

College of Engineering, Computing and Applied Sciences

RESUME – Sapna Sarupria

Associate Professor

Department of Chemical and Biomolecular Engineering

Clemson University, Clemson, SC 29634

864-656-3258, ssarupr@g.clemson.edu

Website: <http://molecularsimulations.sites.clemson.edu/>

EDUCATION

Ph.D., Rensselaer Polytechnic Institute, 2009, Chemical Engineering

M.E., Texas A&M University, College Station, 2004, Chemical Engineering

B. Tech, Chaitanya Bharati Institute of Technology, India, 2002, Chemical Engineering

PROFESSIONAL EXPERIENCE

Clemson University, 08/2018 – , Associate Professor, Chemical and Biomolecular Engineering

Michigan Technological University, 07/2018 – Present, Adjunct Associate Professor, Department of Physics

Clemson University, 2012 – 08/2018, Assistant Professor, Chemical and Biomolecular Engineering

Princeton University, 2009 – 2012, Postdoctoral Researcher, Chemical and Biological Engineering Department

MEMBERSHIPS

Member, American Institute of Chemical Engineers, AIChE (2006-2007, 2008-2009, 2010-2011, 2012-)

Member, American Chemical Society, ACS (2008-2009, 2016-)

HONORS, AWARDS AND OTHERS

- Received International Researcher Fellowship from RESOLV – cluster of excellence on solvation led by Ruhr University.
- Plenary speaker, Thermodynamics 2019 conference, 26-28 June 2019, Huelva, Spain
- Co-Organizer “Molecular engineering of soft matter: Spanning small molecules to macromolecules”, Telluride Science Research Center (TSRC) Workshop, 06/16/2019--06/20/2019, Telluride CO.
- Discussion leader in Power Hour for 2019 Liquids Gordon Research Conference and 2018 Water Gordon Research Conference – to enable discussion on inclusion and equity in science.
- Invited to attend the Telluride Science Research Center Donor Appreciation Dinner. Only about 10 scientists are invited to this event each year. (Dec 2018)
- Elected Vice Chair of The Computational Molecular Science and Engineering Forum of the AIChE (2018--)
- Keynote speaker, 2018 Water and Aqueous Solutions Gordon Research Seminar, 07/21/2018-07/22/2018, Holderness, NH
- Award of Excellence by Clemson University Board of Trustees (2018)
- NSF CAREER Awardee (2017)
- Guest Editor for Journal of Theoretical and Computational Chemistry, Special Issue: Advanced Molecular Simulations: Methods and Applications (2017-2018)

- ACS COMP OpenEye Outstanding Junior Faculty Award in Computational Chemistry (2016)
- College of Engineering and Science Dean's Faculty Fellows Award (2016 -- 2019)
- Co-Organizer "Molecular engineering of soft matter: Spanning small molecules to macromolecules", Telluride Science Research Center (TSRC) Workshop, 06/20/2017--06/24/2017, Telluride CO.
- Co-Organizer "Molecular engineering of soft matter: Spanning small molecules to macromolecules", Telluride Science Research Center (TSRC) Workshop, 06/16/2019--06/20/2019, Telluride CO.
- Co-founder of Departmental New Faculty Mentoring System (since 2016)
- Founder of Computational Materials Science @ Clemson University (CMS@CU) group (since 2017)

STUDENT HONORS AND AWARDS

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

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

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 (2018)

Ryan DeFever, NSF Graduate Research Fellowship Honorable Mention

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

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

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

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

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

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

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 ScaffFS in this conference.

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

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

Luke Rhym, undergraduate researcher was awarded \$500 from Calhoun Honor College in Fall 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.

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

FUNDING

“Clemson Beckman Scholars Program”

Role: Contributor and faculty mentor

Funding Agency: Arnold and Mabel Beckman Foundation

Duration: 2019 -- 2022

“MRI: Development of Enodia: A highly reconfigurable, HPC-backed instrument enabling multifaceted interactive visualization”

Role: Contributor

Funding agency: National Science Foundation

“Discovering colloidal structures using machine learning and advanced sampling methods in molecular simulations”

Role: Principal Investigator

Funding agency: SC EPSCOR

“RII Track-1: Materials Assembly and Design Excellence in South Carolina (MADE in SC)”

Role: Contributor

Funding Agency: National Science Foundation

“Enhancing Rare Events Sampling in Molecular Simulations of Complex Systems”

Role: Principal Investigator (100%)

Funding Agency: Department of Energy

“CAREER: Large Scale Simulations Enabled Materials Engineering for Heterogeneous Ice Nucleation”

Role: Principal Investigator

Funding Agency: National Science Foundation

“Collaborative Proposal: Heterogeneous ice nucleation in clouds: Synergistic experimental and simulation approach”

Role: Principal Investigator

Collaborator: Dr. Will Cantrell, Michigan Technological University

Funding Agency: National Science Foundation

“Predictive Structure-Function Relationships for Enzymes Immobilized on Complex Surfaces”

