**Sapna Sarupria**
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## EDUCATION AND PROFESSIONAL EXPERIENCE

### Education

| | | | |
|---|---|---|---|
| Ph.D. | Rensselaer Polytechnic Institute, Troy, NY | 2009 | Chemical Engineering |
| M.E. | Texas A&M University, College Station, TX | 2004 | Chemical Engineering |
| B. Tech. | Chaitanya Bharati Institute of Technology, India | 2002 | Chemical Engineering |

### Professional Experience

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| 2021 – | Associate Professor, Dept. of Chemistry, U. of Minnesota Twin Cities |
| 2021 – | Graduate Faculty, Dept. of Chemical Engineering and Materials Science, U. of Minnesota Twin Cities |
| 2022 – | Graduate Faculty, Chemical Physics Program, U. of Minnesota Twin Cities |
| 2018 – 2021 | Associate Professor, Chemical and Biomolecular Engineering, Clemson Univ. |
| 2012 – 2018 | Assistant Professor, Chemical and Biomolecular Engineering, Clemson Univ. |
| 2021 – | Adjunct Associate Prof., Chemical and Biomolecular Engineering, Clemson Univ. |
| 2019 – 2024 | Adjunct Associate Professor, Department of Physics, Michigan Technological Univ. |
| 2018 – 2021 | Deans' Faculty Fellow, College of Computing, Engineering and Applied Science, Clemson Univ. |
| 2016 – 2019 | Deans' Faculty Fellow, College of Engineering and Sciences, Clemson Univ. |
| 2009 – 2012 | Postdoctoral Researcher, Chemical Engineering, Princeton University |

### Leadership Positions/Other Professional Positions

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|---|---|
| 2024 – | Computer Aids for Chemical Engineering (CACHE) Trustee |
| 2024 – | Chair, American Chemical Society (ACS) Theory Subdivision of ACS PHYS |
| 2022 – | Co-founder, Institute of Computational Molecular Science Education (NSF-funded) |
| 2022 – 2024 | Vice Chair/Vice Chair-Elect, American Chemical Society (ACS) Theory Subdivision of ACS PHYS |
| 2020 – 2021 | Graduate Program Coordinator, Chemical and Biomolecular Engineering, Clemson Univ. |
| 2020 – 2022 | Chair, Computational Molecular Science and Engineering Forum (CoMSEF), AIChE |
| 2020 – | Editor and Member of the Editorial Board for Living Journal of Computational Molecular Science (LiveCoMS) |
| 2018 – 2020 | Vice Chair, Computational Molecular Science and Engineering Forum (CoMSEF), AIChE |

### Memberships in Professional Organizations

Member, American Institute of Chemical Engineers, AIChE (2006–2007, 2008–2009, 2010–2011, 2012–)
Member, American Chemical Society, ACS (2008–2009, 2016–)

## HIGHLIGHTS: HONORS, AWARDS AND ACHIEVEMENTS

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|---|---|
| 2024 | **AIChE CoMSEF Impact Award** |
| 2024 | Nominated and elected as a Computer Aids for Chemical Engineering (CACHE) trustee |
| 2023- | Elected Chair of American Chemical Society (ACS) Theory Subdivision of ACS PHYS |
| 2019-2020 | Received International Researcher Fellowship from RESOLV – German Cluster of Excellence on Solvation led by Ruhr University |
| 2019 | Our work on ice nucleation was selected for press coverage and highlighted by ACS. The interview is available on YouTube. https://www.acs.org/content/acs/en/pressroom/newsreleases/2019/august/chipping-away-at-how-ice-forms-could-keep-windshields-power-lines-ice-free.html https://www.youtube.com/watch?v=BtMZ5lz15VM&list=PLLG7h7fPoH8L42YLDZk1aySuLs7aUV4iQ&index=15&t=449s |
| 2019 | Invited instructor to teach Transition Interface Sampling and Forward Flux Sampling in Rare Events Summer School organized at IISc, Bangalore, India |
| 2019 | College of Computing, Engineering and Applied Science, Dean's Faculty Fellows Award (2019 – 2024), Clemson University |
| 2019 | Discussion Leader for Power Hour to enable discussion on inclusion and equity in science, 2019 Liquids Gordon Research Conference, Holderness, NH |
| 2019 | Plenary speaker, Thermodynamics 2019 Conference, 26 – 28 June 2019, Huelva, Spain |
| **2018** | **First non-white woman to be granted tenure in the Department (that is >100 years old) (Chemical and Biomolecular Engineering, Clemson Univ.)** |
| 2018 | Invited to attend the Telluride Science Research Center Donor Appreciation Dinner. Only about 10 scientists are invited to this event each year. |
| 2018 | Elected Vice Chair of the Computational Molecular Science and Engineering Forum (CoMSEF) of the AIChE |
| 2018 | Keynote speaker, 2018 Water and Aqueous Solutions Gordon Research Seminar (GRS), July 21—22, 2018, Holderness, NH |
| 2018 | Discussion leader in Power Hour to enable discussion on inclusion and equity in science, 2018 Water Gordon Research Conference, Holderness, NH |
| 2018 | Award of Excellence by Clemson University Board of Trustees |
| 2018 | Guest Editor for Journal of Theoretical and Computational Chemistry, Special Issue: Advanced Molecular Simulations: Methods and Applications (2017–2018) |
| 2017 | NSF CAREER Awardee |
| 2017 | Co-organizer of the first ever "Molecular engineering of soft matter: Spanning small molecules to macromolecules", Telluride Science Research Center (TSRC) Workshop, June 20 – 24, 2017, Telluride, CO. |
| 2017 | Founder of Computational Materials Science @ Clemson University (CMS@CU) group (2017–2020) |

2016 ACS COMP OpenEye Outstanding Junior Faculty Award in Computational Chemistry

2016 College of Engineering and Science Dean's Faculty Fellows Award (2016–2019), Clemson University

## RESEARCH: Grants and Contracts

**Current (External sources) Received at the University of Minnesota**

"Collaborative Research: DMREF: A computationally driven predictive framework for stabilizing viral therapies"
Role: UMN Principal Investigator (100%) (PIs: Caryn Heldt, Michigan Tech; Sarah Perry, UMass Amherst)
Funding agency: National Science Foundation
Amount: $567,653 Duration: 2021 – 2025

"Collaborative Research: CyberTraining: Implementation: Medium: Establishing Sustainable Ecosystem for Computational Molecular Science Training and Education"
Role: UMN Principal Investigator (PI: Neeraj Rai, Mississippi St., Co-PIs: Jindal Shah, OSU, Michael Shirts, UC Boulder; Eric Jankowski, Boise State)
Funding agency: National Science Foundation
Amount: $105,000 (UMN amount) Duration: 09/01/2021 – 08/31/2025

**Current (Internal sources)**
"Generative design of polymer interfaces"
Role: Principal Investigator (100%)
Funding Agency: MnDRIVE DSI Seed Grant
Amount: $10,000 Duration: 03/29/2024 – 03/28/2025

"Atom-level Nucleation Mechanisms from Generalized Features"
Role: Principal Investigator (Co-PI: Michael Steinbach)
Funding Agency: Data Science Initiative (DSI) College of Science and Engineering, UMN
Amount: ~$50,000 (one graduate student for one year) Duration: 08/28/2024 – 08/25/2025

**Past Awards**

**Received at the University of Minnesota UMN**

"CAREER: Large Scale Simulations Enabled Materials Engineering for Heterogeneous Ice Nucleation"
Role: Principal Investigator (100%)
Funding Agency: National Science Foundation
Amount: $503,773 (Clemson University amount) Duration: 09/01/2017 – 08/31/2022

"Predictive Hierarchical Modeling of Chemical Separations and Transformations in Functional Nanoporous Materials: Synergy of Machine Learning, Molecular Simulation, Electronic Structure Theory and Experiment"
Role: Investigator (10%) (PI: Ilja Siepmann, UMN)
Funding Agency: Department of Energy
Amount: $1,500,000 ($89,690 to Sarupria) Duration: 09/01/2021 – 08/31/2022

"Predictive computational framework to design novel peptides for hydrogel formation"
Role: Principal Investigator (100%)
Funding Agency: NSF Materials Research Science and Engineering Center Seed Grant (MRSEC Seed)

Amount: $60,000 Duration: 09/01/2021 – 08/31/2023

"Reactions in Solutions"
Role: Principal Investigator (100%)
Funding Agency: Center of Sustainable Polymers (Seed Grant)
Amount: $45,000 Duration: 09/01/2021 – 08/31/2023

"Integrated molecular simulations and machine learning tools to uncover the treasure trove of hidden structures during crystallization"
Role: Principal Investigator (Co-PI: Michael Steinbach, UMN)
Funding Agency: Data Science Initiative (DSI) College of Science and Engineering, UMN
Amount: ~$50,000 (one graduate student for one year) Duration: 08/28/2023 – 08/25/2024

**Received at Clemson University**

"Clemson University Identifying Chemical Fingerprints present in Gas Chromatography"
Role: Clemson Principal Investigator (100%)
Funding agency: Savannah National River Lab (SRNL Subcontract)
Amount: $225000 Duration: 2020 – 2022 (terminated in 2021 as Sarupria moved to UMN)

"Clemson Beckman Scholars Program"
Role: Contributor and faculty mentor (0%)
Funding agency: Arnold and Mabel Beckman Foundation
Amount: N/A Duration: 2019 – 2022

"MRI: Development of Enodia: A highly reconfigurable, HPC-backed instrument enabling multifaceted interactive visualization"
Role: Contributor (2%)
Funding agency: National Science Foundation
Amount: $1,964,707 Duration: 08/01/2018 to 07/31/2022

"Discovering colloidal structures using machine learning and advanced sampling methods in molecular simulations"
Role: Principal Investigator (100%)
Funding agency: SC EPSCOR
Amount: $50000 Duration: 09/01/2018 to 08/31/2019

"RII Track-1: Materials Assembly and Design Excellence in South Carolina (MADE in SC)"
Role: Contributor (3%) (PI: Raj Bordia, Clemson)
Funding Agency: National Science Foundation
Amount: $19,999,996 (Clemson University amount) Duration: 07/01/2017 – 06/30/2022

"Enhancing Rare Events Sampling in Molecular Simulations of Complex Systems"
Role: Principal Investigator (100%)
Funding Agency: Department of Energy
Amount: $550,000 Duration: 03/01/2016 to 08/31/2020

"Collaborative Proposal: Heterogeneous ice nucleation in clouds: Synergistic experimental and simulation approach"
Role: Principal Investigator (100%)
Collaborator: Dr. Will Cantrell, Michigan Technological University

Funding Agency: National Science Foundation
Amount: $287,789 (Clemson University amount) Duration: 03/01/2016 – 02/28/2019

