SHIKHA NANGIA

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EDUCATION

2006	Ph. D.	Chemistry	University of Minnesota, Twin cities
2000	M.S.	Chemistry	Indian Institute of Technology (IIT), Delhi
1998	B.S.	Chemistry	University of Delhi, Delhi, India

PROFESSIONAL EXPERIENCE

2018-present	Associate Professor	Department of Biomedical and Chemical Engineering *Syracuse University*
2021-present	Associate Editor	ACS Applied Bio Materials *American Chemical Society*
2020-present	Graduate Program Director	Department of Biomedical and Chemical Engineering *Syracuse University*
2014-present	Member	Interdisciplinary Neuroscience Studies *Syracuse University*
2012-2020	Member	Department of Biomedical and Chemical Engineering *Syracuse University*
2012-2018	Assistant Professor	Syracuse Biomaterials Institute *Syracuse University*
2009-220	Research Professor	Department of Biomedical and Chemical Engineering *Syracuse University*
2009-2012	Research Professor	Department of Chemistry *Syracuse University*
2006-2009	Postdoctoral Researcher	Department of Chemistry *Pennsylvania State University*

HONORS AND AWARDS

2019	Chancellor's Citation Award for Outstanding Contributions to Student Experience and University Initiatives, *Syracuse University*
2017	Dean's Award for Excellence in Education, *College of Engineering, Syracuse University*
2017	Meredith Teaching Recognition Award, *Syracuse University*
2016	College Technology Educator of the Year, *Technical Alliance of Central New York*
2016	ACS OpenEye Outstanding Junior Faculty Award, *ACS COMP division*
2015	Nappi Research Competition Award
2015	NSF CAREER award
2015	Faculty Excellence Award, *College of Engineering, Syracuse University*

HONORS AND AWARDS TO UNDERGRADUATE AND GRADUATE MENTEES

2021	Second place Research Talk, ECS Research Day, Syracuse University, N. Rajagopal (G)

2021 Merck Research Award, Women Chemists Committee, American Chemical Society, N. Rajagopal (G)
2020 The Chemical Computing Group Excellence Award for Graduate Students, American Chemical Society, N. Rajagopal (G)
2019 Second place poster, Summer Research Symposium, Syracuse University, V. Bialczak (UG)
2019 Graduate Research Fellowship Program, National Science Foundation, K. Piston (G)
2019 University Scholar, Syracuse University, S. Ebangwese (UG)
2019 All University Doctoral prize, Syracuse University, H. Ma (G)
2019 2019 SBI Distinguished Student Research Award, Syracuse University, H. Ma (G)
2019 Outstanding Graduate Student in Bioengineering Award, Syracuse University, H. Ma (G)
2019 Chancellor's Award for Public Engagement and Scholarship, K. Piston (G)
2019 Third place poster, 4th Annual Neuroscience Day, Syracuse University, N. Rajagopal (G)
2019 Best poster, Stevenson Biomaterials Day, Syracuse University, K. Piston (G)
2019 Second place poster, Stevenson Biomaterials Day, Syracuse University, S. Ebangwese (UG)
2018 First place poster, Summer Research Symposium, Syracuse University, P. Ganesh (UG)
2018 Third place poster, Stevenson Biomaterials Day, Syracuse University, N. Rajagopal (G)
2018 First place research pitch, ECS Research Day, Syracuse University, H. Ma (G)
2017 Graduate School Master of Science Prize, Syracuse University, Nan Wang (G)
2017 First place poster, ECS Research Day, Syracuse University, F. J. Irudayanathan (G)
2017 First place research pitch, ECS Research Day, Syracuse University, F. J. Irudayanathan (G)
2017 First place poster, 3rd Annual Neuroscience Day, F. J. Irudayanathan (G)
2017 Second place poster, Stevenson Biomaterials Day, J. Gomez (UG)
2017 Graduate Research Fellowship Program, National Science Foundation, A. Peña (UG)
2016 Meredith Symposium Finalist, Syracuse University, A. Khan (UG)
2016 Bioengineering Founder's Award, Syracuse University, A. Peña (UG)
2016 The Chemical Computing Group Excellence Award for Graduate Students, American Chemical Society, W. Jiang (G)
2016 First place poster, Stevenson Biomaterials Day, F. J. Irudayanathan (G)
2016 Syracuse Biomaterials Institute Graduate Fellowship, W. Jiang (G)
2016 Graduate School Master of Science Prize, Syracuse University, X. Wang (G)
2015 First Place Poster, Emerging Researchers National Conference, A. Peña (UG)
2015 Graduate School Master of Science Prize, Syracuse University, H. Ma (G)
2015 Graduate Research Fellowship Program, National Science Foundation, J. Woods (UG)
2015 First place poster, Syracuse University Neuroscience Research Day, F. J. Irudayanathan (G)
2014 First place poster, Stevenson Biomaterials Day, F. J. Irudayanathan (G)
2014 Third place poster, Stevenson Biomaterials Poster Day, W. Jiang (G)
2014 Best poster, Biomedical Research Conference for Minority Students, A. Peña (UG)
2014 Third place, LSMCE Conference Roadmap to Action: LSAMP Principles for Broadening Minority Participation in STEM, A. Peña (UG)
2014 Best BMCE poster award, Nunan Research Day, F. J. Irudayanathan (G)
2014 Outstanding Graduate Student in Bioengineering Award, H. Kamani (G)
2014 Graduate School Master of Science Prize, Syracuse University, H. Kamani (G)