Role: Co-investigator

Co-investigators: Dr. Mark Blenner (ChBE, Clemson)

Funding Agency: Defense Threat Reduction Agency

“DMREF: Collaborative Research: An integrated multiscale modeling and experimental approach to design fouling-resistant membranes”

Role: Principal Investigator

Co-investigators: Scott Husson (ChBE, Clemson), David Ladner (EE&ES, Clemson)

Funding Agency: National Science Foundation

“Tackling the “fire-in-ice” problem in the petroleum industry: A molecular approach”,
Funding Agency: American Chemical Society Petroleum Research Fund
Role: Principal Investigator

“TIGER: DMREF: Computer Aided Design of Antifouling Membranes for Water Purification”
Funding Agency: Clemson University
Role: Principal Investigator

PUBLICATIONS

[Corresponding authors are indicated by asterisk and are underlined, and student authors from my research group are bolded]

Refereed Journal Publications

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

2019

1. DeFever, R.S., Targonski, C., Hall, S. W., B., Smith, M.C., Sarupria, S. “A generalized deep learning approach for local structure identification in molecular simulations”, RSc Chemical Science (DOI: 10.1039/c9sc02097g) (2019)
2. 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), (accepted & presented)
3. Dasetty, S., 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)
4. Zhang, X., DeFever, R., Sarupria, S. and Getman, R. B., “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 (DOI: 10.1021/acs.jcim.9b00089) (2019)
5. 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).
6. **Siva Dasetty** and *Sarupria, S., “Adsorption of Amino Acids on Graphene: Assessment of Current Force Fields”, Soft Matter, 15, 2359-2372 (DOI: 10.1039/C8SM02621A); accessible on ChemArxiv (2019) <https://doi.org/10.26434/chemrxiv.7640489.v2>
7. **DeFever, Ryan S.** and *Sarupria, S., “Contour forward flux sampling: Sampling rare events along multiple collective variables”, J. Chem. Phys. 150, 024103 (2019) [<https://doi.org/10.1063/1.5063358>]

2018

8. **Sarupria, S.** “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) [DOI: <https://doi.org/10.1142/S0219633618020017>] (not peer-reviewed)
9. **Glatz, Brittany** and *Sarupria, S., “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. [DOI: 10.1021/acs.langmuir.7b02859, 2018]

2017

10. **DeFever, Ryan S.** and ***Sarupria, S.**, “Nucleation Mechanism of Clathrate Hydrates of Water-Soluble Guest Molecules”, *J. Chem. Phys.*, 147, 204503 (2017) [DOI: <https://doi.org/10.1063/1.4996132>]
11. **Siva Dasetty**, Mark A. Blenner and ***Sarupria, S.**, “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) [DOI: <https://doi.org/10.1088/2053-1591/aa9946>]
12. **DeFever, Ryan S.** and ***Sarupria, S.**, “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) [DOI: <https://doi.org/10.1016/j.jct.2017.08.021>]
13. Xiaohong Zhang, Torrie E. Sewell, **Brittany Glatz**, ***Sapna Sarupria**, and ***Rachel 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)
14. Tianjun Xie, Sapna Sarupria and Rachel 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

15. **Glatz, Brittany** and ***Sarupria, S.** “The surface charge distribution affects ice nucleating efficiency of silver iodide” *J. Chem. Phys.* 145, 211924 (2016)

2015

16. 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)
17. **Ryan S. DeFever** and **Sapna Sarupria**, “Association of small aromatic molecules with PAMAM dendrimers”, *Physical Chemistry Chemical Physics* 17, 29548-29557 (2015) [DOI: [10.1039/C5CP03717D](https://doi.org/10.1039/C5CP03717D)]
18. Cameron J. Bodenschatz, Sapna Sarupria and ***Rachel Getman**, “Molecular-Level Details about Liquid H₂O 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) [DOI: [10.1021/acs.jpcc.5b02333](https://doi.org/10.1021/acs.jpcc.5b02333)]
19. **Ryan 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) [DOI: [10.1021/es505518r](https://doi.org/10.1021/es505518r)]

2014

20. Amir Haji-Akbari, **Ryan S. Defever**, Sapna Sarupria, and ***Pablo 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

21. 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)
22. 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

23. 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) [DOI: 10.1021/jp4050513]
 24. *S. Sarupria and P. Debenedetti, “Homogeneous nucleation of methane hydrate in microsecond molecular dynamics simulations”, *Journal of Physical Chemistry Letters*, **3**: 2942-2947 (2012)
 25. S. Sarupria and *P. G. Debenedetti, “Molecular dynamics study of dissociation of carbon dioxide hydrates”, *Journal of Physical Chemistry A*, **115**: 6102 (2011)
 26. *P. G. Debenedetti and S. Sarupria, “Hydrate molecular ballet”, *Science*, **326**: 1070 (2009)
 27. 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)
 28. 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).
 29. 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)
 30. 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)
 31. 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)
- *High School Students