"Predictive Structure-Function Relationships for Enzymes Immobilized on Complex Surfaces"
Role: Co-Investigator (50%) (Co-PI: Dr. Mark Blenner, Clemson)
Funding Agency: Defense Threat Reduction Agency
Amount: $823,899 Duration: 03/22/2016 – 03/21/2021

"DMREF: Collaborative Research: An integrated multiscale modeling and experimental approach to design fouling-resistant membranes",
Role: Principal Investigator (34%) (Co-PIs: Scott Husson, Clemson; David Ladner, Clemson)
Funding Agency: National Science Foundation
Amount: $969,089 ($323029) (Clemson University) Duration: 1/1/2016 – 12/31/2019

"Tackling the "fire-in-ice" problem in the petroleum industry: A molecular approach",
Funding Agency: American Chemical Society Petroleum Research Fund
Role: Principal Investigator (100%)
Amount: $110,000 ($110,000) Duration: 09/01/2014 - 08/31/2016

"TIGER: DMREF: Computer Aided Design of Antifouling Membranes for Water Purification"
Funding Agency: Clemson University
Tole: Principal Investigator (34%) (Co-PIs: Scott Husson, Clemson; David Ladner, Clemson)
Amount: $10,000 Duration: 06/01/2014 – 06/30/2015

## SERVICE (National Level)

1. **Chair** (2024 – Present), American Chemical Society (ACS) Theory Subdivision of ACS PHYS.
2. **Computer Aids for Chemical Engineering (CACHE) Trustee** (2025 – Present)
3. **Vice Chair/Vice Chair Elect** (2022 – 2024), American Chemical Society (ACS) Theory Subdivision of ACS PHYS.
4. **Past Chair (elected)** of the Computational Molecular Science and Engineering Forum of the AIChE (2022 – Present).
5. **Chair (elected)** of The Computational Molecular Science and Engineering Forum of the AIChE (2020 – 2022).
6. **Co-organizer, Virtual Seminar Series on Statistical Thermodynamics and Molecular Simulations (STMS).** This seminar has been well attended with over 80 to 100 participants from across the world each time. (2020 – Present)
7. **Editorial Board, Living Journal of Computational Molecular Science** (2020 – Present)
8. **Guest Editor:** Journal of Physical Chemistry B: Pablo G. Debenedetti Festschrift (2023)
9. **Co-organizer** of Workshop: Hands on With Molecular Simulation, AIChE National Meeting,
    a. Oct 28, 2018, Pittsburgh, PA
    b. Nov 10, 2019, Orlando, FL
10. **Vice Chair (elected)** of the Computational Molecular Science and Engineering Forum of the AIChE (2018 – 2020).
11. **Conference Organizer:** Telluride Science Research Center (TSRC) workshop on Soft Matter
    a. Molecular Engineering of Soft Matter: Spanning Small Molecules to Macromolecules 06/16/2019 – 06/20/2019
    b. Molecular engineering of soft matter: Spanning small molecules to macromolecules 06/20/2017 – 06/24/2017

12. **Programming Chair** for Area 1A Thermodynamics and Transport Properties AIChE National Meeting (2019)
13. **Guest Editor**: Journal of Theoretical and Computational Chemistry, Special Issue: Advanced Molecular Simulations: Method and Applications (2017 – 2018)
14. **Session Chair** to multiple sessions at AIChE (2012 – Present)
15. **Organizer:** Computational Materials Science Group@Clemson University (2016 – 2020)
16. **Discussion leader** (scientific sessions): Gordon Research Conference Water and Aqueous Solutions; Gordon Research Conference Liquids
17. **Discussion leader of Power Hour**: at Gordon Research Conference (2018, 2019)
18. **Reviewer:**
    a. **Funding agencies:** BBSRC (UK), DOE, NSF, ACS PRF
    b. **Journals:** Proteins: Structure, Function and Bioinformatics, Journal of Physical Chemistry, Applied Energy, Fluid Phase Equilibria, Environmental Science and Technology, Physical Chemistry Chemical Physics, Energies, Scientific Reports, Langmuir, Journal of Chemical Physics, Proceedings of National Academy of Sciences, ACS Sustainable Chemistry & Engineering, Soft Matter, ACS Nano, RSc Chemical Science, Nature Nanotechnology, Philosophical Transactions A. etc
    c. **Others:** American Chemical Society Chemical Computing Group
    d. **External thesis evaluator:** Indian Institute of Science, India; University of British Columbia, Canada; CNRS, France; etc
    e. **Graduate/Undergraduate events:** Poster Judge for 3rd ChBE Departmental Graduate Student Symposium (2015); Poster Judge for 1st ChBE Departmental Graduate Student Symposium (2013); Poster Judge for 1st Graduate Student Symposium at Clemson University (2012)
19. **Organizer:** "2012 Water and Aqueous Solutions Graduate Research Seminar", Conference Chair (August 2012)

## PUBLICATIONS

### Preprints on ArXiv (and similar avenues)

1. S. W. Hall, P. Minh, and S. Sarupria, "LeaPP: Learning Pathways to Polymorphs through machine learning analysis of atomic trajectories" (2024) arXiv:2405.09642
2. J. W. P. Zajac, P. Muralikrishnan, I. Tohidian, X. Zeng, C. L. Heldt, S. L. Perry, S. Sarupria, "Flipping Out: Role of Arginine in Hydrophobic Polymer Collapse". (2024) arXiv:2403.11305
3. J. W. P. Zajac, P. Muralikrishnan, C. L. Heldt, S. L. Perry, S. Sarupria, "Impact of Co-Excipient Selection on Hydrophobic Polymer Folding: Insights for Optimal Formulation Design", (2024) arXiv:2407.00885

### Refereed Journal Publications

**(**http://scholar.google.com/citations?user=OY4-O2AAAAAJ&hl=en**)**

2024

1. V. Gopal, N. Singh, M. Pitz, A. Alexandar-Bryant and S. Sarupria, "Self-assembly of de novo peptides: Insights from experiments and molecular dynamics simulations", (2024) (Submitted to Bioconjugate Chemistry – special issue on Computational Methods in Drug Delivery)

2. J. W. P. Zajac, P. Muralikrishnan, C. L. Heldt, S. L. Perry, S. Sarupria, "Impact of Co-Excipient Selection on Hydrophobic Polymer Folding: Insights for Optimal Formulation Design", (2024) (Submitted to JPCB)
3. J. W. P. Zajac, P. Muralikrishnan, I. Tohidian, X. Zeng, C. L. Heldt, S. L. Perry, S. Sarupria, "Flipping Out: Role of Arginine in Hydrophobic Polymer Collapse". (2024) under review (RSc Chemical Science)
4. S. W. Hall, P. Minh, and S. Sarupria, "LeaPP: Learning Pathways to Polymorphs through machine learning analysis of atomic trajectories" (2024) under review (PNAS)

2023

5. S. Dasetty, J.W.P. Zajac, Y. Zhang, and S. Sarupria, "Exploitation of active site flexibility-low temperature activity relation for engineering broad range temperature active enzymes", Molecular Systems Design and Engineering (Emerging Investigator series) Advanced article, 2023 (**Selected for front cover**) (**Nominated for Best paper award**)
6. 40. T. Yuan, R. S. DeFever, J. Zhou, E. Cortes-Morales, and S. Sarupria, "RSeeds: Rigid seeding method for studying heterogeneous crystal nucleation". Journal of Physical Chemistry (2023)
7. 39. R. A. Garcia Carcamo, X. Zhang, A. Estejab, J. Zhou, B. J. Hare, C. Sievers, S. Sarupria, and R. B. Getman, "Differences in solvation thermodynamics of oxygenates at Pt/Al2O3 perimeter versus Pt(111) terrace sites", iScience, 26, 105980 (2023)

2022

8. S. Sarupria, S. W. Hall, and J. Rogal, "Machine learning for molecular simulations of crystal nucleation and growth", MRS Bulletin, v47 (2022)
9. S. W. Hall, G. D. Leines, S. Sarupria, and J. Rogal, "Practical guide to replica exchange transition interface sampling and forward flux sampling", J. Chemical Physics, 156, 200901 (2022); Selected as **Featured Articl**e by the editors.

2021

10. A. Clark, H. Adams, R. Hernandez, A. Krylov, A. Niklasson, S. Sarupria, Y. Wang, S. Wild, Q. Yang, "The Middle Science: Traversing scale in complex many-body systems", ACS Central Science, 7, 8, 1271–1287 (2021)
11. [&]B. C. Paruchuri, [&]V. Gopal, S. Sarupria, and J. Larsen, "Towards enzyme-responsive polymersome drug delivery", Nanomedicine, 16:30, 2679-2693 (2021) (&: equal author contribution)
12. [&]W. Wang, [&]S. Dasetty, S. Sarupria, and M. Blenner, "Rational engineering of low temperature activity in thermoalkalophilic Geobacillus thermocatenulatus lipase", Biochemical Engineering Journal, 174:10809 (2021) (&: equal author contribution)
13. S. Dasetty, and S. Sarupria, "Advancing rational control of peptide-surface complexes", J. Phys. Chem. B, 125: 2644–2657 (2021)

2020

14. [&]N. N. Lata, [&]J. Zhou, P. Hamilton, M. Larsen, S. Sarupria, and W. Cantrell, "Multivalent Surface Cations Enhance Heterogeneous Freezing of Water on Mica", J. Phys. Chem. Lett., 11, 8682–8689 (2020) (&: equal author contribution)

2019

15. R. S. DeFever, C. Targonski, S. W. Hall, M. C. Smith, and S. Sarupria. "A generalized deep learning approach for local structure identification in molecular simulations", RSc Chemical Science, 10, 7503-7515 (DOI: 10.1039/c9sc02097g) (2019) **Selected as HOT article and selected for cover art.**
16. R. S. DeFever, W. Hanger, J. Kilgannon, A. Apon, S. Sarupria and L. Ngo, "Building A Scalable Forward Flux Sampling Framework using Big Data and HPC", Practice and Experience in Advanced Research Computing (PEARC19) (2019) (accepted & presented)

17. S. Dasetty, P. Meza-Morales, R. B. Getman, S. Sarupria, "Simulations of interfacial processes: Recent advances in force field development", Current Opinion in Chemical Engineering, 23, 138-145 (2019)
18. X. Zhang, R. S. DeFever, S. Sarupria, S. and R. B. Getman, "Free energies of catalytic species adsorbed to Pt(111) surfaces under liquid solvent calculated using classical and quantum approaches", J. Chemical Information and Modeling, 595, 2190-2198 (2019)
19. C. J. Bodenschatz, X. Zhang, T. Xie, J. Arvay, S. Sarupria, and R. B. Getman "Multiscale Sampling of a Heterogeneous Water/Metal Catalyst Interface using Density Functional Theory and Force-Field Molecular Dynamics", J. Vis. Exp. (146), e59284, doi:10.3791/59284 (2019).
20. S. Dasetty, J. K. Barrows and S. Sarupria, "Adsorption of Amino Acids on Graphene: Assessment of Current Force Fields", Soft Matter, 15, 2359-2372; accessible on ChemArxiv (2019) https://doi.org/10.26434/chemrxiv.7640489.v2
21. R. S. DeFever, and S. Sarupria, "Contour forward flux sampling: Sampling rare events along multiple collective variables", J. Chem. Phys. 150, 024103 (2019)