PUBLICATIONS

1. Development of the Computational Antibiotic Screening Platform (CLASP) to Aid in the Discovery of New Antibiotics, Y. Dai, H. Ma, M. Wu, T. A. Welsch, S. Vora, D. Ren, and **S. Nangia**, Soft Matter, 17, 2725-2736 (2021). https://doi.org/10.1039/D0SM02035D

2. High-Level Antibiotic Tolerance of a Clinically Isolated *Enterococcus faecalis* Strain, H. Gu, S. Roy, X. Zheng, T. Gao, H. Ma, Z. Soultan, C. Fortner, **S. Nangia**, D. Ren, Chemical Communications Applied and Environmental Microbiology, **87**, 10281-10284 (2020). https://doi.org/10.1128/AEM.02083-20
3. Non-canonical lipoproteins with programmable assembly and architecture, Md S. Hossain, l. C. Maller, Y. Dai, **S. Nangia**, and D. Mozhdehi, Chemical Communications, **56**, 10281-10284 (2020). https://doi.org/10.1039/D0CC03271A *Featured on the cover.*
4. Paracellular Gatekeeping: What Does it Take for an Ion to pass through a Tight Junction Pore? F. J. Irudayanathan and **S. Nangia**, Langmuir **36**, 6757-6764 (2020). https://doi.org/10.1021/acs.langmuir.0c00877 *Featured on the cover.*
5. Molecular mechanism of ultrasound interaction with a blood brain barrier model, V. H. Man, M. S. Li, P. Derreumaux, J. Wang, T. T Nguyen, **S Nangia**, P. H Nguyen, The Journal of Chemical Physics, 153, 045104 (2020). https://doi.org/10.1063/5.0010667
6. Rational identification and characterization of peptide ligands for targeting polysialic acid, D. G. Shastry, F. J. Irudayanathan, A. Williams, M. Koffas, R. J. Linhardt, **S. Nangia**, P. Karande, Scientific Reports, **10**, 1-15 (2020). https://doi.org/10.1038/s41598-020-64088-z
7. Interaction of amphiphilic coumarin with DPPC/DPPS lipid bilayer: effects of concentration and alkyl tail length, P. Kalyanram, H. Ma, S. Marshall, C. Goudreau, A. Cartaya, T. Zimmermann, I. Stadler, **S. Nangia,** and A. Gupta, Physical Chemistry Chemical Physics, **22**, 15197-15207 (2020). https://doi.org/10.1039/D0CP00696C
8. Predicting selectivity of paracellular pores for biomimetic applications, N. Rajagopal, A. J. Durand, and **S. Nangia**, Molecular Systems Design & Engineering, **5**, 686 - 696 (2020). https://doi.org/10.1039/C9ME00177H
9. Computational Nanoscopy of Tight Junctions at the Blood–Brain Barrier Interface, N. Rajagopal, F. J. Irudayanathan, and **S. Nangia**, International Journal of Molecular Science, **20,** 5583-5613 (2019). https://doi.org/10.3390/ijms20225583
10. The ghrelin O-acyltransferase structure reveals a catalytic channel for transmembrane hormone acylation, M. B. Campaña, F. J. Irudayanathan, T. R. Davis, K. R. McGovern-Gooch, R. Loftus, M. A., N. Escoffery, M. Navarro, M. A. Sieburg, **S. Nangia**, J. L. Hougland, Journal of Biological Chemistry, **294**, 14166-14174 (2019). http://dx.doi.org/10.1074/jbc.AC119.009749
11. Obtaining Protein Association Energy Landscape for Integral Membrane Proteins, N. Rajagopal and **S. Nangia**, *Journal of Chemical Theory and Computation*, **15**, 6444-6455 (2019). *Featured on the cover.* https://doi-org.libezproxy2.syr.edu/10.1021/acs.jctc.9b00626
12. The Influence of Water on Choline-Based Ionic Liquids, E. E. L. Tanner, K. M. Piston, H. Ma, K. N. Ibsen, **S. Nangia**, S. Mitragotri, *ACS Biomaterials Science & Engineering*, **5**, 3645–3653 (2019). https://doi.org/10.1021/acsbiomaterials.9b00243
13. Molecular architecture of a membrane-spanning hormone acyltransferase required for metabolic regulation, M. B. Campaña, F. J. Irudayanathan, T. R. Davis, K. R. McGovern-Gooch, R. Loftus, M. A., N. Escoffery, M. Navarro, M. A. Sieburg, **S. Nangia**, J. L. Hougland, *BioRxiv* (2019). https://doi.org/10.1101/556233
14. Palmitoylation of Claudin-5 proteins influences their lipid domain affinity and tight junction assembly at the blood–brain barrier interface, N. Rajagopal, F. J. Irudayanathan, and **S. Nangia**, *Journal of Physical Chemistry B*, **123**, 983–993 (2019). https://doi.org/10.1021/acs.jpcb.8b09535
15. Development of effective stochastic potential method using random matrix theory for efficient conformational sampling of semiconductor nanoparticles at non-zero temperatures, J. Scher, M. Bayne, A. Srihari, **S. Nangia**, and A. Chakraborty, *Journal of Chemical Physics*, **149,** 014103 (2018). https://doi.org/10.1063/1.5026027

