

## Santanu Roy, R & D Associate

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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 presence of magnetic field

**Advisor** Prof. Anil D. Gangal

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

## Research and Professional Experience

2020–Current **R & D Associate, Chemical Sciences Division, ORNL**

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<sub>2</sub>, (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**

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, Pacific Northwest National Laboratory**

Development of rate theory and classical and *ab initio* molecular dynamics of 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

## Predocutorial Research Experience

2008 **Guest Researcher, Free 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 F<sub>0</sub>-F<sub>1</sub> ATP Synthase.

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

## Achievements: Awards, Grants, 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.**
- 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 **Supervising 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 **Mentoring**, 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 Liquid
  - (g) ACS Catalysis
  - (h) International Journal of Molecular Sciences
  - (i) ACS Omega

## Seminar and Poster Presentations

### Oral Invited Presentations

- 2023 **Invited to a workshop at Telluride** "Ions in Solution: Biology, Energy, and Environment"
- 2021 **Invited contribution**, 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 Perspective 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

- 2018 256<sup>th</sup> 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 253<sup>rd</sup> 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  $\beta$ -Hairpin.*”
- 2009 The winter School for Theoretical Chemistry and Spectroscopy, Han sur Lesse, Belgium: “*The Structural Heterogeneity of a  $\beta$ -hairpin peptide.*”

### Poster Presentations

- 2016 251<sup>st</sup> 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 Aggregates, 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  $\beta$ -hairpin peptide with 2DIR spectroscopy.*"

2009 We Heraeus Summer School at Jacobs University, Bremen, Germany: "*Structural Heterogeneity of a  $\beta$ -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 of condensed phase systems from molecular dynamics trajectory.

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

## List of Publications

38. 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<sub>2</sub> Direct Air Capture.", under review.
37. R Chahal, **S Roy**, M Brehm, S Banerjee, V Bryantsev, ST Lam., "Transferable Deep Learning Potential Reveals Intermediate-Range Ordering Effects in LiF–NaF–ZrF<sub>4</sub> Molten Salt", **J. Am. Chem. Soc. Au** 2, 2693 (2022)
36. **S Roy**, V Bocharova, AG Stack, VS Bryantsev., "Nucleation Rate Theory for Coordination Number: Elucidating Water-Mediated Formation of a Zigzag Na<sub>2</sub>SO<sub>4</sub> Morphology", **ACS Applied Materials & Interfaces** 14, 53213 (2022)
35. MS Emerson, S Sharma, **S Roy**, VS Bryantsev, A S Ivanov, R Gakhar, et al., "Complete Description of the LaCl<sub>3</sub>–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, WC Phillips, J F Wishart, D. Leshchev, P. Halstenberg, S. Dai, Simerjeet 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, DS 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, WV Karunaratne, F Wu, R Gakhar, DS 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, ..... **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<sub>2</sub> 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<sub>2</sub>", *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, AG Stack, A Navrotsky, VS 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<sub>2</sub>-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<sup>+</sup> and Fr<sup>+</sup>" *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 (YPO<sub>4</sub>) 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  $\text{H}_3\text{O}^+$  and  $\text{OH}^-$  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  $\beta$ -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  $\beta$ -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).