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)

ORAL PRESENTATIONS

(speaker is underlined)

Invited

2019

1. *Sarupria, S. “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**)
2. *Sarupria, S. “Molecular ballet of water near interfaces: Elucidating the mechanisms of heterogeneous ice nucleation”, *Thermodynamics’2019*, Huelva, Spain 26-28 June 2019 (**Invited**)
3. *Sarupria, S. and S. Dasetty, “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 (**Invited**)
4. *Sarupria, S. and S. Dasetty, “Towards computer aided engineering of proteins and protein–surface complexes”, *CECAM Biomolecular mechanisms at functionalized solid surfaces*, Paris, France, May 14-17, 2019

5. *Sarupria, S. “Freezing water and aqueous solutions: Elucidating the molecular ballet using computer simulations”, Department of Chemical Engineering, University of Houston, March 1, 2019, Houston, TX **(Invited)**

2018

6. *Sarupria, S. “Freezing water and aqueous solutions: Elucidating the molecular ballet using computer simulations”, Department of Chemical Engineering, University of Rochester, Dec 5, 2018, Rochester, NY **(Invited)**
7. *Sarupria, S. “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 **(Invited)**
8. *Sarupria, S. “Freezing water and aqueous solutions: Elucidating the molecular ballet using computer simulations”, Department of Chemistry, University of Florida, Feb 13, 2018, Gainesville, FL **(Invited)**
9. *Sarupria, S., R. DeFever, W. Hanger, Linh Ngo and A. Apon, “SAFFIRE: Enabling Large Scale Simulations of Rare Events”, AIChE National Meeting, Oct 28- Nov 2, 2018, Pittsburgh, PA **(Invited)**
10. *Sarupria, S. “Molecular simulations of ice and hydrate nucleation”, Heterogeneous Ice Nucleation: The ultimate challenge for molecular modeling, CECAM-HG-EPFL, Lausanne, Switzerland 18-21 September, 2018 **(Invited)**
11. *Sarupria, S. **Keynote Speaker** for Water and Aqueous Solutions Gordon Research Seminar, 2018 **(Invited)**
12. Ryan DeFever and Sapna Sarupria*, “Elucidating the Nucleation Mechanism of Clathrate Hydrates of Soluble Guest Molecules”, Twentieth Symposium On Thermophysical Properties, Boulder, CO, June 24–29, 2018 **(Invited)**
13. *Sarupria, S. “Freezing water and aqueous solutions: Elucidating the molecular ballet using computer simulations”, Ohio University, Feb 5, 2018, Athens, OK **(Invited)**

2017

14. *Sarupria, S. “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 **(Invited)**
15. *Sarupria, S. “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 **(Invited)**
16. *Sarupria, S., Ryan S. DeFever, and Brittany Glatz, “Freezing water and aqueous solutions: Elucidating the molecular ballet using computer simulations”, 9th Sino-US Joint Conference of Chemical Engineering (SUCE2017) Beijing, China, October 14-20, 2017 **(Invited)**
17. *Sarupria, S. “Elucidating the molecular ballet of gas hydrates using computer simulations”, Gas Hydrates Workshop, Telluride Science Research Center, June 20-24, 2017 **(Invited)**
18. *Sarupria, S. “Using molecular simulations and experiments to engineer robust enzymes”, Soft matter: Workshop, Telluride Science Research Center, June 20-24, 2017, Telluride CO **(Invited)**
19. *Sarupria, S. “Freezing water and aqueous solutions: Elucidating the molecular ballet using computer simulations”, Oklahoma State University, Mar 28, 2017, Stillwater, OK **(Invited)**
20. *Sarupria, S. “Freezing water and aqueous solutions: Elucidating the molecular ballet using computer simulations”, Lehigh University, Mar 22, 2017, Bethlehem, PA **(Invited)**
21. *Sarupria, S. “Freezing water and aqueous solutions: Elucidating the molecular ballet using computer simulations”, The University of Virginia, Mar 16, 2017, Charlottesville, VA **(Invited)**
22. *Sarupria, S. “Freezing water and aqueous solutions: Elucidating the molecular ballet using computer simulations”, Worcester Polytechnic Institute, Mar 1, 2017, Worcester, MA **(Invited)**

23. *Sarupria, S. “Freezing water and aqueous solutions: Elucidating the molecular ballet using computer simulations”, Chemistry Department, Virginia Commonwealth University, Feb 9, 2017 Richmond, VA **(Invited)**

2016

24. *Sarupria, S. “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 **(Invited)**