16. Self-Assembly Simulations of Classic Claudins–insights into the Pore Structure, Selectivity and Higher Order Complexes, F. J. Irudayanathan, X. Wang, N. Wang, S. Willsey, I. Seddon, and **S. Nangia**, *Journal of Physical Chemistry B*, **122**, 7463–7474 (2018). *Featured on the cover.* http://dx.doi.org/10.1021/acs.jpcb.8b03842
17. Mechanism of Antibacterial Activity of Choline-Based Ionic Liquids (CAGE), Kelly N. Ibsen, H. Ma, A. Banerjee, E. E. L. Tanner, **S. Nangia**, and S. Mitragotri, *ACS Biomaterials Science & Engineering* **4**, 2370–2379 (2018). http://dx.doi.org/10.1021/acsbiomaterials.8b00486
18. Dynamics of OmpF trimer formation in the bacterial outer membrane of *Escherichia coli*, H. Ma, A. Khan, and **S. Nangia**, *Langmuir*, **34**, 5623–5634 (2018). *Featured on the cover.* http://dx.doi.org/10.1021/acs.langmuir.7b02653
19. Architecture of the paracellular channels formed by Claudins of the blood-brain barrier tight junctions, F. J. Irudayanathan, N. Wang, X. Wang, and **S. Nangia**, *Annals of the New York Academy of Sciences***,** 1–16 **(2017).** http://dx.doi.org/10.1111/nyas.13378
20. Modeling diversity in structures of bacterial outer membrane lipids, H. Ma, D. D. Cummins, N. B. Edelstein, J. Gomez, A. Khan, M. D. Llewellyn, T. Picudella, S. R. Willsey and **S. Nangia**, *Journal of Chemical Theory and Computation*, **13,** 811–824 (2017). http://dx.doi.org/10.1021/acs.jctc.6b00856
21. Drug-specific design of telodendrimer architecture for effective Doxorubicin encapsulation, W. Jiang, X. Wang, D. Guo, J. Luo, and **S. Nangia**, *Journal of Physical Chemistry B*, **120**, 9766–9777 (2016). http://dx.doi.org/10.1021/acs.jpcb.6b06070
22. Molecular architecture of the blood-brain barrier tight junction proteins–A synergistic computational and *in vitro* approach, F. J. Irudayanathan, J. P. Trasatti, P. Karande, and **S. Nangia**, *Journal of Physical Chemistry B*, **120**, 77–88 (2016). http://dx.doi.org/10.1021/acs.jpcb.5b09977
23. Combinatorial approaches to evaluate nanodiamonds uptake and induced cellular fate, R. Eldawud, M. Reitzig, J. Opitz, Y. Rojanasakul, W. Jiang, **S. Nangia**, and C. Dinu, *Nanotechnology*, **27**, 085107 (2016). http://dx.doi.org/10.1088/0957-4484/27/8/085107
24. Simulating gram-negative bacterial outer membrane: A coarse grain model, H. Ma, F. J. Irudayanathan, W. Jiang, and **S. Nangia**, *Journal of Physical Chemistry B*, **119**, 14668–14682 (2015). *Featured on the cover.* http://dx.doi.org/10.1021/acs.jpcb.5b07122
25. Signaling factor interactions with polysaccharide aggregates of bacterial biofilms, S. C. DeSalvo, Y. Liu, G. Choudhary, D. Ren, **S. Nangia**, and R. Sureshkumar, *Langmuir*, **31** 1958-1966 (2015). http://dx.doi.org/10.1021/la504721b
26. Multiscale approach to investigate self-assembly of telodendrimer based nanocarriers for anticancer drug-delivery, W. Jiang, J. Luo, and **S. Nangia**, *Langmuir*, 31 4270-4280 (2015). http://dx.doi.org/10.1021/la503949b
27. Optical signature of formation of protein corona in the firefly luciferase-CdSe quantum dot complex, J.M. Elward, F.J. Irudayanathan, **S. Nangia**, and A. Chakraborty, *Journal of Chemical Theory and Computation*, **10**, 5534-5524 (2014). *Featured on the cover.* http://dx.doi.org/10.1021/ct500681m
28. A Structure–Property Relationship Study of the Well-Defined Telodendrimers to Improve Hemocompatibility of Nanocarriers for Anticancer Drug Delivery, C. Shi, D. Yuan, **S. Nangia**, G. Xu, K. S. Lam, and J. Luo, *Langmuir*, **30**, 6878-6888 (2014). http://dx.doi.org/10.1021/la5003513

