College of Engineering, Computing and Applied Sciences

RESUME – Sapna Sarupria
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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

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)

HONORS AND AWARDS

- ACS COMP OpenEye Outstanding Junior Faculty Award in Computational Chemistry.
- College of Engineering and Science Dean's Faculty Fellows Award
- 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.

STUDENT HONORS AND AWARDS

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

Ryan DeFever, NSF Graduate Research Fellowship Honorable Mention

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

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

Ryan DeFever, Professional Enhancement Grant from Clemson University ($750) April 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 ScaFFS 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

"CAREER: Large Scale Simulations Enabled Materials Engineering for Heterogeneous Ice Nucleation"
Role: Principal Investigator
Funding Agency: National Science Foundation
Duration: 9/1/2017 – 08/31/2022

"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
Duration: 3/1/2016 – 2/28/2019

"Predictive Structure-Function Relationships for Enzymes Immobilized on Complex Surfaces"
Role: Co-investigator (50%)
Co-investigators: Dr. Mark Blenner (ChBE, Clemson)
Funding Agency: Defense Threat Reduction Agency
Duration: 5 years

"Sampling Rare Events In Aqueous Systems Using Molecular Simulations"
Role: Principal Investigator
Co-investigator: Linh Ngo (Computer Science, Clemson University)
Funding Agency: Department of Energy
Duration: 03/01/2016 – 08/31/2017

"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
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
Duration: 9/1/2014 - 8/31/2016 (one year no-cost extension granted)

"TIGER: DMREF: Computer Aided Design of Antifouling Membranes for Water Purification"
Funding Agency: Clemson University
Role: Principal Investigator
Duration: 6/1/2014 – 6/30/2015

PUBLICATIONS

Refereed Journal Publications

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

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

1. 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)
2. 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)
3. **Glatz, Brittany** and *Sarupria, S. "The surface charge distribution affects ice nucleating efficiency of silver iodide" J. Chem. Phys. 145, 211924 (2016)
4. 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)
5. **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]
6. Cameron J. Bodenschatz, Sapna Sarupria and *Rachel 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 [DOI: 10.1021/acs.jpcc.5b02333]
7. **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]
8. 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, 2014,16, 25916-25927
9. 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)
10. 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

11. 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)
12. *S. Sarupria and P. Debenedetti, "Homogeneous nucleation of methane hydrate in microsecond molecular dynamics simulations", Journal of Physical Chemistry Letters, 3: 2942-2947 (2012)
13. S. Sarupria and *P. G. Debenedetti, "Molecular dynamics study of dissociation of carbon dioxide hydrates", Journal of Physical Chemistry A, 115: 6102 (2011)
14. *P. G. Debenedetti and S. Sarupria, "Hydrate molecular ballet", **Science**, 326: 1070 (2009)
15. 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)

16. 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).
17. 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)
18. 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)
19. 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)

PRESENTATIONS

(speaker is underlined)

1. *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)**
2. *Sarupria, S. "Freezing water and aqueous solutions: Elucidating the molecular ballet using computer simulations", Worchester Polytechnic Institute**,** Mar 1, 2017, Worchester, MA **(Invited)**
3. *Sarupria, S. "Freezing water and aqueous solutions: Elucidating the molecular ballet using computer simulations", The University of Viginia**,** Mar 16, 2017, Charlottesville, VA **(Invited)**
4. *Sarupria, S. "Freezing water and aqueous solutions: Elucidating the molecular ballet using computer simulations", Lehigh University**,** Mar 22, 2017, Bethlehem, PA **(Invited)**
5. *Sarupria, S. "Freezing water and aqueous solutions: Elucidating the molecular ballet using computer simulations", Oklahoma State University**,** Mar 28, 2017, Stillwater, OK **(Invited)**
6. 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
7. *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
8. *Glatz, B and Sarupria, S, "Heterogeneous Ice Nucleation Using Forward Flux Sampling", AIChE Annual Meeting, Nov 13-16, 2016, San Francisco, CA
9. *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
10. *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

11. *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**
12. *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
13. *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
14. *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
15. *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)**
16. 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
17. 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
18. 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
19. 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
20. Ryan DeFever and Sapna Sarupria, "Nucleation of Gas Hydrates in Interfacial Systems", Nov 8-13, 2015, AIChE Annual Meeting, Salt Lake City, UT
21. 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
22. 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.**
23. 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
24. 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
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, "Hydrate nucleation near SAM surfaces", Nov 16-21, 2014, AIChE National Meeting, Atlanta, GA