2015

25. *Sapna Sarupria “Molecular modeling of Gas Hydrates”, National University of Singapore, 29 May 2015, Singapore **(Invited)**
26. *Sapna Sarupria, “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 **(Invited)**
27. *Sapna Sarupria, “Simulation studies of gas hydrates”, Microscopic Description of Gas Clathrate Telluride Science Research Center Workshop, Telluride CO (July 9-13, 2012) **(Invited)**
28. *Sarupria, S., Jiarun Zhou, Nurun Nahar Lata, Brittany Glatz and Will Cantrell, “Water Structure on Mica Surfaces: Synergistic Insights from Experiments and Molecular Simulations”, AIChE National Meeting, Oct 28-Nov 2, 2018, Pittsburgh, PA
29. *Sarupria, S., “Uncovering Heterogeneous Ice Nucleation using Advanced Molecular Simulations”, Twentieth Symposium On Thermophysical Properties, Boulder, CO, June 24–29, 2018
30. *Sarupria, S. “Bridging experiments and molecular simulations to elucidate heterogeneous ice nucleation”, Session: Atmospheric Surface Science, EGU General Assembly, Vienna, 8-13 April, 2018
31. Brittany G., Zhou, J. and *Sarupria S., “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
32. *Siva Dasetty, Maxwell Hilbert, Mark Blenner and Sapna Sarupria, “Impact of Linker Attachment Site on Structure and Dynamics of Enzymes”, AIChE National Meeting, Oct 29–Nov 3, 2017, Minneapolis, MN
33. *Ryan DeFever and Sapna Sarupria, “Nucleation Mechanism of Clathrate Hydrates of Soluble Guest Molecules”, AIChE National Meeting, Oct 29–Nov 3, 2017, Minneapolis, MN
34. *Anna Malakian, Steven Weinman, Sapna Sarupria, and Scott M. Husson, Colloidal Fouling Behavior on Membrane Surfaces with Controlled Chemistry and Ordered Roughness, AIChE National Meeting, Oct 29–Nov 3, 2017, Minneapolis, MN
35. Malakian, A., Sarupria, S., Ladner, D., and Husson, S. M., “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
36. Malakian, A., Sarupria, S., Ladner, D., and Husson, S. “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
37. Ryan DeFever and *Sapna 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
38. *Brittany Glatz and Sapna Sarupria, "Heterogeneous Ice Nucleation: What About the Surface Affects Ice?", April 11, 2017, Graduate Symposium, Chemical Engineering, Clemson University, Clemson SC.

39. *Siva Dasetty, Weigao Wang, Mark Blenner, Sapna Sarupria, “Engineering Robust Activity in Extremophilic Enzymes”, April 11, 2017, Graduate Symposium, Chemical Engineering, Clemson University, Clemson SC
40. Glatz, B and *Sarupria, S, “Bridging experiments and molecular simulations to elucidate heterogeneous ice nucleation”, Atmospheric Ice Nucleation Conference Focus Meeting, Jan 16-17, 2017, Leeds, UK
41. *Glatz, B and Sarupria, S, “Impact of Surfaces Charge Distribution on the Mechanism of Heterogeneous Ice Nucleation”, AIChE Annual Meeting, Nov 13-16, 2016, San Francisco, CA
42. *Glatz, B and Sarupria, S, “Heterogeneous Ice Nucleation Using Forward Flux Sampling”, AIChE Annual Meeting, Nov 13-16, 2016, San Francisco, CA
43. *Dasetty, S., Barrows, J. and Sarupria, S. “Binding Affinities of Amino Acids on Graphene: Assessment of Force Fields”, AIChE Annual Meeting, Nov 13-16, 2016, San Francisco, CA
44. *Dasetty, S., Wang, W., Blenner, M. A., and Sarupria, S. “Understanding the Structural Differences Between Psychrophilic and Thermophilic Enzymes: A Molecular Dynamics Study”, AIChE Annual Meeting, Nov 13-16, 2016, San Francisco, CA
45. *DeFever, R. and Sarupria, S. “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**
46. *DeFever, R. and Sarupria, S. “Molecular Dynamics Studies of Structure II Hydrate Nucleation Using Advanced Sampling Techniques”, AIChE Annual Meeting, Nov 13-16, 2016, San Francisco, CA
47. *Boateng, L., Monk, R., Xie, P., Malakian, A., Weinman, S., Ladner, D., Battiato, I., Husson, S. M. and Sarupria, S., “An Integrated Multiscale Modeling and Experimental Approach to Design Fouling-Resistant Membranes”, AIChE Annual Meeting, Nov 13-16, 2016, San Francisco, CA
48. *Wang, W., Dasetty, S, Sarupria, S. and Blenner, M. A., 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
49. Sarupria, S. “Sampling Rare Events in Aqueous Systems Using Molecular Simulations”, DOE CPIMS Annual Meeting, Nov 1-4, 2016, B, MD
50. *Malakian, A., Weinman, S., Monk, R., Boateng, L., Sarupria, S., Ladner, D., and Husson, S. “Understanding the Roles that Patterning and Chemistry Play on Membrane Fouling”, North American Membrane Society 26th Annual Meeting, May 21- 25, 2016, Bellevue, WA
51. 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, Nov 20, 2015, Austin, TX
52. Siva Dasetty and Sapna 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
53. Brittany Glatz and Sapna Sarupria, “Heterogeneous Ice Nucleation and Growth: What Effects Do Surfaces Have?”, Nov 8-13, 2015, AIChE Annual Meeting, Salt Lake City, UT
54. Ryan DeFever, David Barton, Danielle Jacobs and Sapna 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
55. Ryan DeFever and Sapna Sarupria, “Nucleation of Gas Hydrates in Interfacial Systems”, Nov 8-13, 2015, AIChE Annual Meeting, Salt Lake City, UT
56. Ryan DeFever, Danielle Jacobs and Sapna Sarupria, “Molecular Dynamics Investigations of Dendrimer–Aromatic Hydrocarbon Interactions”, Nov 8-13, 2015, AIChE Annual Meeting, Salt Lake City, UT