29. Effect of nanoparticle charge and shape anisotropy on translocation through cell membranes, **S. Nangia** and R. Sureshkumar, *Langmuir*, **28**, 17666-17671 (2012). *Featured on the cover.* http://dx.doi.org/10.1021/la303449d
30. Theoretical advances in the dissolution studies of mineral-water interfaces, **S. Nangia** and B. J. Garrison, *Theoretical Chemistry Accounts.* **127**, 271-284 (2010). *Invited feature article.* http://dx.doi.org/10.1007/s00214-010-0770-2
31. Role of intrasurface hydrogen bonding on dissolution of silica, **S. Nangia** and B. J. Garrison, *J. Physical Chemistry C* **114**, 2267-2272 (2010). http://dx.doi.org/10.1021/jp909878b
32. Advanced Monte Carlo approach to study evolution of quartz surface during the dissolution process, S. Nangia and B. J. Garrison, *Journal of American Chemical Society* **131**, 9538-9546 (2009). http://dx.doi.org/10.1021/ja901305y
33. Ab-initio study of dissolution of quartz from edge, kink, and surface sites, **S. Nangia** and B. J. Garrison, *Molecular Physics (invited)*, **107**, 831–843 (2009). http://dx.doi.org/10.1080/00268970802665621
34. Dissolution mechanisms of aluminosilicates, C. P. Morrow, **S. Nangia**, and B. J. Garrison, *Journal of Physical Chemistry A*, **113**, 1343–1352 (2009). http://dx.doi.org/10.1021/jp8079099
35. Reaction rates and dissolution mechanisms of quartz as a function of pH, **S. Nangia** and B. J. Garrison, *Journal of Physical Chemistry A* **112**, 2077–2033 (2008). http://dx.doi.org/10.1021/jp076243w
36. Study of a family of 40 hydroxylated beta-cristobalite surfaces using empirical potential energy functions, **S. Nangia**, N. M. Washton, K. T. Mueller, J. D. Kubicki, and B. J. Garrison, *Journal of Physical Chemistry C* **111**, 5169–5177 (2007). http://dx.doi.org/10.1021/jp0678608
37. Direct calculation of coupled diabatic potential-energy surfaces for ammonia and mapping of a four-dimensional conical intersection seam, **S. Nangia** and D. G. Truhlar, *Journal of Chemical Physics* **124**, 124309–13 (2006). http://dx.doi.org/10.1063/1.2168447
38. Non-Born–Oppenheimer molecular dynamics, A. W. Jasper, **S. Nangia**, CY. Zhu, and D. G. Truhlar, *Accounts of Chemical Research* **39** 101–108 (2006). http://dx.doi.org/10.1021/ar040206v
39. A new form of $MgTa_2O_6$ obtained by the molten salt method, A. K. Ganguly, **S. Nangia**, M. Thirumal, and P. L. Gai, *Journal of Chemical Science*, **118** 37–42 (2006). http://dx.doi.org/10.1007/BF02708763
40. Can a single-reference approach provide a balanced description of ground and excited states? A comparison of the completely renormalized equation-of-motion coupled-cluster method with multireference quasidegenerate perturbation theory near a conical intersection and along a photodissociation coordinate in ammonia, **S. Nangia** and D. G. Truhlar, M. J. McGuire, and P. Piecuch, *Journal of Physical Chemistry A* **109**, 11643–11646 (2005). http://dx.doi.org/10.1021/jp0556355
41. Introductory lecture: Nonadiabatic effects in chemical dynamics, A. W. Jasper, CY. Zhu, **S. Nangia**, and D. G. Truhlar, *Faraday Discussions* **127**, 1–22 (2004). http://dx.doi.org/10.1039/b405601a
42. Coherent switching with decay of mixing: An improved treatment of electronic coherence for non-Born-Oppenheimer trajectories, CY. Zhu, **S. Nangia**, A. W. Jasper, and D. G. Truhlar, *Journal of Chemical Physics* **121**, 7658–7670 (2004). http://dx.doi.org/10.1063/1.1793991
43. Army ants algorithm for rare event sampling of delocalized nonadiabatic transitions by trajectory surface hopping and the estimation of sampling errors by the bootstrap method, **S. Nangia**, A. W. Jasper, T. F. Miller III, and D. G. Truhlar, *Journal of Chemical Physics* **120**, 3586–3597 (2004).