2018

22. B. Glatz and S. Sarupria, "Heterogeneous ice nucleation: Interplay of surface properties and their impact on water orientations", Invited submission to the special issue of Langmuir, Early Career Authors in Fundamental Colloid and Interface Science, Langmuir, 34(3), 1190-1198 (2018)

2017

23. R. S. DeFever, and S. Sarupria, "Nucleation Mechanism of Clathrate Hydrates of Water-Soluble Guest Molecules", J. Chem. Phys., 147, 204503 (2017)
24. S. Dasetty, M. A. Blenner and S. Sarupria, "Review: Engineering Lipases: Walking the Fine Line Between Activity and Stability", **Invited submission to Materials Research Express 'Emerging Investigators' Awards** Collection, Mater. Res. Express, 4 114008 (2017)
25. R. S. DeFever, and S. Sarupria, "Surface Chemistry Effects on Heterogeneous Clathrate Hydrate Nucleation: A Molecular Dynamics Study", Invited submission to Gas Hydrates Special Issue of the Journal of Chemical Thermodynamics, 117, 205-213 (2017)
26. X. Zhang, T. E. Sewell, B. Glatz, S. Sarupria, and R. B. Getman, "On the water structure at hydrophobic interfaces and the roles of water on transition-metal catalyzed reactions: A short review", Catalysis Today, 285, 57-64, (2017)
27. T. Xie, S. Sarupria and R. B. Getman, "A DFT and MD study of aqueous-phase dehydrogenation of glycerol on Pt(1 1 1): comparing chemical accuracy versus computational expense in different methods for calculating aqueous-phase system energies", Mol. Sim., 43, 370-378 (2017)

2016

28. B. Glatz and S. Sarupria. "The surface charge distribution affects ice nucleating efficiency of silver iodide" J. Chem. Phys. 145, 211924 (2016)

2015

29. B. Sengupta, W. Gregory, J. Zhu, S. Dasetty, J. Brown, A. Rao, J. Barrows, S. Sarupria, and R. Podila, "Influence of carbon nanomaterials defects on the formation of protein corona", RSc Advances, 5, 82395-82402 (2015)
30. R. S. DeFever, and S. Sarupria, "Association of small aromatic molecules with PAMAM dendrimers", Physical Chemistry Chemical Physics 17, 29548-29ß557 (2015)
31. C. J. Bodenschatz, S. Sarupria and R. B. Getman, "Molecular-Level Details about Liquid $H_2O$ Interactions with CO and Sugar Alcohol Adsorbates on Pt(111) Calculated Using Density Functional Theory and Molecular Dynamics", Journal of Physical Chemistry C, 119 (24), 13642–13651, (2015)
32. R. S. DeFever, N.K. Geitner, P. Bhattacharya, F. Ding, P.C. Ke, and S. Sarupria, "PAMAM dendrimers and graphene: Materials for removing aromatic contaminants from water", Environmental Science & Technology 49 (7), 4490-4497, (2015)

2014

33. A. Haji-Akbari, R. S. DeFever, S. Sarupria, and P. G. Debenedetti, "Suppression of sub-surface freezing in free-standing films of a coarse-grained model of water", Physical Chemistry Chemical Physics, 16, 25916-25927, (2014)

2013

34. O. Kaunwi, *C. Baldwin, *G. Greisheimer, S. Sarupria and A. Guiseppi-Elie, "Molecular dynamics simulations of peptide-SWCNT interactions related to enzyme conjugates for biosensors and biofuel cells", Nano LIFE, **03**, 1343007 (2013) (*High school students)
35. P. Bhattacharya, N.K. Geitner, S. Sarupria, and P.C. Ke, Exploiting the Physicochemical Properties of Dendritic Polymers for Environmental and Biological Applications, Physical Chemistry Chemical Physics 15 (2013), 4477. **Featured as Cover Art of PCCP**.

**Prior to Clemson**

36. S. Vembanur, A. J. Patel, S. Sarupria and S. Garde, "On the thermodynamics and kinetics of hydrophobic interactions at interfaces", Journal of Physical Chemistry B, **117** (35), 10261–10270 (2013)
37. S. Sarupria and P. Debenedetti, "Homogeneous nucleation of methane hydrate in microsecond molecular dynamics simulations", Journal of Physical Chemistry Letters, 3: 2942-2947 (2012)
38. S. Sarupria and P. G. Debenedetti, "Molecular dynamics study of dissociation of carbon dioxide hydrates", Journal of Physical Chemistry A, 115: 6102 (2011)
39. P. G. Debenedetti and S. Sarupria, "Hydrate molecular ballet", **Science**, 326: 1070 (2009)
40. S. Sarupria, T. Ghosh, A. E. Garcia and S. Garde, "Studying pressure denaturation of a protein by molecular dynamics simulations", Proteins: Structure, Function and Bioinformatics, 78:1641-1651 (2010)
41. S. Sarupria and S. Garde, "Quantifying water density fluctuations and compressibility of hydration shells of hydrophobic solutes and proteins", Physical Review Letters. 103:037803 (2009). Featured in Virtual Journal of Biological Physics Research (74 citations as of Sep 10, 2014).
42. C. J. Fennell, A. Bizjak, V. Vlachy, K. A. Dill, S. Sarupria, S. Rajamani, and S. Garde, "Ion pairing in molecular simulations of aqueous alkali halide solutions", Journal of Physical Chemistry B, 113: 14837 (2009)
43. M. Athawale, S. Sarupria and S. Garde, "Enthalpy-entropy contributions to salt and osmolyte effects on molecular-scale hydrophobic hydration and interactions", Journal of Physical Chemistry B, 112: 5661 (2008)
44. B. Pereira, S. Jain, S. Sarupria, L. Yang and S. Garde, "Pressure dependence of the compressibility of a micelle and a protein: insights from cavity formation analysis", Molecular Physics, 105: 189-199 (2007)

**Peer reviewed conference proceedings**

1. W. Hanger, R. S. DeFever, L. Ngo, A. Apon and S. Sarupria, "Scalable Forward Flux Sampling, ScaFFS: Software platform to study rare events in molecular simulations", Supercomputing 2015 (SC15) Workshop: Producing High Performance and Sustainable Software for Molecular Simulation
2. P. Xuan, Y. Zheng, S. Sarupria, and A. Apon, "SciFlow: A Dataflow-Driven Model Architecture for Scientific Computing using Hadoop", IEEE BigData Conference: Big Data and Science Workshop Proceedings, (2013)

**Non-peer reviewed articles**

1. J. C. Palmer, S. Sarupria and T. M. Truskett, "Tribute to Pablo G. Debenedetti", J. Phys. Chem. B, 127, 38, 8075-8078 (2023)
2. S. Sarupria, "A Broader View: Towards a culturally competent academic experience for all", CoMSEF Newsletter, November 2020 (link to PDF)

3. Sapna Sarupria, “Introduction to the special issue on advanced molecular simulations: Methods and applications”, Editorial to Special Issue “Advanced molecular simulations: Methods and application” Journal of Theoretical and Computational Chemistry, 17 (2018)

## INVITED PRESENTATIONS

2024

1. “Heterogeneous ice nucleation: What can simulations tell us?”, Telluride Science & Innovation Center (TSRC) Cryopreservation Grand Challenges: Fundamental Molecular Science to Applications, Sep 22– 27, 2024, Telluride, CO
2. “Seeing the invisible in nucleation”, A Time Warp in Digital Chemical Discoveries, Lorentz Center workshop. 2–6 Sep 2024 Lorentz Center@Snellius - Leiden, The Netherlands
3. “Learning pathways to polymorphs”, Enhanced Sampling Methods symposium, ACS National Meeting, Denver, CO, 18 –22 Aug 2024
4. “Molecular engineering of materials: Combining the power of molecular simulations and machine learning”, IPRIME Annual Meeting, UMN Twin Cities, Minneapolis, MN May 28–30, 2024
5. “Symphony of interactions: Interfacial water, ions, and phase transitions”, Chemistry of Ice Symposium, ACS National Meeting, New Orleans, 17–21 March 2024
6. “Walking the surfaces with AI-powered MD simulations”, American Physical Society (APS) March Meeting 2024, Minneapolis, MN
7. “Learning Pathways to Polymorphs”, 1st ViRAPID (Vienna Research Platform on Accelerating Photoreaction Discovery) Workshop, University of Vienna, Vienna, Austria. Feb 26–29 2024
8. “Overcoming barriers without bias: Studying nucleation of crystals in molecular simulations”, Greater Boston Area Theoretical Chemistry Seminar Series, Feb 6–8, 2024

2023

1. “A Symphony of Interactions: Interfacial Water, Ions, and Phase Transitions”, Wayne State University, Chemical Engineering Department Seminar, Dec 2023
2. “Molecular Design of Materials: From Clouds to Brain Tumors”, University of Washington Department of Chemical Engineering Fall 2023 Seminar Series on Computational Theory and Molecular Simulation, Oct 2023
3. "Mica, Water, Ice: It's complicated", INP Colloquium, Virtual, Oct 2023
4. “A Symphony of Interactions: Interfacial Water, Ions, and Phase Transitions”, GRC Chemistry and Physics of Liquids, Jul 30–Aug 4, 2023, Holderness, NH
5. “A Symphony of Interactions: Interfacial Water, Ions, and Phase Transitions”, Liquids, Glasses and Other Adventures in Thermodynamics and Statistical Mechanics, Jun 15–17, 2023, Princeton University, Princeton, NJ: Symposium celebrating Dr. Pablo Debendetti’s 70th Birthday!
6. “Finding hidden dimensions in structural transitions”, NSF MolSSI Workshop: Machine learning and Chemistry: Are we there yet?, May 31–Jun 2, 2023, University of Maryland, College Park MD
7. “In Silico Engineering of Enzymes and Peptides”, University of Central Arkansas, April 7th, 2023
8. “Path sampling of rare events: applications to nucleation”, Rare Events: Analysis, Numerics, and Applications, Feb 27–Mar 3, 2023 Brin Mathematics Research Center, University of Maryland College Park, MD
9. Telluride Research Science Center Workshop: “Water Structure, Dynamics, and Thermodynamics in Biology” June 25–29, 2023 (invitation declined)
10. Telluride Research Science Center Workshop: Gas Hydrates June 6–9, 2023 (invitation declined)

