netherlands. *Supervised a **Solid-State Physics** tutorial course for the 3rd year B. Sc. students.*

2012 Zernike Institute for Advanced Materials, University of Groningen, The Netherlands. ***Supervised an M. Sc. student** in his research on effects of ions on a peptide's conformation and its IR spectra.*

Professional Service

1. Member of the American Chemical Society
2. Reviewer of
   (a) PNAS
   (b) Nature Communication
   (c) Journal of Chemical Physics
   (d) Journal of Physical Chemistry
   (e) Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy
   (f) Journal of Molecular Liquids
   (g) ACS Catalysis
   (h) International Journal of Molecular Sciences
   (i) ACS Omega

Seminar and Poster Presentations

Oral Invited Presentations

2023 **Invited talk**, American Chemical Society National Meeting and Exposition, Virtual Meeting: Molten Salt Symposium "*Structural and dynamical heterogeneity of La^{3+} containing molten salts*"

2023 **Invited seminal** at Research Explorations for Nuclear Energy in Wyoming "**RENEW**" Academic Workshop hosted by the University of Wyoming School of Energy Resources Nuclear Energy Research Center (**NERC**), Presentation title, "*Molten salts at the atomic*

level: A computational perspective"

2023 **Invited talk at a Telluride Science Research Center workshop**: Ions in Solution: Biology, Energy, and Environment**,** "*Collective Reaction Coordinates for Rate Processes"*

2021 **Invited talk**, American Chemical Society National Meeting and Exposition, Virtual Meeting: Molten Salt Symposium "*Elucidating local structure, dynamics, and speciation in structurally disordered molten salts*"

2019 **Invited Seminar** at Oak Ridge National Laboratory, Oak Ridge, TN, USA: "*Computational spectroscopy and rate theory: A predictive framework for soft materials.*"

2017 **Invited Seminar** at Oak Ridge National Laboratory, Oak Ridge, TN, USA: "*Structure, Dynamics, and Solvent Properties of Water: A Perpective from Vibrational Spectroscopy and Reaction Rate Theory.*"

2014 **Invited seminar** at Pacific Northwest National Laboratory, Richland, Washington, USA: "*Bridging the Gap between Theory and Experiment in the World of Molecular Vibration: Case Studies on Peptides and Membrane-Confined water.*"

2008 **Invited seminar** at Zernike Institute for Advanced Materials, University of Groningen, The Netherlands and the Department of Mathematics, Free University of Berlin, Germany: *"A Trip to Bio-computing from Path Integral Formulation."*

2007 **Invited seminar** at Max Planck Institute for Nuclear Physics/International Max Planck Research School, Heidelberg, Germany: "*Formulation of Path Integral in Presence of. Magnetic Field Using Higher Order Trotter Product Formula.*"

Oral Contributed Presentations

2019 258th American Chemical Society National Meeting and Exposition, San Diego, CA, USA: "*Bridging the gap between theory and experiments on the structure, dynamics, and thermodynamics of molten salts*"

2018 256th American Chemical Society National Meeting and Exposition, Boston, MA, USA: "*Structure and exchange kinetics of water at xenotime mineral interface: An application to beneficiation of rare earth elements*"

2017 253rd American Chemical Society National Meeting and Exposition, San Francisco, CA, USA: "*Rate theory in two-dimensional reaction coordinate space: Applications to ion-pairing*"

2016 Physical Science Division seminar at Pacific Northwest National Laboratory, Richland, Washington, USA: "*Two-Dimensional Reaction Rate Theory for Ion-Pairing and Solvation.*"

2014 Postdoctoral seminar at University of Wisconsin, Dept. of Chemistry, Madison, Wisconsin, USA: *"Structure and Dynamics of Membrane-Confined Water: Vibrational Spectroscopic Study."*

2012 The physics meeting (FOM Veldhoven) in The Netherlands: *"'Resolving the Heterogeneous Configuration Space of Elastic Biopolymers."*

2010 Optical Science Meeting at Zernike Institute for Advanced Materials, University of Groningen, The Netherlands: *"Structural Classification of the Amide-I Sites of a β-Hairpin."*

2009 The winter School for Theoretical Chemistry and Spectroscopy, Han sur Lesse, Belgium: *"The Structural Heterogeneity of a β-hairpin peptide."*