http://dx.doi.org/10.1063/1.1641019

CONFERENCE PAPERS AND OTHER INDEXED JOURNAL PUBLICATIONS

1. Peer mentoring for women in STEM, A. Rauh, M. Blum, N. Russo, M. A. Green, and **S. Nangia**, *ASEE Annual Conference and Exposition, Conference Proceedings*, 1087, (2020).
2. Multiscale simulations to characterize the blood brain barrier tight junctions, F.J. Irudayanathan, **S. Nangia** *Journal of Biomolecular Structure and Dynamics* 33, 138-139 (2015). http://dx.doi.org/10.1080/07391102.2015.1038135
3. Probing mechanisms of bacterial infection through molecular dynamics simulations, S. C. DeSalvo,† Y. Liu, **S. Nangia**, and R. Sureshkumar, *Bioengineering Conference (NEBEC), 2013 39th Annual Northeast*. http://dx.doi.org/10.1109/NEBEC.2013.129
4. ChemXSeer digital library Gaussian search, S. Lahiri, J. P. Fernández-Ramírez, S. Nangia, P. Mitra, C. L. Giles, K. T Mueller, 2011. *arXiv:1104.4601*

CITATION METRICS

	Total Citations	h-index
Google Scholar	1568	18
Scopus	1501	18
Web of Science	1514	18

RESEARCH AWARDS

NIH R01
Co-Investigator — $348,000 (total)
Project Title: Defining the Molecular Architecture for Transmembrane Acylation by a Membrane Bound O-Acyltransferase — 9/1/2019- 8/31/2022