2022

1. "In silico nanoscopy to probe biomolecular systems – Enzyme engineering to designing bio-nano systems", Center for Biological Physics, Arizona State University, Oct 19, 2022
2. "Understanding phase transitions in silico: ice nucleation to peptide assembly", Department of Chemistry (Theoretical Chemistry Group), Ecole Normale Superieure, Oct 7th, 2022
3. "In Silico Engineering of Enzymes and Peptides", CECAM Immobilizing peptides and proteins: Interplay between theoretical and experimental approaches, CECAM-FR-MOSER, Institut de Biologie Physico-Chimique, Paris, Oct 4–7, 2022
4. "Saffire to polymerizeIt: Our lab's journey in software development", Open-source software in Chemistry session, ACS National Meeting, August 23–25, 2022
5. "Pushing the Frontiers of Simulations to Study Crystallization in Complex Systems", Foundations of Molecular Modeling and Simulation July 17–21, 2022, Devlan, WI
6. "Towards machine learning enabled studies of heterogeneous nucleation", Machine learning augmented sampling for the molecular sciences, CECAM Lausanne, May 11–13, 2022
7. "Navigating complex energy landscapes: Can ML help us climb mountains?", The Mathematics of Soft Matter: Structure and Dynamics, Feb 28–Mar 4, 2022
8. "The many faces of heterogenous ice nucleation: A complicated water-surface relationship", Department of Chemistry, Stanford University, Stanford CA, Feb 22, 2022
9. "Decoding nature on a computer: From clouds to vaccines", Department of Chemistry, Macalester College, St Paul, MN. Feb 16, 2022

2021

1. "Navigating the paths towards nucleation in complex systems", Recent Advances in Modeling Rare Events (RARE): Methods and Applications Symposium, Dec 9-12, 2020, Coorg, India. (postponed to 2021 due to COVID, held virtually Dec 14–18, 2021)
2. "Leveraging Advanced Simulations and Machine Learning to Overcome Free Energy Barriers in Molecular Systems (Keynote)", Cyberloop Workshop on Nano/Bio-Materials Modeling and Validation Nov. 18–19, 2021
3. "Molecular Engineering of Ice Responsive Materials: Decoding Heterogeneous Ice Nucleation", PICS Colloquium, University of Pennsylvania, April 2, 2021
4. "Phase Transitions, Molecular Simulations and Machine Learning", APS Meeting, March 15–19, 2021
5. "Path sampling methods for studying rare events including nucleation and crystallization", CECAM: Simulation of open systems in Chemistry, Pharma, Food Science and Immuno-diagnostics, Feb 25, 2021–Mar 25, 2021
6. "Molecular Engineering of Ice Responsive Materials: Decoding Heterogeneous Ice Nucleation", Department Seminar, Dept. of Chemical Engineering, The Ohio State University, Feb 18, 2021

2020

1. "Molecular Ballet of Water on Surfaces: Implications in Heterogeneous Ice Nucleation", Department Seminar, McKetta Department of Chemical Engineering, The University of Texas at Austin, Oct 20, 2020
2. WELCOME – Women ExceLling in COmputational Molecular Engineering seminar series, October 14, 2020.
3. "Nano-diving into the clouds: Uncovering molecular mechanisms of heterogeneous ice nucleation", Department seminar, Chemistry, University of Minnesota, Oct 5, 2020 (Virtual)
4. "Can surface charges promote ice nucleation?", Pitzer Center Theoretical Chemistry seminar, University of California Berkeley, August 4, 2020

5. "Probing protein-surface interactions using molecular dynamics", Dynamics in correlated systems: Chemical and Biological (DCSCB) 16-19 September 2020, Indian Institute of Technology, Bombay, India (postponed to 2021 due to COVID)
6. "Forward Flux methods: the good, the bad, the ugly", MolSSI School on Open Source Software for Rare-Event Sampling Strategies, June 8-9, 2020, University of Pittsburgh, Pittsburgh, PA (postponed to 2021 due to COVID)
7. "Heterogeneous ice nucleation: Prediction of nucleators", WaterX workshop, May 31-June 5, 2020, La Maddalena, Sardinia (Italy) (postponed to 2021 due to COVID)
8. "Water at interfaces", CECAM: Metastability and multiscale effects in interfacial phenomena, April 14-17, 2020, Lausanne, Switzerland. (postponed to 2021 due to COVID)
9. "Gas hydrate nucleation and growth", Gordon Research Conference on Natural Gas Hydrate Systems, Feb 23-28, 2020, Galveston, TX
10. "Pushing the limits of simulations of complex systems - from nucleation to biomolecules; from rare event sampling to multiscale modeling", Cluster of Excellence RESOLV Ruhr-Universität, Feb 5, 2020, Bochum, Germany

2019

1. "Building and applying *in silico* nanoscopes for gas hydrates and ice", University of Kansas, Lawrence KS, November 22, 2019 (**Invited: White Lecture**)
2. "Advanced sampling techniques and machine learning to overcome barriers in simulations of nucleation", NSF MolSSI workshop "Machine learning and chemistry: challenges on the way forward", Nov 16–18, 2019
3. "Molecular perspective of gas hydrate nucleation and growth", Colorado School of Mines, Golden CO, Nov 1, 2019
4. "Building and applying *in silico* nanoscopes for gas hydrates and ice", University of Maryland, College Park MD, Oct 23, 2019
5. "*In silico* nanoscopes for gas hydrates, ice and proteins", Rochester Institute of Technology, Rochester NY, 17 Oct 2019
6. "*In silico* nanoscopes for gas hydrates, ice and proteins", Stevens Institute of Technology, Hoboken NJ, 16 Oct 2019
7. "Understanding heterogeneous ice nucleation through synergistic simulations and experimental studies", ENVR: Water in the Solid State: Reactions & Interactions with Impurities, ACS National Meeting, San Diego CA, 25–29, Aug 2019
8. "Homogeneous and heterogeneous nucleation of gas hydrates: Interplay of water structure, dynamics, and guest solubility", GEOC: Water, Ice, & Clathrate Hydrate, ACS National Meeting, San Diego CA, 25–29, Aug 2019
9. "Understanding heterogeneous ice nucleation through water structure and dynamics", PHYS: Hydration from the Gas to the Condensed Phase, ACS National Meeting, San Diego CA, 25–29, Aug 2019
10. "Building and applying in silico nanoscopes for gas hydrates and ice nucleation", The 19th MERCURY Conference, Furman University, Greenville SC, 13–17 July 2019 (**Keynote talk**)
11. "Transition Interface Sampling and Forward Flux Sampling" – one-day workshop as part of the Rare Events Summer School, July 7-13, 2019, Indian Institute of Science, Bangalore, India **(Invited instructor)**
12. "Molecular ballet of water near interfaces: Elucidating the mechanisms of heterogeneous ice nucleation", Thermodynamics'2019, Huelva, Spain 26–28 June 2019
13. "Towards computer aided engineering of proteins and protein–surface complexes", TSRC Molecular Engineering of Soft Matter: Spanning Small Molecules to Macromolecules, Telluride, CO, June 16–20, 2019
14. "Towards computer aided engineering of proteins and protein–surface complexes", CECAM Biomolecular mechanisms at functionalized solid surfaces, Paris, France, May 14-17, 2019

15. "Freezing water and aqueous solutions: Elucidating the molecular ballet using computer simulations", Department of Chemical Engineering, University of Houston**,** March 1, 2019, Houston, TX

2018

1. "Freezing water and aqueous solutions: Elucidating the molecular ballet using computer simulations", Department of Chemical Engineering, University of Rochester**,** Dec 5, 2018, Rochester, NY
2. "Freezing water and aqueous solutions: Elucidating the molecular ballet using computer simulations", Department of Chemical and Biomolecular Engineering, Michigan Technological University**,** Nov 28, 2018, Houghton, MI
3. "Freezing water and aqueous solutions: Elucidating the molecular ballet using computer simulations", Department of Chemsitry, University of Florida**,** Feb 13, 2018, Gainseville, FL
4. "SAFFIRE: Enabling Large Scale Simulations of Rare Events", AIChE National Meeting, Oct 28– Nov 2, 2018, Pittsburgh, PA
5. "Molecular simulations of ice and hydrate nucleation", Heterogeneous Ice Nucleation: The ultimate challenge for molecular modeling, CECAM-HG-EPFL, Lausanne, Switzerland Sep 18–21, 2018
6. Water and Aqueous Solutions Gordon Research Seminar, July 21–22, 2018, Holderness, NH, US (**Keynote Speaker**)
7. "Elucidating the Nucleation Mechanism of Clathrate Hydrates of Soluble Guest Molecules", Twentieth Symposium On Thermophysical Properties, Boulder, CO, June 24–29, 2018
8. "Freezing water and aqueous solutions: Elucidating the molecular ballet using computer simulations", Ohio University**,** Feb 5, 2018, Athens, OK

2017

1. "Accessing the inaccessible: Studying the Liquid-to-Solid Transition in Molecular Simulations", AIChE Session: Forum Plenary: Computational Molecular Science and Engineering Forum, AIChE National Meeting, Oct 29–Nov 3, 2017, Minneapolis, MN
2. "Uncovering Heterogeneous Ice Nucleation Using Advanced Molecular Simulations", AIChE Session: Molecular Modeling of Industrially Relevant Interfacial Phenomena, AIChE National Meeting, Oct 29–Nov 3, 2017, Minneapolis, MN
3. "Freezing water and aqueous solutions: Elucidating the molecular ballet using computer simulations", 9$^{th}$ Sino-US Joint Conference of Chemical Engineering (SUCE2017) Beijing, China, October 14–20, 2017
4. "Elucidating the molecular ballet of gas hydrates using computer simulations", Gas Hydrates Workshop, Telluride Science Research Center, June 20–24, 2017
5. "Using molecular simulations and experiments to engineer robust enzymes", Soft matter: Workshop, Telluride Science Research Center, June 20–24, 2017, Telluride CO
6. "Freezing water and aqueous solutions: Elucidating the molecular ballet using computer simulations", Oklahoma State University**,** Mar 28, 2017, Stillwater, OK
7. "Freezing water and aqueous solutions: Elucidating the molecular ballet using computer simulations", Lehigh University**,** Mar 22, 2017, Bethlehem, PA
8. "Freezing water and aqueous solutions: Elucidating the molecular ballet using computer simulations", The University of Virginia**,** Mar 16, 2017, Charlottesville, VA
9. "Freezing water and aqueous solutions: Elucidating the molecular ballet using computer simulations", Worchester Polytechnic Institute**,** Mar 1, 2017, Worchester, MA
10. "Freezing water and aqueous solutions: Elucidating the molecular ballet using computer simulations", Chemistry Department, Virginia Commonwealth University**,** Feb 9, 2017 Richmond, VA

2016

1. "Large scale forward flux studies of ice and hydrate nucleation", Water and Aqueous Solutions Gordon Research Conference**,** July 31–Aug 5, 2016 Holderness School, Holderness NH

2015

1. "Molecular modeling of Gas Hydrates", National University of Singapore, 29 May 2015, Singapore
2. "Towards bottom-up design of materials: Molecular simulation studies of processes relevant to the environment", Tata Institute of Fundamental Research, June 2, 2015, Hyderabad, Telangana, India
3. "Simulation studies of gas hydrates", Microscopic Description of Gas Clathrate Telluride Science Research Center Workshop, July 9–13, 2015, Telluride CO

## Service (Department, College, University level)

**COLLEGE AND UNIVERSITY LEVEL**

UNIVERSITY OF MINNESOTA

- 2022 – Present: Data Science Initiative: Executive Committee
- 2021 – Present: Mental Health Advocate
- 2023 – Co-organizer, "Advancing Molecules and Materials via Data Science" Workshop, Sep 22, 2023.