57. Ryan DeFever, Walter Hanger, Linh Ngo, Amy Apon and Sapna 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.**
58. Ryan DeFever, Danielle Jacobs and Sapna 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
59. Ryan DeFever, Walter Hanger, Linh Ngo, Amy Apon and Sapna 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
60. Sapna Sarupria, “Hydrate nucleation near SAM surfaces”, Nov 16-21, 2014, AIChE National Meeting, Atlanta, GA
61. Ryan DeFever, Nicholas Geitner, Priyanka Bhattacharya, Pu-Chun Ke, Feng Ding and Sapna Sarupria, “Molecular Dynamics Study of Hydrocarbon Adsorption on Dendrimers and Graphene Oxide for Water Purification”, Nov 16-21, 2014, AIChE National Meeting, Atlanta, GA
62. Brittany Glatz, and Sapna Sarupria, “Effects of Lattice Spacing on Water Films: Implications for Ice Nucleation?”, Nov 16-21, 2014, AIChE National Meeting, Atlanta, GA
63. Sapna Sarupria, “Molecular Modeling & Computer Simulations in Materials Engineering”, Western South Carolina Section, AIChE, 18 February 2014, Greenville, SC
64. Sapna Sarupria, “Water Structure and dynamics in thin films on mineral surfaces”, AIChE National Meeting, San Francisco CA, (Nov 3-8, 2013)
65. Sapna Sarupria, “A brief overview of molecular simulations”, Invited talk at Summer Program for Research Interns (SPRI), 11 July 2013, Clemson University
66. Sapna 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
67. David Barton, Ryan DeFever and Sapna Sarupria, “Molecular Simulations of PAMAM Dendrimers for Oil Dispersion”, AIChE Southern Regional Conference, Mar 31-Apr 2, 2016 Tuscaloosa, AL
68. 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.**
69. Dylan Bruckner and Sapna Sarupria, “Molecular Dynamics Studies to Understand Early Events in Virus Capsid Formation”, April 5-7, 2013, AIChE Southern Regional Conference, Lexington, Kentucky

Prior to Clemson

70. Sapna Sarupria, “Mathematical modeling and the beauty of molecules”, Invited talk in Polymer Composites Laboratory, Seattle WA (March 19-20, 2012)
71. Sapna Sarupria, “Hydration phenomena in proteins and gas hydrates”, Invited department seminar, University of Michigan, Ann Harbor MI (March 9-11, 2011)
72. Sapna Sarupria, “Hydration phenomena in proteins and gas hydrates”, Invited department seminar, Virginia Tech, Blacksburg VA (March 1-3, 2011)
73. Sapna Sarupria, “Hydration phenomena in proteins and gas hydrates”, Invited department seminar, University of Kentucky, Lexington KY (February 16, 2011)
74. Sapna Sarupria, “Hydration phenomena in proteins and gas hydrates”, Invited department seminar, University of Rochester, Rochester NY (February 23, 2011)
75. Sapna Sarupria, “Hydration phenomena in proteins and gas hydrates”, Invited department seminar, Clemson University, Clemson SC (February 6-8, 2011)

76. Sapna Sarupria, “Molecular dynamics study of carbon dioxide hydrate decomposition”, AIChE National Meeting, Salt Lake City UT, (November 7-12, 2010)
77. Sapna Sarupria, “Probing hydrophobic interactions at interfaces”, AIChE National Meeting, Salt Lake City UT (November 7-12, 2010)
78. Sapna Sarupria, “Can polar surfaces be hydrophobic? Molecular simulation study of model silica surfaces”, AIChE National Meeting, Salt Lake City UT, (November 7-12, 2010)
79. Sapna Sarupria, “Studying decomposition of CO₂ hydrates using molecular dynamics simulations”, Gordon Research Conference (Water and Aqueous Solutions), Holderness NH, (August 7-12, 2010) (Invited talk part of the Best Poster Award)
80. Sapna Sarupria, “Quantifying pressure effects on water-mediated ion-ion interactions”, AIChE National Meeting, Philadelphia PA (November 16-21, 2008)
81. Sapna Sarupria, “Hydrophobic hydration and interaction in extended thermodynamic space”, Invited talk at international conference titled Proteins Under Pressure, Santa Fe NM, (January 21-25, 2008). The conference was focused on state of the art studies on the effects of hydrostatic pressure on biomolecules and was attended by world’s top experts in the field.
82. Sapna Sarupria, “Lengthscale dependence of hydrophobic hydration – Exploring the pressure dimension”, Gordon Research Conference (Liquids, Chemistry and Physics of), Holderness NH (July 29-August 3, 2007) (Invited talk part of the Best Poster Award)
83. Sapna Sarupria, “Effect of high pressures on proteins”, AIChE National Meeting, San Francisco CA (November 12-17, 2006)
84. Sapna Sarupria, “Pressure denaturation of proteins – A molecular dynamics study”, Midwest Thermodynamics and Statistical Mechanics Conference, Akron OH (May 25-26, 2006)