NSF Engineering Research Center Planning Grant
Co-PI — $100,000 (total)
Planning Grant: Engineering Research Center for Innovative Materials and Processes for Antimicrobial Control Technologies (IMPACT) — 9/1/2019- 8/31/2020

CUSE Grant — $20,000 (total)
PI — $20,000
Cancer epigenetics: Molecular and structural interplay of histone modifications — 3/1/2019- 4/31/2021

CUSE Grant — $30,000 (total)
Co-PI — $10,000
Bringing a membrane enzyme into structural focus: Interdisciplinary computational-biochemical modeling of ghrelin O-acyltransferase — 5/1/2018- 4/31/2020

NSF CBET Award (Award # 1706061) — $321,000 (total)
Co-PI — $62,769
Integrating synthetic biology approaches with patterned biofilm formation to investigate bacterial persistence in heterogeneous structures — 7/15/2017- 7/14/2020

NSF REU Site — $318,863 (total)
Co-PI — 5/1/2018 - 4/30/2021
Interactive Biomaterials: REU Site

NIH R21 — $213,000 (total)
Co-Investigator — $74,000
Rational Design and High Throughput Synthesis of Nanocarriers for Efficient Drug Delivery — 8/1/2015 - 7/31/2017

NSF CAREER — $530,000 (total)
PI — $530,000
Enabling Transport Across the Blood-Brain Barrier by Engineering Thermodynamically Favorable Pathways — 4/1/2015 - 3/31/2020

NSF REU Site — $297,506 (total)
Senior Personal — 5/1/2015 - 4/30/2018
Interactive Biomaterials: REU Site

NSF EFRI — $2,000,000 (total)
Co-PI — $ 253,750
Deciphering and Controlling the Signaling Processes in Bacterial Multicellular Systems and Bacteria-Host Interactions — 1/01/2012 –12/31/2016

COMPUTER ALLOCATION AWARDS

XSEDE Supercomputer Allocation MCB140216 (renewal) — 1.3 million hours
PI — (equivalent to $27,052)
Multiscale Molecular Modeling of the Biomolecular Interfaces for Enhancing Drug Delivery and Designing Antimicrobial Peptides

Anton2 (PSCA18067P) — 120,000 Units
PI — 12/7/2018 –11/30/2019
Role of S-Palmitoylation on the Blood-Brain Barrier Tight Junction Interface

100,000 Units

Anton2 (PSCA17073P) — 12/7/2017 –11/30/2018
PI
Role of S-Palmitoylation on the Blood-Brain Barrier Tight Junction Interface — 2.9 million hours
(equivalent to $65,006)

XSEDE Supercomputer Allocation MCB140216 (renewal) — 7/1/2017 –6/30/2018
PI
Multiscale Molecular Modeling of the Biomolecular Interfaces for Enhancing Drug Delivery and Designing Antimicrobial Peptides — 1.3 million hours
(equivalent to 46,267.71)

XSEDE Supercomputer Allocation MCB140216 — 10/01/2015 –09/30/2016
PI
Multiscale Molecular Modeling of the Biomolecular Interfaces for Enhancing Drug Delivery and Designing Antimicrobial Peptides

TEACHING AWARDS

Faculty Excellence Award, Syracuse University — $17,000
Enhancing the Teaching and Learning of Chemical Thermodynamics using Active-Learning Pedagogies — 5/1/2015 –4/31/2016