CLEMSON

2019

- Selected to be the *Executive Member of the Advocate Advisory Board*. The ADVOCATES program is intended to train faculty members about gender inequity, underrepresented race and ethnic inequity and provide them with training and tools to both recognize white male privilege and how to be better allies for women and other underrepresented faculty members in their departments and colleges. (2019–2021)
- Member of search committee for Associate Dean for Excellence in Inclusion and Equity (2019–2020) for College of Computing, Engineering and Applied Science.
- *Clemson University Computational Advisory Team (CU-CAT) committee*: The committee in involved in Palmetto and High-Performance Computing related issues and is part of a communication stream that flows from faculty to Provost to CCIT to CIO. (2015 – 2021)

2018

- Member of *Faculty Senate* Ad Hoc Committee on the Status of Women (2018)
- Selected to participate in the *Clemson TIGERS ADVANCE Trailblazers Program*, a unique initiative at Clemson to prepare senior assistant professors and tenured faculty for leadership roles in academic or professional organizations while furthering institutional diversity.
- *Elected faculty senate* (alternate) member and serving on financial committee (2017, 2018)

2017 and earlier

- *Organized the CAREER writing workshop* at Clemson University in Spring 2017 with Drs. Karen High and Cindy Lee.
- Served on Associate Dean for Research and Graduate Studies in CECAS search committee (2016).
- Contributor to the EPSCoR RII-Track 1 proposal (2014, 2015, 2016)
- Served on Associate Dean of Undergraduate Studies Search Committee (Oct – Jan 2015)

DEPARTMENT LEVEL

University of Minnesota

- Co-chair, Diversity and Inclusion Department Committee (2021 – Present)
- Department Chair Search Committee (2022–2023)
- Faculty Search Committee (2023 – 2024)
- Graduate student PhD qualifier and PhD defense committees in Chemistry and Chemical Engineering & Materials Science department

Clemson University

- **Graduate Program Coordinator, Chemical and Biomolecular Engineering (2020 – 2021)**
- Graduate studies committee (2017 – 2021)
- Graduate recruitment committee (2017 – 2021)
- Undergraduate committee (2016)
- Honor's Committee Chair (2015)
- Honor's Committee (2014, 2015)
- Oral Examination Committee member
- Doctoral Committee Member of several graduate students
- Departmental Qualifier Examination Committee (2012–2015)
- Member, Faculty Search Committee (2012–2013, 2013–2014, 2016–2017)

## ADVISING AND MENTORING

**Postdoctoral Fellows Supervised**

1. Dr. Neetu Singh, Project: Peptide self-assembly (2020 – 2023)
2. Dr. Ernesto Carlos Cortes Morales, Project: Ice nucleation (2021 – 2023)

**Doctoral Students Advised (Current)**

1. Porhouy Minh "Developing rare event methods to study crystallization" (2021 – Present)
2. Naomi Trampe (coadvised with Dr. Ilja Siepmann) "Studying transport through porous media for chemical separations", (2021 – Present)
3. Praveen Muralikrishnan "Computational discovery small molecules to stabilize viral therapeutics", (2021 – Present)
4. Jonathan Zajac, "Discovering molecular strategies of stabilizing therapeutics", (2021 – Present)
5. Varun Gopal, "Understanding protein-polymer interactions for drug delivery applications" (2020 – Present)
6. Steven Hall, "Machine learning applied to rare event methods" (2018 – Present)

**Doctoral Dissertations Directed**

1. Salman Bin Kashif, "Fouling Mechanisms and Selectivity of Polyamide Membranes: Insights from Molecular Simulations" (2017 – 2024) PhD
2. Sina Chiniforoush; co-advised with Dr. Chris Cramer, "Combined Application of Density Functional Theory and Molecular Mechanics Sampling Techniques to study Chemical Systems, from Intramolecular Rearrangements to Polymerization Reactions", (2017 -- 2023) PhD
3. Jiarun Zhou, "Probing the structure of water near surfaces: From water absorption to ice nucleation", (2016 – 2023) PhD
4. Ryan DeFever, "Advancing molecular simulations of crystal nucleation: Applications to clathrate hydrates", (2014 – 2019) PhD
5. Siva Dasetty, "Towards computer aided engineering of proteins and protein–surface complexes", (2015 – 2019) PhD

6. Brittany Glatz, “Molecular simulation studies of ice nucleation”, (2012 – 2018) PhD

**Masters’ Theses Directed and Others**

1. Youchi Zhang “Computational discovery of peptide self-assembly for drug delivery applications” (2021 – 2023) Masters’
2. Jiexin Shi, “Using machine learning to identify pollutants in air” (2020 – 2021, changed groups because the group moved from Clemson to UMN & he remained in Clemson)
3. Siva Dasetty, “Understanding molecular interactions between proteins and carbon nanomaterials” Masters’ (with Thesis) (2013 – 2015)
4. Tianmu (Tim) Yuan, “Molecular Dynamics Simulations of Ice Nucleation on Soft Surfaces” (2018 – 2019)
5. Yen Yen Nguyen Edalgo, “Simulation studies of self-assembly of magnetic colloidal particles” (2018 – 2019)

## UNDERGRADUATE STUDENT ACTIVITIES

Creative Inquiry is the platform to engage undergraduates in research at Clemson University.

Creative Inquiry titled “Developing Project Based Learning Modules to Enhance Education Experiences” 2020 – 2021.

Creative Inquiry titled “Molecular Modeling of Biological and Polymer Systems” 2013-2018. I have trained over 27 undergraduate students in molecular simulations through this Creative Inquiry program, several are now in graduate schools like MIT, Rensselaer Polytechnic Institute, MUSC and Clemson University.

Creative Inquiry titled “Games for the Education in Materials Science” comprising 5 students in the first semester (Spring 2013), 10+ students in Fall 2013 and 5 students in Spring 2014

Hosted students in various REU programs: Biophysics REU (Physics), VisREU (Computer Science), School of Computing REU, COMSEF Advanced Materials REU (Materials Science)

**Undergraduate Honors Thesis (students from Clemson)**

1. Waring Hills, “Molecular Dynamics Simulations of the Anthrax Toxin”, May 2018
2. Brandon Alverson, “Molecular Dynamics Simulations for Studying Nucleation in Aqueous Solutions”, May 2017
3. Danielle Jacobs, “Role of Polymeric Materials in Solute Separations and Phase Transitions: A Molecular Dynamics Study”, May 2017
4. David Barton, “Molecular Simulations of PAMAM Dendrimers for Oil Dispersion”, May 2016
5. Luke H. Rhym “Analysis of Hydrate Growth Order Parameters and Preparation of Systems for Forward Flux Sampling”, April 2015
6. Ryan DeFever “Molecular Simulation Studies of Dendrimers and Graphene Oxide for Water Purification Applications”, August 2014
7. Dylan M. Bruckner “Molecular Dynamics Studies To Understand Early Events In Virus Capsid Formation”, April 2014

**Departmental Honor’s Students (shown with asterisk) and Undergraduate researchers (from Clemson)**

1. Aarin Henning, ChBE (May 2019—Dec 2020)
2. Kate Tolleson, ChBE (Aug 2019-Nov 2019)
3. *Garrett Buchmann, ChBE (May 2018-Nov 2018)

4. *Natalie Rodgers, ChBE (Oct 2017–Dec 2017)
5. *Waring Hills, ChBE (Jan 2017–May 2018)
6. Tara Brooks, ChBE (Oct 2017–Dec 2017)
7. Kamryn Kant, ChBE (Jan 2017–May 2018)
8. Christian Summerville, ChBE (Jan–May 2017)
9. Steven Hall, ChBE (May 2016–May 2018)
10. Dylan Weber, ChBE (May 2016–Aug 2016)
11. Judge Walter Hanger, Computer Engineering (May 2014-May 2017)
12. John Barrows, Biochemistry (Sep 2014–May 2016)
13. Tyler Slonecki, VisREU (June-July 2014)
14. *David Barton, ChBE (Sep 2014–May 2016)
15. *Brandon Alverson, ChBE (Jan 2015–May 2017)
16. *Danielle Jacobs, ChBE (Jan 2014–May 2017)
17. *Steve Cotty, ChBE (Jan 2015–Summer 2016)
18. *Luke Rhym, ChBE (May 2012–May 2015)
19. *Ryan DeFever, ChBE (Aug 2012–May 2014)
20. *Dylan Bruckner, ChBE (May 2012–May 2014)
21. Emily Voyles, ChBE (May 2013–May 2014)
22. BreAnn Janvier, ChBE (Jan 2014–May 2014)
23. Matthiew Filanova, ChBE (May 2012–May 2013)
24. Stephanie Chui, ChBE (Feb 2013–May 2014)
25. Julianne McLeod, Calhoun College Honor Student (Aug–Dec 2012)
26. Joshua John, ChBE (Sep 2012–Apr 2013)
27. Clayton Hammontree, ChBE (May–Aug, 2012)

**Visiting undergraduate scholars and summer REU students**

University of Minnesota:

1. Jack Hoppe, University of Minnesota (Summer 2024)
2. Anika Nagpal, Bowdoin College (Summer 2024, NSF CSP REU)
3. Aashish Agarwal, Indian Institute of Technology Delhi, India (December 2024, undergraduate research visit)
4. Cameron Khan, Princeton University (Summer 2022, SURF-CTC)
5. Brian Lee, St. John's University, NY (Summer 2022, NSF/Lando REU)
6. Aniruddha Seal, National Institute of Science Education and Research, Odisha, India (Summer 2022, SURF-CTC)
7. Daniel Pert, University of Michigan (Summer 2022, CSP REU)
8. Cal Mergendahl, University of Minnesota Morris (Summer 2021, SURF-CTC)
9. Sophie Holliday, University of Cambridge, Churchill College, UK (Summer 2021, SURF CTC)

Clemson:

1. Gabriel Orlando Brito, Mercer University, GA (Summer 2021, COMSET Adv Matl REU)
2. Stephanie Strain, California State Polytechnic University, CA (Summer 2021, CoMSEF Scholars)
3. Kristin Frailey, Greenville University, IL (Summer 2020, Biophysics REU)
4. Jake Ballard, Texas A&M University (Summer 2020, Biophysics REU)
5. Braden Holst, Clemson University (Summer 2020, COMSET Adv Matl REU)
6. Diego Losada Rubio, Wofford College (Summer 2019, COMSET REU)
7. Vatsa Shah, Indian Institute of Technology, Guwahati, India (2019, Visiting)
8. Eliel Akinbami, Howard University, Washington D.C., (2018, Visiting)
9. Harshit Arora, Indian Institute of Technology Chennai, India (2015, Visiting)
10. Tyler Slonecki, Wofford College, S.C. (2014, VisREU)

**High School Students**

1. Milan Darji, Minnetonka High School (2024)
2. *Gisela Griesheimer, SC Governor's School for Science & Mathematics
3. *Cassidy Baldwin, SC Governor's School for Science & Mathematics

*6-week interns in Sarupria research group as part of the SPRI program at Clemson

## TEACHING

### Courses Taught

#### University of Minnesota

Chem 4501, Introduction to Thermodynamics, Kinetics, and Statistical Mechanics (S22, S23, S24)
Chem 8561, Thermodynamics, Statistical Mechanics, and Reaction Dynamics I (F22, F23)
Data Science in Chemistry (Lab Class) – New course being designed in Spring 2024

#### Clemson University

ChE 2300, Fluid Flow and Heat Transfer, S12, S13, S14
ChE 8040, Advanced Thermodynamics, F12, F13, F14, F15, F19
ChE H3000/H8950 Department Seminar, F14, S15
ChE 3070, Unit Operations Lab I, F12 (Co-instructor), S17
ChE 3210, Thermodynamics II, S16, F16, F17, F18, F20 (online)
ChE 8450, Multiscale Modeling, S18
ChE 8450, Statistical Mechanics, S19

### Teaching Development Activities

Attended the Chemical Engineering Summer School, July 21-26, 2012, University of Maine, ME

Participated in Thermodynamics Virtual Communities of Practice Program (2013) – an activity funded by National Science Foundation.

## STUDENT HONORS AND AWARDS

2024 Jonathan Zajac received **First Place for poster** in Life Sciences and Engineering category in the 2024 Research Computing Exhibition, MSI, UMN (received $2000 travel award)

2024 Steven Hall and Porhouy Minh received **First Place for poster presentation** in 2024 Stahl Forum held by UMN and Medtronics, Minneapolis (they received $100 giftcard)

2024 Steven Hall and Porhouy Minh were the Finalist for the 2024 Research Computing Exhibition, MSI, UMN (received $1000 travel award)

2023 Steven Hall received the **Data Science Initiative ADC Graduate Fellowship** (UMN)

2023 Varun Gopal was the Finalist for the 2023 Research Computing Exhibition, MSI, UMN (received $1000 travel award)

2023 Jonathan Zajac and Praveen Muralikrishnan was the Finalist for the 2023 Research Computing Exhibition, MSI, UMN (received $1000 travel award)

2023 Varun Gopal received the NSF CSP travel award

2023 Varun Gopal and Salman Bin Kashif were selected as one of the top 45 posters to present at the 3M Poster Session

2022 Neetu Singh Yadav received the UMN Postdoc Associate Career Development Award ($500)

2022 Neetu Singh Yadav received the Postdoc Award Honorable Mention under impactful research category for 2022 UMN National Postdoc Appreciation Week Award

2022 Neetu Singh Yadav was the Finalist for the 2022 Research Computing Exhibition, MSI, UMN (received $1000 travel award)

2022 Porhouy Minh (PH) received **travel grant** from i-CoMSE to attend the 2022 i-CoMSE Summer School on MC/MD methods

2019 Steven Hall received **travel grant** from GRC & GRS Crystal Growth and Assembly to attend and present at the conference

2019 Jiarun Zhou received partial **travel grant** from GRC & GRS Crystal Growth and Assembly to attend and present at the conference. (2019)

2019 Ryan DeFever received the **Outstanding Graduate Researcher Award** at Clemson University

2019 Ryan DeFever received the **ACS Chemical Computing Group (CCG) Excellence Award**

2019 Steven Hall and Kamryn Kant were selected for NIST SURF program (2019)

2018 Eliel Akinbami, **Best poster award**, 6th Summer Undergraduate Research Symposium, Clemson

2017 **Ryan DeFever, NSF Graduate Research Fellowship Honorable Mention**

2017 Ryan DeFever, Professional Enhancement Grant from Clemson University ($750) Sep 2017

2017 Ryan DeFever, Professional Enhancement Grant from Clemson University ($550) April 2017

2017 Ryan DeFever received the Best Presentation in the Session award at AIChE 2017 for his presentation on gas hydrate nucleation

2016 Ryan DeFever, Professional Enhancement Grant from Clemson University ($750) Sep 2016

2016 Siva Dasetty, Professional Enhancement Grant from Clemson University ($750) Sep 2016

2016 Brittany Glatz, **Best poster award** at Gordon Research Seminar Water and Aqueous Solutions, Holderness School, Holderness, NH (Aug 2016)

2015 Judge (Walter) Hanger was selected to attend the XSEDE 2015 conference and received travel grant from the conference covering all costs of the travel and boarding. He presented his work on ScaFFS in this conference.

2015 David Barton, undergraduate researcher received the **NASA Undergraduate Student Research Fellowship** (stipend of $6000) from South Carolina Space Grant Consortium (May 2015)

2015 David Barton, undergraduate researcher was awarded $500 from Calhoun Honor College in Spring 2015

2014 Luke Rhym, undergraduate researcher was awarded $500 from Calhoun Honor College (Fall 2014)

2014 *Ryan DeFever, Nicholas Geitner, Priyanka Bhattacharyya, Pu-Chun Ke and Sarupria, Sapna; "Investigating Dendrimers and Graphene Oxide for Hydrocarbon Adsorption: A Molecular Dynamics Study", March 21-23, 2014 Student Southern Regional AIChE Conference; San Juan, Puerto Rico. Awarded the **second prize for best oral presentation**.

2014 Ryan DeFever and Dylan Bruckner, undergraduate researchers were awarded $750 from Calhoun Honor College in Spring 2013

## CONTRIBUTED PRESENTATIONS

(speaker/presenter is underlined)
2024

1. N. Trampe; S. Bin Kashif; I. J. Siepmann, S. Sarupria, “High Throughput Simulations of Monovalent Cation Selectivity in Zeolite Membranes” APS March Meeting, Minneapolis, March 4 – 8, 2024
2. S. Bin Kashif, V. Gopal, S. Sarupria, “Understanding molecular underpinnings of water purification membranes using molecular simulations”, APS March Meeting, Minneapolis, March 4 – 8, 2024
3. J. W. P. Zajac, P. Muralikrishnan, S. Sarupria, “Designing Protein Stabilizers: Small Molecule Effects on Protein Folding are Driven by Direct Interactions and Solvent Rearrangement”, APS March Meeting, Minneapolis, March 4 – 8, 2024
4. P. Minh, S. W. Hall, R. DeFever, S. Sarupria, “Effect of interaction potential on crystal nucleation mechanisms and kinetics for Lennard-Jones-like particles”, APS March Meeting, Minneapolis, March 4 – 8, 2024
5. P. Minh, S. W. Hall, S. Sarupria, “Crystal Nucleation Analysis from the Time Evolution of Local Particle Environments”, APS March Meeting, Minneapolis, March 4 – 8, 2024
6. V. Gopal, S. Bin Kashif, S. Sarupria, "Breaking barriers: A machine learning approach to efficiently explore the free energy surface of protein-surface systems", APS March Meeting, Minneapolis, March 4 – 8, 2024
7. P. Muralikrishnan, J. W. P. Zajac, S. Sarupria, "Enhancing Protein Stability: Tuning Hydrophobic Interactions with Additives", APS March Meeting, Minneapolis, March 4 – 8, 2024
8. J. W. P. Zajac, S. Sarupria, "Investigating the effects of arginine on hydrophobic collapse: insights towards temperature-stable vaccine design", Chemical Biology Interface Grant Meeting, Minneapolis, March 13, 2023
9. J. W. P. Zajac, P. Muralikrishnan, S. Sarupria, "Navigating Complex Design Space in Modeling Temperature-Stable Therapeutics", 2024 Research Computing Exhibition, Minneapolis, April 23, 2024
10. S. W. Hall, P. Minh, S. Sarupria, “LeaPP: Learning Pathways to Polymorphs with Time Analysis of Crystallizing Particles”, 54th Midwest Theoretical Chemistry Conference (MWTCC), Madison, WI, May 31, 2024
11. N. Trampe; S. Bin Kashif; I. J. Siepmann, S. Sarupria, “High Throughput Simulations of Monovalent Cation Selectivity in Zeolite Membranes” IPRIME Annual Meeting, Minneapolis, May 30, 2024
12. P. Minh, S. W. Hall, S. Sarupria, “LeaPP: Learning Pathways to Polymorphs with Time Analysis of Crystallizing Particles”, IPRIME Annual Meeting, Minneapolis, May 30, 2024

2023

1. V. Gopal, S. Bin Kashif, D. Pert, A. Seal, B. Lee, S. Sarupria, “Overcoming near-sightedness in protein-surface molecular simulations using ML lenses”, 3M Poster Session, Minneapolis, April 25, 2023
2. J. W. P. Zajac, P. Muralikrishnan, S. Sarupria, “Investigating the Effects of Arginine on Hydrophobic Interactions: Insights Towards Temperature-Stable Vaccine Design”, Chemical Biology Interface Training Grant Symposium, Minneapolis, May 24, 2023
3. E. Cortes-Morales, S. Sarupria, “How is ice formed? A search for physical descriptors of heterogeneous ice nucleation using MD and ML”, 3rd Annual Jeannette Brown Lectureship, Minneapolis, MN, April 27, 2023
4. J. W. P. Zajac, P. Muralikrishnan, S. Sarupria, "Investigating the Effects of Arginine on Hydrophobic Interactions: Insights Towards Temperature-Stable Vaccine Design", 2023 Research Computing Exhibition, Minneapolis, April 25, 2023
5. V. Gopal, S. Bin Kashif, D. Pert, A. Seal, B. Lee, S. Sarupria, “Overcoming near-sightedness in protein-surface molecular simulations using ML lenses”, 2023 Research Computing Exhibition, Minneapolis, April 25, 2023