POSTER PRESENTATIONS

(presenter indicated by asterisk and is underlined)

1. *Steven Hall, Ryan S. DeFever, and 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
2. *Jiarun Zhou, Nurun N. Lata, Sapna Sarupria, and Will H. 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
3. *Tim Yuan, Ryan S. DeFever, and S. Sarupria, “RSeeds: Rigid seeding method for studying heterogeneous crystal nucleation”, GRC Crystal Growth and Assembly, June 23 - 28, 2019, Manchester, NH
4. *Steven Hall, Ryan S. DeFever, Colin Targonski, Melissa C. Smith, and Sapna 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.
5. *Jiarun Zhou, Nurun Nahar Lata, Will Cantrell and Sarupria, S, “Water Structure and Correlation to Heterogeneous Ice Nucleation on Mineral Surfaces”, 2019 SC EPSCoR/IDeA State Conference, April 12th, 2019, Greenville, SC
6. *Steven Hall, Ryan DeFever and Sarupria, S., “Effect of interaction potential on crystal nucleation kinetics of Lennard-Jones like particles”, 2019 SC EPSCoR/IDeA State Conference April 12th, 2019, Greenville, SC.
7. *Jiarun Zhou, Nurun Nahar Lata, Will Cantrell and Sarupria, S, “Heterogeneous Ice Nucleation on Mineral Surfaces: Study of Surface Effects”, 2018 SC EPSCoR/IDeA State Conference, April 7th, 2018, Columbia, SC
8. *Steven Hall, Ryan DeFever and Sarupria, S., “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. *Waring Hills, *Kamryn Kant and Sarupria, S., Molecular Dynamics of the Anthrax Pore-forming Toxin, Clemson University Creative Inquiry Poster Symposium, April 2nd, 2018.
10. *Siva Dasetty, Weigao Wang, Mark Blenner and Sapna Sarupria, “Engineering Robust Activity in Extremophilic Enzymes”, AIChE National Meeting, Oct 29–Nov 3, 2017, Minneapolis, MN.
11. *Ryan DeFever and Sapna 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.
12. *Ryan DeFever and Sapna 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.
13. *Siva Dasetty, Weigao Wang, Mark Blenner, Sapna Sarupria, “Engineering Robust Activity in Extremophilic Enzymes”, February 25, 2017, Clemson Biological Sciences Annual Student Symposium, Biological Sciences, Clemson University, Clemson SC
14. *Siva Dasetty, Weigao Wang, Mark Blenner, Sapna Sarupria, “Engineering Robust Activity in Extremophilic Enzymes”, April 29, 2017, The Future of Integrative Structural Biology, Physics, Clemson University, Clemson SC (poster)
15. *Ryan DeFever and Sapna Sarupria, "Nucleation Mechanism of Clathrate Hydrates of a Water Soluble Guest Molecule", April 11, 2017, Graduate Symposium, Chemical Engineering, Clemson University, Clemson, SC. (Poster) [Received the first place for the best poster award](#)
16. *Brittany Glatz, and Sapna 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.](#)
17. Ryan DeFever and *Sapna 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
18. *Sarupria, S., “Sampling Rare Events in Aqueous Systems Using Molecular Simulations”, 15-18 May 2016, DOE CTC PI Meeting, Gaithersburg, MD.
19. *Siva Dasetty and Sapna Sarupria, “What drives the adsorption of peptides on carbon nanomaterials”, February 23, 2016, Graduate Symposium, Chemical Engineering, Clemson University, Clemson SC (poster)
20. *Sarupria, S., Husson, S.M., Ladner, D.A. and Battiato, I. “DMREF: An integrated multiscale modeling and experimental approach to design fouling-resistant membranes.” Materials Genome Initiative Annual Meeting, Jan 2016, Bethesda, MD.
21. *Walter Hanger, Sapna Sarupria, Ryan DeFever, Amy Apon and Linh Ngo, “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.](#)
22. *Brittany Glatz, and Sapna 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
23. *Ryan DeFever and Sapna 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
24. *Ryan DeFever and Sapna 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](#)
25. *Danielle Jacobs, *David Barton, Ryan DeFever and Sapna Sarupria, “Dendrimers for Water Purification: Molecular Dynamics Studies”, Clemson University Creative Inquiry Poster Symposium (April 8th, 2015) (poster)