28. *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
29. *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
30. *Sapna Sarupria, "Molecular Modeling & Computer Simulations in Materials Engineering", Western South Carolina Section, AIChE, 18 February 2014, Greenville, SC
31. *Sapna Sarupria, "Water Structure and dynamics in thin films on mineral surfaces", AIChE National Meeting, San Francisco CA, (Nov 3-8, 2013)
32. *Sapna Sarupria, "A brief overview of molecular simulations", Invited talk at Summer Program for Research Interns (SPRI), 11 July 2013, Clemson University
33. *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
34. *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
35. *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.
36. Sapna Sarupria, "Simulation studies of gas hydrates", Microscopic Description of Gas Clathrate Telluride Science Research Center Workshop, Telluride CO (July 9-13, 2012) **(Invited)**

Prior to Clemson

Sapna Sarupria, "Mathematical modeling and the beauty of molecules", **Invited talk** in Polymer Composites Laboratory, Seattle WA (March 19-20, 2012)

Sapna Sarupria, "Hydration phenomena in proteins and gas hydrates", **Invited department seminar**, University of Michigan, Ann Harbor MI (March 9-11, 2011)

Sapna Sarupria, "Hydration phenomena in proteins and gas hydrates", **Invited department seminar**, Virginia Tech, Blacksburg VA (March 1-3, 2011)

Sapna Sarupria, "Hydration phenomena in proteins and gas hydrates", **Invited department seminar**, University of Kentucky, Lexington KY (February 16, 2011)

Sapna Sarupria, "Hydration phenomena in proteins and gas hydrates", **Invited department seminar,** University of Rochester, Rochester NY (February 23, 2011)

Sapna Sarupria, "Hydration phenomena in proteins and gas hydrates", **Invited department seminar**, Clemson University, Clemson SC (February 6-8, 2011)

Sapna Sarupria, "Molecular dynamics study of carbon dioxide hydrate decomposition", AIChE National Meeting, Salt Lake City UT, (November 7-12, 2010)

Sapna Sarupria, "Probing hydrophobic interactions at interfaces", AIChE National Meeting, Salt Lake City UT (November 7-12, 2010)

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)

Sapna Sarupria, "Studying decomposition of CO_2 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)

Sapna Sarupria, "Quantifying pressure effects on water-mediated ion-ion interactions", AIChE National Meeting, Philadelphia PA (November 16-21, 2008)

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.

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)

Sapna Sarupria, "Effect of high pressures on proteins", AIChE National Meeting, San Francisco CA (November 12-17, 2006)

Sapna Sarupria, "Pressure denaturation of proteins – A molecular dynamics study", Midwest Thermodynamics and Statistical Mechanics Conference, Akron OH (May 25-26, 2006)

Posters

(presenter indicated by asterisk and is underlined)

National and International Conferences

1. *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.**
2. *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.
3. *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)
4. *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
5. *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
6. 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
7. 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

Local Conferences:

8. 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
9. Ryan DeFever and Sapna Sarupria, "sII clathrate-hydrate nucleation: The effects of hydrophobic and hydrophilic surfaces", February 23, 2015, Graduate Symposium, Chemical Engineering, Clemson University, Clemson SC – **Received the second place for the best poster award**

10. *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)
11. *Ryan DeFever and Sapna Sarupria, "Dendrimer-Guest Interactions: Challenging Conventional Wisdom", March 4, 2015, Graduate Symposium, Chemical Engineering, Clemson University, Clemson SC
12. *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
13. *Brittany Glatz, Luke Rhym and Sapna Sarupria, "Ice Nucleation and Growth on Kaolinite Surfaces", Departmental Graduate Student Symposium (ChBE), 5 March 2014
14. *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
15. *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

(presented by Sapna Sarupria prior to Clemson)

- "Capturing the birth of gas hydrates", 2012 Water and Aqueous Solutions Gordon Research Conference, Holderness, NH August 11-17, 2012
- "Studying decomposition of CO_2 hydrates using molecular dynamics simulations", Gordon Research Conference (Water and Aqueous Solutions), Holderness NH, August 7-12, 2010 – received the Best Poster Award.
- "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.
- "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.
- "Quantifying pressure dependence of water mediated ion-ion interactions", Gordon Research Conference (Biopolymers), Newport RI, June 8-13, 2008.
- "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).
- "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.
- "Proteins under stress: Molecular simulations of pressure denaturation of proteins", Gordon Research Conference (Water and Aqueous solutions), Holderness NH, Jul 30-Aug 4, 2006.
- "Proteins under stress: Molecular simulations of pressure denaturation of proteins", Key Executives Conference, Troy NY, April 6-7, 2006.

OTHER SPONSORED ACTIVITY

Creative Inquiry titled "Molecular Modeling of Biological and Polymer Systems" in Fall 2013, Spring 2014, Fall 2014, Spring 2015, Spring 2016, Fall 2016, Spring 2017. I have trained over 20 undergraduate students in molecular simulations through this Creative Inquiry program, three of which are in graduate school at MIT, Rensselaer Polytechnic Institute and Clemson University.

Travel Grant from Materials Computation Center, UIUC/NSF program to attend CECAM Workshop on "Microscopic view of CO_2 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

Updated: March 20, 2017