6. V. Gopal, S. Bin Kashif, D. Pert, A. Seal, B. Lee, S. Sarupria, "Overcoming near-sightedness in protein-surface molecular simulations using ML lenses", NSF Center for Sustainable Polymers Annual Meeting, Minneapolis, April 20, 2023
7. S. Bin Kashif, V. Gopal, D. Pert, A. Seal, B. Lee, S. Sarupria, "Protein adsorption on surfaces: Improving phase space exploration using Machine Learning", Clemson ChBE Graduate Symposium, Clemson, April 11, 2023
8. J. W. P. Zajac, S. Sarupria, "Investigating the effects of arginine on hydrophobic collapse: insights towards temperature-stable vaccine design", Chemical Biology Interface Grant Meeting, Minneapolis, March 13, 2023
9. P. Muralikrishnan, P.; J. W. P. Zajac, X. Zeng, D. Amponsah-Berko, C. Heldt, S. Perry, S. Sarupria, "Towards machine learning-enabled discovery of thermostable vaccines", Peter O. Stahl Advanced Design Forum, Minneapolis, March 6, 2023

2021

1. S. Bin Kashif, S. Dasetty, S. Sarupria, "PolyPlex: A generalized and open-source Python software for generating all-atom cross-linked polymer structures", ACS Fall 2021, Atlanta, August 24, 2021
2. S. Bin Kashif, S. Dasetty, S. Sarupria, "Towards a generalized tool for atomistic cross-linked polymer generation", Midwest Thermodynamics and Statistical Mechanics Conference, University of Wisconsin-Madison, June 14, 2021
3. S. Bin Kashif, S. Dasetty, S. Sarupria, "PolyPlex: A generalized, extendable tool for atomistic cross-linked polymer generation", Clemson ChBE Graduate Symposium, Clemson, April 13, 2021
4. J. Zhou, N. N. Lata, P. Hamilton, M. Larsen, S. Sarupria, W. Cantrell, "Effects of Cations on Hydration and Ice Nucleation on Mica", ChBE Symposium, April 13, 2021
5. V. Gopal, S. Sarupria, "A Molecular Dynamics study into the Catalytic Mechanism of Hyaluronidase", Clemson ChBE Graduate Symposium, Clemson, April 13, 2021
6. R. S. DeFever, C. Targonski, S. W. Hall, M. C. Smith, S. Sarupria, "Rare Event Simulations of Nucleation Phenomena", Clemson ChBE Graduate Symposium, Clemson, April 13, 2021

2020

1. J. Zhou, N. N. Lata, S. Sarupria, W. Cantrell, "Effects of cations on heterogenous ice nucleation through studies of mica surfaces", 3rd AINC, Boston, January 10 – 12, 2020
2. J. Zhou, N. N. Lata, P. Hamilton, M. Larsen, S. Sarupria, and W. Cantrell, "Multivalent Cations on Mica Promote Ice Nucleation", M3DC, July 22, 2020

2019

1. R. S. DeFever, C. Targonski, S. W. Hall, M. C. Smith, S. Sarupria, "A Generalized Deep Learning Approach for Local Structure Identification in Molecular Simulations", Rare Events Summer School, July 7 – 13, 2019, Indian Institute of Science, Bangalore, India. Received the best poster award; gave an oral presentation as part of the award.
2. S. W. Hall, R. S. DeFever, S. Sarupria, "Effect of Interaction Potential on Crystal Nucleation Kinetics for Lennard-Jones-like Particles", GRC Crystal Growth and Assembly, June 23 – 28, 2019, Manchester, NH
3. J. Zhou, N. N. Lata, S. Sarupria, W. Cantrell, "Initiation site of heterogeneous ice nucleation can be a sign of surface nucleating propensity", GRC Crystal Growth and Assembly, June 23 – 28, 2019, Manchester, NH
4. T. Yuan, R. S. DeFever, S. Sarupria, "RSeeds: Rigid seeding method for studying heterogeneous crystal nucleation", GRC Crystal Growth and Assembly, June 23 – 28, 2019, Manchester, NH
5. R. S. DeFever, C. Targonski, S. W. Hall, M. C. Smith, S. Sarupria, "A Generalized Deep Learning Approach for Local Structure Identification in Molecular Simulations", Workshop: Foundational & Applied Data Science for Molecular and Material Science & Engineering, May 22 – 24, 2019, Lehigh University, PA.

6. J. Zhou, N. N. Lata, S. Sarupria, W. Cantrell, "Water Structure and Correlation to Heterogeneous Ice Nucleation on Mineral Surfaces", 2019 SC EPSCoR/IDeA State Conference, April 12th, 2019, Greenville, SC
7. S. W. Hall, R. S. DeFever, S. Sarupria, "Effect of interaction potential on crystal nucleation kinetics of Lennard-Jones like particles", 2019 SC EPSCoR/IDeA State Conference April 12th, 2019, Greenville, SC.

2018

4. J. Zhou, N. N. Lata, B. Glatz, S. Sarupria, W. Cantrell, "Water Structure on Mica Surfaces: Synergistic Insights from Experiments and Molecular Simulations", AIChE National Meeting, Oct 28 – Nov 2, 2018, Pittsburgh, PA
5. D. Sarupria, "Uncovering Heterogeneous Ice Nucleation using Advanced Molecular Simulations", Twentieth Symposium On Thermophysical Properties, Boulder, CO, June 24 – 29, 2018
6. S. Sarupria, "Bridging experiments and molecular simulations to elucidate heterogeneous ice nucleation", Session: Atmospheric Surface Science, EGU General Assembly, Vienna, 8 – 13 April, 2018
7. J. Zhou, N. N. Lata, S. Sarupria, W. Cantrell, "Heterogeneous Ice Nucleation on Mineral Surfaces: Study of Surface Effects", 2018 SC EPSCoR/IDeA State Conference, April 7th, 2018, Columbia, SC
8. S. W. Hall, R. S. DeFever, S. Sarupria, "Effect of interaction potential on crystal nucleation kinetics of Lennard-Jones like particles", 2018 SC EPSCoR/IDeA State Conference April 7th, 2018, Columbia, SC
9. W. Hills, K. Kant, S. Sarupria, Molecular Dynamics of the Anthrax Pore-forming Toxin, Clemson University Creative Inquiry Poster Symposium, April 2nd, 2018

2017

10. B. Glatz, J. Zhou, S. Sarupria, "Using Simulations and Experiments to Characterize Water Structure Near Mica Surfaces for Heterogeneous Ice Nucleation", AIChE National Meeting, Oct 29 – Nov 3, 2017, Minneapolis, MN
11. S. Dasetty, M. Hilbert, M. Blenner, S. Sarupria, "Impact of Linker Attachment Site on Structure and Dynamics of Enzymes", AIChE National Meeting, Oct 29 – Nov 3, 2017, Minneapolis, MN
12. R. S. DeFever, S. Sarupria, "Nucleation Mechanism of Clathrate Hydrates of Soluble Guest Molecules", AIChE National Meeting, Oct 29 – Nov 3, 2017, Minneapolis, MN
13. A. Malakian, S. Weinman, S. Sarupria, S. M. Husson, Colloidal Foulant Behavior on Membrane Surfaces with Controlled Chemistry and Ordered Roughness, AIChE National Meeting, Oct 29 – Nov 3, 2017, Minneapolis, MN
14. A. Malakian, S. Sarupria, D. Ladner, S. M. Husson, "Influence of patterning and chemistry on membrane fouling by colloidal nanoparticles", 2017 International Congress on Membranes and Membrane Processes, July 29 – August 4, 2017, San Francisco, CA
15. A. Malakian, S. Sarupria, D. Ladner, S. M. Husson, "Understanding the Roles that Patterning and Chemistry Play on Membrane Fouling", 2017 International Congress on Membranes and Membrane Processes, July 29 – August 4, 2017, San Francisco, CA
16. R. S. DeFever and S. Sarupria, "Understanding the Role of Surface Chemistry on Heterogeneous Nucleation of Clathrate Hydrates Using Extensive Molecular Dynamics Simulations", International Conference on Gas Hydrates (ICGH9), June 25 – 30, 2017, Denver, CO
17. B. Glatz and S. Sarupria, "Heterogeneous Ice Nucleation: What About the Surface Affects Ice?", April 11, 2017, Graduate Symposium, Chemical Engineering, Clemson University, Clemson SC.
18. S. Dasetty, W. Wang, M. Blenner, S. Sarupria, "Engineering Robust Activity in Extremophilic Enzymes", April 11, 2017, Graduate Symposium, Chemical Engineering, Clemson University, Clemson SC

19. B. Glatz, S. Sarupria, “Bridging experiments and molecular simulations to elucidate heterogeneous ice nucleation”, Atmospheric Ice Nucleation Conference Focus Meeting, Jan 16 – 17, 2017, Leeds, UK
20. S. Dasetty, W. Wang, M. Blenner, S. Sarupria, “Engineering Robust Activity in Extremophilic Enzymes”, AIChE National Meeting, Oct 29 – Nov 3, 2017, Minneapolis, MN
21. R. S. DeFever, S. Sarupria, “Homogeneous and Heterogeneous Nucleation of Clathrate Hydrates of a Water-Soluble Guest Molecule”, August 7 – 8, 2017, Gordon Research Conference: Chemistry and Physics of Liquids, Holderness, NH
22. R. S. DeFever, S. Sarupria, “Probing Mechanisms of Homogeneous and Heterogeneous Nucleation of Clathrate Hydrates”, July 12, 2017, CECAM Workshop: Building links between experiments and computer simulations of crystallization, CECAM-HQ, EPFL, Lausanne, Switzerland.
23. S. Dasetty, W. Wang, M. Blenner, S. Sarupria, “Engineering Robust Activity in Extremophilic Enzymes”, February 25, 2017, Clemson Biological Sciences Annual Student Symposium, Biological Sciences, Clemson University, Clemson SC
24. S. Dasetty, W. Wang, M. Blenner, S. Sarupria, “Engineering Robust Activity in Extremophilic Enzymes”, April 29, 2017, The Future of Integrative Structural Biology, Physics, Clemson University, Clemson SC
25. R. S. DeFever, S. Sarupria, "Nucleation Mechanism of Clathrate Hydrates of a Water Soluble Guest Molecule", April 11, 2017, Graduate Symposium, Chemical Engineering, Clemson University, Clemson, SC Received the first place for the best poster award