Poster Presentations

2024 Gordon Research Conference, Separation, "*Reaction Mechanism and Rate Limiting Steps of CO_2 Capture by Aqueous Glycine: An Ab Initio Free Energy Study*"

2023 Gordon Research Conference, Chemistry and Physics of Liquids, "*Quantifying Speciation in Molten Salts*"

2016 251st American Chemical Society National Meeting and Exposition, San Diego, CA, USA: "*Reaction Rate Theory in Coordination Number Space: An Application to Ion Solvation.*"

2011 Time-resolved Vibrational Spectroscopy XV, Centro Stefano Franscini, Monte Verità, Ascona, Switzerland: "*Solvent and Conformation Dependence of Amide-I Vibrations in Proteins with Proline.*"

2011 CECAM conference on Spectroscopy and Quantum Phenomena in Large Molecular Aggre-gates, University of Bremen, Germany: "*Solvent and Conformation Dependence of Amide-I Vibrations in Proteins with Proline.*"

2011 The physics meeting (FOM Veldhoven) in The Netherlands: "*Analysis of 2DIR Spectra for Systems with Non-Gaussian Dynamics.*"

2011 International Workshop on Ultrafast Chemical Physics & Physical Chemistry, University of Strathclyde, Glasgow, UK: "*Resolving the Heterogeneous Configuration Space of Elastic biopolymers*"

2010 CECAM workshop on Protein Folding Dynamics: Bridging the Gap between Theory and Experiment, CECAM-HQ-EPFL, Lausanne, Switzerland: "*Structural Heterogeneity of a hairpin Revealed Isotope Label 2DIR Spectroscopy"*

2010 Theory and Spectroscopy section in "Scientific meeting on Chemistry Related to Physics and Material Science" ,Veldhoven, The Netherlands: "*Classifying the amide-I sites of a β-hairpin peptide with 2DIR spectroscopy.*"

2009 We Heraeus Summer School at Jacobs University, Bremen, Germany: "*Structural Heterogeneity of a β-hairpin Revealed by Isotope Label 2DIR Spectroscopy.*"

Computer skills

Programming language Fortran 90, C

Code Development Written codes to calculate IR, 2DIR, SFG, and 2DSFG spectra, free energy surfaces, and reaction rates for condensed phase systems from molecular dynamics trajectory.

Softwares (a) Molecular dynamics packages such as GROMACS, AMBER, CP2K
(b) Electronic structure calculation packages such as VASP, ORCA, GAUSSIAN

List of Publications

(google scholar: https://scholar.google.com/citations?user=1V6ACgUAAAAJ&hl=en)

*** indicates corresponding authorship**

39. U. I. Premadasa, D. Dong, D. Stamberga, R. Custelcean, **S. Roy**, Y. Ma, V. Bocharova, V. S. Bryantsev, and B. Doughty, "Chemical Feedback in the Self-Assembly and Function of Air-Liquid Interfaces: Insight into the Bottlenecks of CO_2 Direct Air Capture, ***ACS Appl. Mater. Interfaces*** 15, 19634(2023)
38. X. Ma, V. S. Bryantsev, **S. Roy***, "An ab initio free energy study of the reaction mechanism and rate-limiting steps of CO_2 capture by aqueous glycine", ***Cell Reports Physical Science*** 4,101642 (2023)
37. R. Chahal, **S. Roy**, M. Brehm, S. Banerjee, V. Bryantsev, S. T. Lam., "Transferable Deep Learning Potential Reveals Intermediate-Range Ordering Effects in LiF–NaF–ZrF_4 Molten Salt", ***J. Am. Chem. Soc. Au*** 2, 2693 (2022)
36. **S. Roy***, V. Bocharova, A. G. Stack, V. S. Bryantsev., "Nucleation Rate Theory for Coordination Number: Elucidating Water-Mediated Formation of a Zigzag Na_2SO_4 Morphology", ***ACS Applied Materials & Interfaces*** 14, 53213 (2022)
35. M. S. Emerson, S. Sharma, **S. Roy***, V. S. Bryantsev, A. S. Ivanov, R. Gakhar, et al., "Complete Description of the $LaCl_3$–NaCl Melt Structure and the Concept of a Spacer Salt That Causes Structural Heterogeneity", ***J. Am. Chem. Soc*** 144, 21751 (2022)