Teaching Recognition Award, Meredith Professors — $3,000
8/1/2017 –5/15/2018

PRESENTATIONS

- (Oral, Invited, Virtual) New Breakthrough in blood-brain barrier tight junctions, Shikha Nangia, *Eli Lilly* (March 3, 2021).
- (Oral, Invited) New Breakthrough in blood-brain barrier tight junctions, Shikha Nangia, 4th *International Tight Junction Conference*, Berlin, Germany (October 8-10, 2021).
- (Oral, Invited, Virtual) Treating Alzheimer's Diseases: A molecular challenge, Shikha Nangia, *University of Pennsylvania* (October 21, 2020).
- (Oral, Invited, Virtual) Molecular challenges to treating Alzheimer's disease, Shikha Nangia, *Women Excelling in Computational Molecular Engineering*, (September 16, 2020).
- (Oral, Invited) Membrane Protein Structure Prediction using Co-evolutionary Analysis, Shikha Nangia, FASEB, PA (July 7-11, 2019).
- (Oral, Invited) Protein Crowding in Complex Lipid Environment, Shikha Nangia, Molecular engineering of soft matter: Spanning small molecules to macromolecules, Telluride, CO (June 15-20, 2019).
- (Oral, Invited) Engineering Pathways across Biological Barriers, Shikha Nangia, *AIChE Annual Meeting*, Pittsburgh, PA (October 29-November 3, 2018).
- (Oral, Invited) Molecular perspective on protein-protein interactions at the tight junctions interface, Shikha Nangia, *256th ACS National Meeting*, Boston, MA (August 19-23, 2018).
- (Poster) Engineering pathways across biological barriers, Shikha Nangia, *FOMMS*, Delavan, WI (July 15-20, 2018).
- (Oral, Invited) Engineering pathways across biological barriers, Shikha Nangia, *Tulane University*, New Orleans, LA (January 25-26, 2018).
- (Oral, Invited) Modeling the protein-protein interactions at the blood-brain barrier interface, Shikha Nangia, *Application of Molecular Modeling to Study Interfacial Phenomena*, *AIChE Annual Meeting*, Minneapolis (October 29-November 2, 2017).
- (Oral, Invited) Multiscale modeling of complex biological interfaces, Shikha Nangia, Molecular engineering of soft matter: Spanning small molecules to macromolecules, Telluride, CO (June 19-23, 2017).
- (Oral, Invited) Breaking through the blood-brain barrier, Shikha Nangia, *Material Science and Engineering, University of Michigan*, Ann Arbor, MI (December 4, 2016).
- (Oral, Invited) Breaking through the blood-brain barrier, Shikha Nangia, *Chemical and Biological Engineering, Rensselaer Polytechnic Institute*, Troy, NY (October 19, 2016).
- (Oral, Invited) Breaking through the blood-brain barrier, Shikha Nangia, *Research Colloquy, Information Technology Services and Research Computing Advisory Council (RCAC) , Syracuse University, Syracuse*, NY (October 24, 2016).
- (Oral, Invited) Breaking through the blood-brain barrier, Shikha Nangia, *Syracuse Biomaterials Seminar Series, SBI, Syracuse University, Syracuse*, NY (October 4, 2016).
- (Oral, Invited) Breaking through the blood-brain barrier, Shikha Nangia, *School of Chemical and Biomolecular Engineering, Cornell University, Ithaca*, NY (September 26, 2016).
- (Oral, Invited) Breaking through the blood-brain barrier, Shikha Nangia, *SyracuseCoE Symposium, Syracuse University, Syracuse*, NY (September 22, 2016).
- (Oral, Invited) Breaking through the blood-brain barrier, Shikha Nangia, *Biomedical Engineering, Binghamton University, Binghamton*, NY (September 20, 2016).
- (Oral, Invited) Breaking through the blood-brain barrier, Shikha Nangia, *Chemical and Biomolecular Engineering, Clemson University, Clemson*, SC (September 15, 2016).
- (Oral, Invited) Multiscale simulations to characterize the blood-brain barrier tight junctions, Shikha Nangia, *2016 Middle Atlantic Regional Meeting MARM, Riverdale, NY* (June 9–12, 2016).
- (Oral, Invited) Engineering nanocarriers for brain tumor treatment, Shikha Nangia and Juntao Luo, *Nappi Research Award Competition, Syracuse University, Syracuse*, NY (December 11, 2015).
- (Oral) Coarse grained parameterization of gram-negative bacterial outer membrane, Shikha Nangia, *AIChE Annual Meeting, Salt Lake City, UT* (November 8–13, 2015).