26. *Ryan DeFever and Sapna Sarupria, “Dendrimer-Guest Interactions: Challenging Conventional Wisdom”, March 4, 2015, Graduate Symposium, Chemical Engineering, Clemson University, Clemson SC (poster)
27. *Tyler Slonecki, Ryan DeFever, Brittany Glatz, Sapna Sarupria and Joshua Levine, “Visualization to Enhance Rare Event Simulations of Ice Nucleation”, XSEDE Conference, Atlanta, GA (July 13-18, 2014)
28. Matthiew Filanova and *Sapna Sarupria, “Birth of gas hydrates: Effect of surface chemistry”, 2014 Water and Aqueous Solutions Gordon Research Conference, Holderness, NH July 27 - August 1, 2014
29. Matthiew Filanova and *Sapna 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
30. *Walter Hanger, Ryan S. DeFever, Linh Ngo, Amy Apon and Sapna Sarupria, “ScaFFS: Scalable Forward Flux Sampling”, July 2014, BigData Research Experience for Undergraduates, Clemson University, Clemson, SC (poster)
31. *Brittany Glatz, Luke Rhym and Sapna Sarupria, “Ice Nucleation and Growth on Kaolinite Surfaces”, Departmental Graduate Student Symposium (ChBE), 5 March 2014 (poster)
32. *Ryan DeFever, Nick Geitner, Priyanka Bhattacharya and Pu Chun Ke, “Dendrimers and Graphene Oxide: Molecular Simulation Studies”, Departmental Graduate Student Symposium (ChBE), 13 Feb 2013 (poster)
33. *Ryan DeFever, Pengfei Xuan, Amy Apon and Sapna Sarupria, “Capturing ice nucleation with a SciFlow DFFS implementation”, Research Experience for Undergraduates, School of Computing, Clemson University, 26 July 2013 (poster)

(presented by Sapna Sarupria prior to Clemson)

34. “Capturing the birth of gas hydrates”, 2012 Water and Aqueous Solutions Gordon Research Conference, Holderness, NH August 11-17, 2012
35. “Studying decomposition of CO₂ hydrates using molecular dynamics simulations”, Gordon Research Conference (Water and Aqueous Solutions), Holderness NH, August 7-12, 2010 – received the Best Poster Award.
36. “Hydration shells of hydrophobic solutes and proteins: Exploring the pressure dimension”, Faraday Discussion 146: Wetting Dynamics of Hydrophobic and Structured Surfaces, Richmond VA, April 12-14, 2010.
37. “Ion pairing preferences in water and volcano plot: A molecular perspective”, Gordon Research Conference (Liquids, Chemistry and Physics of), Holderness NH, August 2-7, 2009.
38. “Quantifying pressure dependence of water mediated ion-ion interactions”, Gordon Research Conference (Biopolymers), Newport RI, June 8-13, 2008.
39. “Using computer simulations to explore pressure effects on proteins”, 235th ACS National Meeting, New Orleans LA, April 6-10, 2008. (Part of ACS Chemical Computing Group Award of Excellence in computing research).
40. “Lengthscale dependence of hydrophobic hydration – Exploring the pressure dimension”, Gordon Research Conference (Liquids, Chemistry and Physics of), Holderness NH, July 29-August 3, 2007 – received the Best Poster Award.
41. “Proteins under stress: Molecular simulations of pressure denaturation of proteins”, Gordon Research Conference (Water and Aqueous solutions), Holderness NH, Jul 30-Aug 4, 2006.
42. “Proteins under stress: Molecular simulations of pressure denaturation of proteins”, Key Executives Conference, Troy NY, April 6-7, 2006.

Undergraduate Honors Thesis

1. Waring Hills, “Molecular Dynamics Simulations of the Anthrax Toxin”, May 2018

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

Current Doctoral Students

- Yen Yen Nguyen Edalgo, “Simulation studies of self-assembly of magnetic colloidal particles” (2018 – Present)
- Kamryn Kant, “Enabling simulations of large biological systems” (2018 – Present)
- Steven Hall, “Machine learning applied to rare event methods” (2018 – Present)
- Tianmu (Tim) Yuan, “Molecular Dynamics Simulations of Ice Nucleation on Soft Surfaces” (2018 – Present)
- Salman Bin Kashif, “Molecular Dynamics Simulations of Fouling on Water Purification Membranes” (2018 – Present)
- Jiarun Zhou, “Molecular Dynamics Simulations of Ice Nucleation Near Mineral Surfaces”, (2016 – Present)

Previous Graduate Students

- Ryan DeFever, “Advancing molecular simulations of crystal nucleation: Applications to clathrate hydrates”, (2014 – 2019)
- Siva Dasetty, “Towards computer aided engineering of proteins and protein–surface complexes”, (2015 – 2019)
- Brittany Glatz, “Molecular simulation studies of ice nucleation”, (2012-2018)
- Siva Dasetty, “Understanding molecular interactions between proteins and carbon nanomaterials” Maters’ (with Thesis) (2013-2015)