2016

26. B. Glatz, S. Sarupria, “Impact of Surfaces Charge Distribution on the Mechanism of Heterogeneous Ice Nucleation”, AIChE Annual Meeting, Nov 13 – 16, 2016, San Francisco, CA
27. B. Glatz, S. Sarupria, “Heterogeneous Ice Nucleation Using Forward Flux Sampling”, AIChE Annual Meeting, Nov 13 – 16, 2016, San Francisco, CA
28. S. Dasetty, J. Barrows, S. Sarupria, “Binding Affinities of Amino Acids on Graphene: Assessment of Force Fields”, AIChE Annual Meeting, Nov 13 – 16, 2016, San Francisco, CA
29. S. Dasetty, W. Wang, M. Blenner, S. Sarupria, “Understanding the Structural Differences Between Psychrophilic and Thermophilic Enzymes: A Molecular Dynamics Study”, AIChE Annual Meeting, Nov 13 – 16, 2016, San Francisco, CA
30. R. S. DeFever, S. Sarupria, “Molecular Dynamics Simulations of Clathrate Hydrate Nucleation Near Model Hydrophobic and Hydrophilic Surfaces”, AIChE Annual Meeting, Nov 13 – 16, 2016, San Francisco, CA – Received the best presentation award
31. R. S. DeFever, S. Sarupria, “Molecular Dynamics Studies of Structure II Hydrate Nucleation Using Advanced Sampling Techniques”, AIChE Annual Meeting, Nov 13 – 16, 2016, San Francisco, CA
32. L. Boateng, R. Monk, P. Xie, A. Malakian, S. Weinman, D. Ladner, I. Battiato, S. M. Husson, S. Sarupria, “An Integrated Multiscale Modeling and Experimental Approach to Design Fouling-Resistant Membranes”, AIChE Annual Meeting, Nov 13 – 16, 2016, San Francisco, CA
33. S. Dasetty, W. Wang, M. Blenner, S. Sarupria, Improving the Activity of a Thermophilic Lipase By Increasing the Flexibility Proximal to the Active Site”, AIChE Annual Meeting, Nov 13 – 16, 2016, San Francisco, CA
34. S. Sarupria, “Sampling Rare Events in Aqueous Systems Using Molecular Simulations”, DOE CPIMS Annual Meeting, Nov 1 – 4, 2016, B, MD
35. A. Malakian, S. Weinman, R. Monk, L. Boateng, S. Sarupria, D. Ladner, S. Husson, “Understanding the Roles that Patterning and Chemistry Play on Membrane Fouling”, North American Membrane Society 26th Annual Meeting, May 21– 25, 2016, Bellevue, WA
36. R. S. DeFever, D. Jacobs, S. Sarupria, “Dendrimers for water purification and oil dispersion: Atomistic and coarse-grained molecular dynamics investigations of dendrimer-hydrocarbon

interactions", Mar 10 – 17, 2016, 251st American Chemical Society National Meeting, San Diego, CA

37. W. Hanger, R. S. DeFever, L. Ngo, A. Apon, S. Sarupria, "Sampling rare events in molecular simulations: Heterogeneous ice nucleation – a case study", Mar 10 – 17, 2016, 251st American Chemical Society National Meeting, San Diego, CA
38. D. Barton, R. S. DeFever, S. Sarupria, "Molecular Simulations of PAMAM Dendrimers for Oil Dispersion", AIChE Southern Regional Conference, Mar 31 – Apr 2, 2016 Tuscaloosa, AL
39. B. Glatz, S. Sarupria, Water and Aqueous Solutions Gordon Research Conference, Holderness School, Holderness NH, July 31 – Aug 5, 2016 – Brittany received the best poster award for her poster in the Gordon Research Seminar**.**
40. R. S. DeFever, S. Sarupria, "Understanding gas hydrates nucleation using molecular simulations", 14th International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD), May 22 – 26, 2016, Porto, Portugal
41. S. Sarupria, "Sampling Rare Events in Aqueous Systems Using Molecular Simulations", 15-18 May 2016, DOE CTC PI Meeting, Gaithersburg, MD
42. S. Dasetty, S. Sarupria, "What drives the adsorption of peptides on carbon nanomaterials", February 23, 2016, Graduate Symposium, Chemical Engineering, Clemson University, Clemson SC
43. S. Sarupria, S. M. Husson, D. A. Ladner, I. Battiato, "DMREF: An integrated multiscale modeling and experimental approach to design fouling-resistant membranes." Materials Genome Initiative Annual Meeting, Jan 2016, Bethesda, MD
44. W. Hanger, R. S. DeFever, L. Ngo, A. Apon, S. Sarupria, "Experiences Using XSEDE Resources for Scalable Rare Event Simulation", XSEDE Conference, St. Louis, MO, July 26 – 30, 2015 Walter Hanger was awarded a student travel grant from the conference to cover all his travel and stay expenses
45. R. S. DeFever, S. Sarupria, "sII clathrate-hydrate nucleation: The effects of hydrophobic and hydrophilic surfaces", February 23, 2016, Graduate Symposium, Chemical Engineering, Clemson University, Clemson SC – Received the second place for the best poster award

2015

46. W. Hanger, R. S. DeFever, L. Ngo, A. Apon, S. Sarupria, "Scalable Forward Flux Sampling, ScaFFS: Software platform to study rare events in molecular simulations", Supercomputing 2015 (SC15) Workshop: Producing High Performance and Sustainable Software for Molecular Simulation, Nov 20, 2015, Austin, TX
47. S. Dasetty, S. Sarupria, "Role of Protein Sequence in Driving Molecular Interactions Between Proteins and Carbon Nanomaterials: A Molecular Dynamics Study", Nov 8 – 13, 2015, AIChE Annual Meeting, Salt Lake City, UT
48. B. Glatz, S. Sarupria, "Heterogeneous Ice Nucleation and Growth: What Effects Do Surfaces Have?", Nov 8 – 13, 2015, AIChE Annual Meeting, Salt Lake City, UT
49. R. S. DeFever, D. Barton, D. Jacobs, S. Sarupria, "Dendrimers for Oil Dispersion: Atomistic and Coarse-Grained Molecular Dynamics Investigations of Dendrimer–Hydrocarbon Interactions", Nov 8 – 13, 2015, AIChE Annual Meeting, Salt Lake City, UT
50. R. S. DeFever, S. Sarupria, "Nucleation of Gas Hydrates in Interfacial Systems", Nov 8 – 13, 2015, AIChE Annual Meeting, Salt Lake City, UT
51. R. S. DeFever, D. Jacobs, S. Sarupria, "Molecular Dynamics Investigations of Dendrimer–Aromatic Hydrocarbon Interactions", Nov 8 – 13, 2015, AIChE Annual Meeting, Salt Lake City, UT
52. W. Hanger, R. S. DeFever, L. Ngo, A. Apon, S. Sarupria, "Scalable Forward Flux Sampling, ScaFFS: Enabling Large Scale Simulations of Rare Events", Nov 8 – 13, 2015, AIChE Annual Meeting, Salt Lake City, UT – Received the best presentation award**.**

53. B. Glatz, S. Sarupria, "Heterogeneous Ice Nucleation and Growth: What Effects do Surfaces Have?", Aug 2 – 7, 2015 Gordon Research Conference 2015 Liquids, Chemistry & Physics of, Holderness School, Holderness NH
54. R. S. DeFever, S. Sarupria, "Heterogeneous Gas Hydrate Nucleation: The Effects of Hydrophobic and Hydrophilic Surfaces", Aug 2 – 7, 2015, Gordon Research Conference 2015 Liquids, Chemistry & Physics of, Holderness School, Holderness NH
55. D. Jacobs, D. Barton, R. S. DeFever, S. Sarupria, "Dendrimers for Water Purification: Molecular Dynamics Studies", Clemson University Creative Inquiry Poster Symposium, April 8th, 2015
56. R. S. DeFever, S. Sarupria, "Dendrimer-Guest Interactions: Challenging Conventional Wisdom", March 4, 2015, Graduate Symposium, Chemical Engineering, Clemson University, Clemson SC

2014

57. S. Sarupria, "Hydrate nucleation near SAM surfaces", Nov 16 – 21, 2014, AIChE National Meeting, Atlanta, GA
58. R. S. DeFever, N. Geitner, P. Bhattacharya, P. C. Ke, F. Ding, S. Sarupria, "Molecular Dynamics Study of Hydrocarbon Adsorption on Dendrimers and Graphene Oxide for Water Purification", Nov 16 – 21, 2014, AIChE National Meeting, Atlanta, GA
59. B. Glatz, S. Sarupria, "Effects of Lattice Spacing on Water Films: Implications for Ice Nucleation?", Nov 16 – 21, 2014, AIChE National Meeting, Atlanta, GA
60. S. Sarupria, "Molecular Modeling & Computer Simulations in Materials Engineering", Western South Carolina Section, AIChE, 18 February 2014, Greenville, SC
61. R. S. DeFever, N. Geitner, P. Bhattacharya, P. C. Ke, S. Sarupria "Investigating Dendrimers and Graphene Oxide for Hydrocarbon Adsorption: A Molecular Dynamics Study", March 21 – 23, 2014 Student Southern Regional AIChE Conference; San Juan, Puerto Rico. Awarded the second prize for best oral presentation
62. T. Slonecki, R. S. DeFever, B. Glatz, S. Sarupria, J. Levine, "Visualization to Enhance Rare Event Simulations of Ice Nucleation", XSEDE Conference, Atlanta, GA, July 13 – 18, 2014
63. M. Filanova and S. Sarupria, "Birth of gas hydrates: Effect of surface chemistry", 2014 Water and Aqueous Solutions Gordon Research Conference, Holderness, NH, July 27 – August 1, 2014
64. M. Filanova and S. Sarupria, "Birth of gas hydrates: Effect of surface chemistry", WATER 2014 - Metastability and nucleation in water: theory, experiments, and applications, 1 – 6 Jun 2014, Les Houches, France
65. W. Hanger, R. S. DeFever, L. Ngo, A. Apon, S. Sarupria, "ScaFFS: Scalable Forward Flux Sampling", July 2014, BigData Research Experience for Undergraduates, Clemson University, Clemson, SC
66. B. Glatz, L. Rhym, S. Sarupria, "Ice Nucleation and Growth on Kaolinite Surfaces", Departmental Graduate Student Symposium (ChBE), 5 March 2014

2013

67. S. Sarupria, "Water Structure and dynamics in thin films on mineral surfaces", AIChE National Meeting, San Francisco CA, (Nov 3 – 8, 2013)
68. S. Sarupria, "A brief overview of molecular simulations", Invited talk at Summer Program for Research Interns (SPRI), 11 July 2013, Clemson University
69. S. Sarupria, "A brief overview of molecular simulations", Invited talk at Research Experience for Undergraduates Enrichment Lecture Series, 25 June 2013, School of Computing, Clemson University
70. D. Bruckner, S. Sarupria, "Molecular Dynamics Studies to Understand Early Events in Virus Capsid Formation", April 5 – 7, 2013, AIChE Southern Regional Conference, Lexington, Kentucky
71. R. S. DeFever, N. Geitner, P. Bhattacharya, S. Sarupria, P. C. Ke, "Dendrimers and Graphene Oxide: Molecular Simulation Studies", Departmental Graduate Student Symposium (ChBE), 13 Feb 2013

72. R. S. DeFever, P. Xuan, A. Apon, S. Sarupria, “Capturing ice nucleation with a SciFlow DFFS implementation”, Research Experience for Undergraduates, School of Computing, Clemson University, 26 July 2013

**Updated:** July 20, 2024