34. **S. Roy***, Y. Liu, M. Topsakal, E. Dias, R. Gakhar, W. C. Phillips, J. F. Wishart, D. Leshchev, P. Halstenberg, S. Dai, S. K Gill, A. I. Frenkel, V. S. Bryantsev, “A Holistic Approach for Elucidating Local Structure, Dynamics, and Speciation in Molten Salts with High Structural Disorder”, ***J. Am. Chem. Soc*** 143, 15298 (2021)
33. **S. Roy**, M. Brehm, S. Sharma, F. Wu, D. S. Maltsev, P. Halstenberg, L. C Gallington, S. M Mahurin, S. Dai, A. S Ivanov, C. J Margulis, V. S Bryantsev “Unraveling Local Structure of Molten Salts via X-ray Scattering, Raman Spectroscopy, and Ab Initio Molecular Dynamics”, ***J. Phys. Chem. B*** 125, 5971 (2021)
32. **S. Roy**, S. Sharma, W. V. Karunaratne, F. Wu, R. Gakhar, D. S. Maltsev, P. Halstenberg, M. Abeykoon, S. K. Gill, Y. Zhang, S. M Mahurin, S. Dai, V. S. Bryantsev, C. J. Margulis, A. S. Ivanov, “X-ray scattering reveals ion clustering of dilute chromium species in molten chloride medium” ***Chemical Science 12***, 8026 (2021)
31. H. Wang, R. S DeFever, Y. Zhang, F. Wu, **S. Roy**, V. S Bryantsev, C. J Margulis, E. J Maginn, “Comparison of fixed charge and polarizable models for predicting the structural, thermodynamic, and transport properties of molten alkali chlorides”, ***J. Chem. Phys. 153***, 214502 (2020)
30. R. C Chapleski Jr, A. U Chowdhury, A. K Wanhala, V. Bocharova, **S. Roy**, P. C Keller, D. Everly, S. Jansone-Popova, A. Kisliuk, R L Sacci, A. G Stack, C. G Anderson, B. Doughty, V. S. Bryantsev,, “A Molecular-Scale Approach to Rare-Earth Beneficiation: Thinking Small to Avoid Large Losses”, ***Iscience*** **23**, 101435 (2020)
29. C. Biaz, ……M. Cho,…... **S. Roy**, ……. M. T. Zanni,, “Vibrational spectroscopic map, vibrational spectroscopy, and intermolecular interaction”, ***Chem. Rev.*** 120, 7152 (2020)
28. **S Roy***, G. K Schenter, J. A Napoli, M. D. Baer, T. E. Markland, C. J. Mundy, “Resolving heterogeneous dynamics of excess protons in aqueous solution with rate theory”, ***J. Phys. Chem. B*** 124, 5665 (2020)
27. J. E. Sutton, **S. Roy**, A. U. Chowdhury, L. Wu, A. K. Wanhala, 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, V. S. Bryantsev, “Molecular recognition at mineral interfaces: implications for the beneficiation of rare earth ores”, ***ACS Applied Materials & Interfaces*** 12, 16327 (2020)
26. F. Wu, S. Sharma, **S. Roy**, P. Halstenberg, L. C Gallington, S. M Mahurin, S. Dai, V. S Bryantsev, A. S. Ivanov, C. J. Margulis, “Temperature Dependence of Short and Intermediate Range Order in Molten $MgCl_2$ and Its Mixture with KCl”, ***J. Phys. Chem. B*** 124, 2892 (2020)
25. S. K Gill, J. Huang, J. Mausz, R. Gakhar, **S. Roy**, F. Vila, M. Topsakal, W. C. Phillips, B. Layne, S. Mahurin, P. Halstenberg, S. Dai, J. F. Wishart, V. S. Bryantsev, A. I. Frenkel, “Connections between the Speciation and Solubility of Ni(II) and Co(II) in Molten $ZnCl_2$”, ***J. Phys. Chem. B*** 124, 1253 (2020)
24. **S Roy***, F. Wu, et al, “Structure and dynamics of the molten alkali-chloride salts from an X-ray, simulation, and rate theory perspective”, ***Phys. Chem. Chem. Phys.*** 22, 22900 (2020)
23. **S Roy***, L. Wu, S. G. Srinivasan, A. G. Stack, A. Navrotsky, V. S. Bryantsev, “Hydration structure and water exchange kinetics at xenotime–water interfaces: implications for rare earth minerals separation”, ***Phys. Chem. Chem. Phys.*** 22, 7719 (2020)
22. 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)
21. N. J. Williams, **S. Roy**, C. O. Reynolds, R. Custelcean, V. S. Bryantsev, B. A. Moyer, “Enhancing

selectivity of cation exchange with anion receptors" **Chem. Com.** 55 3590 (2019).