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

Aarin Henning, ChBE (May 2019--)
 *Garrett Buchmann, ChBE (May 2018-Nov 2018)
 *Natalie Rodgers, ChBE (Oct 2017–Dec 2017)
 *Waring Hills, ChBE (Jan 2017–May 2018)
 *David Barton, ChBE (Sep 2014–May 2016)
 *Brandon Alverson, ChBE (Jan 2015–May 2017)
 *Danielle Jacobs, ChBE (Jan 2014–May 2017)
 *Steve Cotty, ChBE (Jan 2015–Summer 2016)
 *Luke Rhym, ChBE (May 2012–May 2015)
 *Ryan DeFever, ChBE (Aug 2012–May 2014)
 *Dylan Bruckner, ChBE (May 2012–May 2014)
 Tara Brooks, ChBE (Oct 2017–present)
 Kamryn Kant, ChBE (Jan 2017–May 2018)
 Christian Summerville, ChBE (Jan–May 2017)

Steven Hall, ChBE (May 2016–May 2018)
 Dylan Weber, ChBE (May 2016–Aug 2016)
 Judge Walter Hanger, Computer Engineering (May 2014–May 2017)
 John Barrows, Biochemistry (Sep 2014–May 2016)
 Tyler Slonecki, VisREU (June–July 2014)
 Emily Voyles, ChBE (May 2013–May 2014)
 BreAnn Janvier, ChBE (Jan 2014–May 2014)
 Matthiew Filanova, ChBE (May 2012–May 2013)
 Stephanie Chui, ChBE (Feb 2013–May 2014)
 Julianne McLeod, Calhoun College Honor Student (Aug–Dec 2012)
 Joshua John, ChBE (Sep 2012–Apr 2013)
 Clayton Hammontree, ChBE (May–Aug, 2012)

Visiting undergraduate scholars and summer REU students

Diego Losada Rubio, Wofford College (May 28 – July 28, 2019)
Vatsa Shah, Indian Institute of Technology, Guwahati, India (May 22 – July 13, 2019)
Eliel Akinbami, Howard University, Washington D.C., (May 15 – 10 Aug 2018)
Harshit Arora, Indian Institute of Technology Chennai, India (20 June - 22 July 2015)

High School Students

*Gisela Griesheimer, SC Governor's School for Science & Mathematics
*Cassidy Baldwin, SC Governor's School for Science & Mathematics

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

OTHER SPONSORED ACTIVITY

Creative Inquiry titled “Molecular Modeling of Biological and Polymer Systems” 2013-2018. I have trained over 22 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.

Travel Grant from Materials Computation Center, UIUC/NSF program to attend CECAM Workshop on "Microscopic view of CO₂ sequestration" at CECAM-HQ-EPFL, Lausanne, Switzerland (July 2011)

NSF Fellowship to attend Faraday Discussions 146: Wetting Dynamics of Hydrophobic and Structured Surfaces and associated graduate research seminar (Richmond VA, April 9-14, 2010).

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

TEACHING

Courses Taught (Beginning Spring 2012)

ChE 2300, Fluid Flow and Heat Transfer, S12, S13, S14
ChE 8040, Advanced Thermodynamics, F12, F13, F14, F15
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
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) – a funded activity by National Science Foundation.

SERVICE

1. **Co-organizer** of Workshop: Hands On With Molecular Simulation, AIChE National Meeting, Oct 28, 2018, Pittsburgh, PA.
2. **Session Chair** to multiple sessions at AIChE (2012, 2013, 2014, 2015, 2016, 2017)
3. **Vice Chair (elected)** of The Computational Molecular Science and Engineering Forum of the AIChE (2018--).
4. **Programming Chair** for Area 1a AIChE National Meeting
5. **Guest Editor:** Journal of Theoretical and Computational Chemistry, Special Issue: Advanced Molecular Simulations: Method and Applications
6. **Organizer:** Computational Materials Science Group@Clemson University
7. **Organizer:** Telluride Science Research Center (TSRC) workshop on Soft Matter
8. **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, ACS Chemical Science, Nature Nanotechnology, Philosophical Transactions A.
 - c. **Others:** American Chemical Society Chemical Computing Group

Continuing Education

- “2012 Water and Aqueous Solutions Graduate Research Seminar”, Conference Chair (August 2012)
- 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)

Committees

College/University

- Member of Faculty Senate Ad Hoc Committee on the Status of Women (F2018)
- 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.
- Clemson University Computational Advisory Team (CU-CAT) committee: The committee is 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-)
- Elected faculty senate (alternate) member and serving on financial committee (2017, 2018)
- 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

- Graduate studies committee (2017,2018)
- Graduate recruitment committee (2017)
- 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)

Updated: August 9, 2019