20. C. R. Heathman, T. S. Grimes, S. Jansone-Popova, **S. Roy**, V. S. Bryantsev, and P. Zalupski, “Influence of Pre-organized N-Donor Group on the Coordination of Trivalent Actinides and Lanthanides by Aminopolycarboxylate Complexant", ***Chemistry-A European*** 25, 2545 (2019)
19. **S. Roy*** and V. S. Bryantsev, “Finding order in the disordered hydration shell of rapidly exchanging water molecules around the heaviest alkali Cs^+ and Fr^+" ***J. Phys. Chem. B*** 122, 12067 (2018).
18. A. G. Stack, J. E. Stubbs, S. G. Srinivasan, **S. Roy**, V. S. Bryantsev, P. J. Eng, R. Custelcean, A. D. Gordon, and C. R. Hexel, “Mineral-Water Interface Structure of Xenotime (YPO4) 100", ***J. Phys. Chem. C*** DOI: 10.1021/acs.jpcc.8b04015 (2018).
17. T. S. Grimes, C. R. Heathman, S. Jansone-Popova, A. S. Ivanov, **S. Roy**, V. S. Bryantsev , and P. R. Zalupski,“Influence of a Heterocyclic Nitrogen-Donor Group on the Coordination of Trivalent Actinides and Lanthanides by Aminopolycarboxylate Complexants", ***Inorg. Chem.*** 57, 1373 (2018)
16. **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)
15. **S. Roy***, M. D Baer, C. J. Mundy, and G. K. Schenter, “Marcus Theory of Ion-Pairing”, ***J. Chem. Theory. Comput.*** 13, 3470 (2017)
14. **S. Roy***, M. D Baer, C. J. Mundy, and G. K. Schenter, "Reaction rate theory in coordination number space: An application to ion solvation", ***J. Phys. Chem. C*** 120, 7597 (2016)
13. **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).
12. **S. Roy** and L. X. Dang, "Computer simulation of methanol exchange dynamics around cations and anions", ***J. Phys. Chem. B*** 120, 1440 (2016).
11. **S. Roy** and L. X. Dang, "Water exchange dynamics around H_3O^+ and OH^- ions", ***Chem. Phys. Lett.*** 628, 30 (2015).
10. J. K. Carr, L. Wang, **S. Roy**, and J. L. Skinner, "Theoretical Sum Frequency Generation Spectroscopy of Peptides", ***J. Phys. Chem. B*** 119, 8969 (2015).
9. **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).
8. **S. Roy**, S. M. Gruenbaum, and J. L. Skinner, "Theoretical vibrational sum-frequency generation spectroscopy of water near lipid and surfactant monolayer interfaces: II. Two-dimensional spectra", ***J. Chem. Phys.*** 141, 22D505 (2014).
7. J. K. Carr, A. V. Zabuga, **S. Roy**, T. R. Rizzo, and J. L. Skinner, "Assessment of amide I spectroscopic maps for a gas-phase peptide using IR-UV double-resonance spectroscopy and density functional theory calculations", ***J. Chem. Phys.*** 140, 224111 (2014).
6. 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).
5. **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).
4. **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).
3. A. W. Smith, J. Lessing, Z. Ganim, C. S. Peng, A. Tokmakoff, **S. Roy**, T. L. C. Jansen, and Jasper Knoester, "Melting of *β*-hairpin peptide using isotope-edited 2DIR spectroscopy and simulations", ***J. Phys. Chem. B*** 114, 10913 (2010).

2. **S. Roy**, T. L. C. Jansen, and J. Knoester, "Structural classification of the amide I sites of a *β*-hairpin with isotope label 2DIR spectroscopy", ***Phys. Chem. Chem. Phys.*** 12, 9347 (2010).
1. H. Zhu, M. Blom, I. Compagnon, A. M. Rijs, **S. Roy**, G. Von Helden, and B. Schmidt, "Conformations and vibrational spectra of a model tripeptide: change of secondary structure upon micro-solvation", ***Phys. Chem. Chem. Phys.*** 12, 3415 (2010).