- (Oral) Multiscale simulations to characterize the blood brain barrier tight junctions, Shikha Nangia, *AIChE Annual Meeting, Salt Lake City, UT* (November 8–13, 2015).
- (Oral, Invited) Insights into the blood brain barrier tight junctions for treatment of Alzheimer's disease, Shikha Nangia, 2015 *West Virginia University*, Morgantown, WV (August 28, 2015).
- (Oral, Invited) Synergistic experimental and multiscale modeling approaches for optimizing anticancer drug nanocarriers, Shikha Nangia, *250th ACS National Meeting, Boston MA* (August 16–20, 2015).
- (Oral) Molecular characterization of the blood brain barrier tight junctions, *Young Investigator Symposium*, Shikha Nangia, *250th ACS National Meeting, Boston MA* (August 16–20, 2015).
- (Oral) Spectroscopic properties of semiconductor quantum dots embedded in biological medium, B. Ellis, W. Jiang, J. Elward, F. J. Irudayanathan, Shikha Nangia, A. Chakraborty, *250th ACS National Meeting, Boston MA* (August 16–20, 2015).
- (Oral, Invited) Multiscale simulations to characterize the blood brain barrier tight junctions, Shikha Nangia, *Neuroscience Research Day*, Syracuse, NY (April 3, 2015).
- (Oral, Invited) Multiscale simulations to characterize the blood brain barrier tight junctions, Shikha Nangia, *Albany 2015: Conversation 19*, Albany, NY (June 9-13, 2015).
- (Oral) Introduction of computational simulations to high school students will increase their STEM knowledge and interest, Suzanne DeTore and Shikha Nangia, *2015 Emerging Researchers National (ERN) Conference in STEM* , Washington, D.C. (February 19-21, 2015).
- (Oral, Invited) Multiscale modeling approach to determine the role of amphiphilic building block in the stability of paclitaxel drug delivery nanocarriers**,** at *AIChE Annual Meeting, Atlanta, GA* (Nov. 16–22, 2014).
- (Oral), Cellular uptake of nanoparticles with protein coronas: A coarse-grained molecular dynamics simulations study, Ayten Ay, Haarika Kamani, Sydney Mendez, and Shikha Nangia, 2014 Emerging Researchers National (ERN) Conference in STEM , Washington, D.C. February 20-22, 2014.
- (Oral, Invited) Effect of protein corona on nanoparticle cellular uptake, at *AIChE Annual Meeting, San Francisco* (Nov. 2-8, 2013).
- (Oral) Effect of nanoparticle shape and charge on cytotoxicity**,** at *AIChE Annual Meeting, Pittsburgh PA* (October 28– Nov. 2, 2012).
- (Oral) Effect of nanoparticle shape and charge on cytotoxicity**,** at *243rd ACS National Meeting, San Diego CA* (March 25–29, 2012).
- (Oral) Viscoelastic properties of bacterial biofilms using coarse-grained molecular dynamics simulations**,** at *AIChE Annual Meeting, Minneapolis MN* (October 16–21, 2011).
- (Oral) Coarse-grained molecular dynamics simulations of bacterial polysaccharides for studying flow-induced fragmentation mechanisms**,** at *241 ACS National Meeting, Anaheim CA* (March 27–31, 2011).
- (Oral, Invited) Theoretical and Computational Modeling of Dissolution Processes, at *SUNY-ESF, Syracuse, NY* (March 11, 2011)
- (Oral, Invited) Computational approaches of modeling dissolution of rocks and evolution of Earth surface, at *Rensselaer Polytechnic Institute, Troy, NY* (Feb. 8–9, 2010)
- (Oral) Dissolution studies of mineral-water interfaces using newly developed Monte Carlo algorithm, at *237th ACS National Meeting, Salt Lake City UT* (March 22–26, 2009).

NEWS AND MEDIA

2019

- "*How Research Enhances Students' Educational Experience"*- https://news.syr.edu/blog/2019/07/25/how-research-enhances-students-educational-experience/

2017

- "*Professors Honored with Prestigious Meredith, Teaching Recognition, Scholar and Teacher Awards*

https://news.syr.edu/2017/05/professors-honored-with-prestigious-meredith-teaching-recognition-and-scholar-and-teacher-awards/

- *"Teaching Awards Program to Honor 10 Faculty"* https://news.syr.edu/2017/04/teaching-awards-program-to-honor-10-faculty/

2016

- "*Nangia Lab's Blood-Brain Barrier Research Recognized at International Conference*"- https://news.syr.edu/2016/10/nangia-labs-blood-brain-barrier-research-recognized-at-international-conference-21801/
- "*Nangia Wins ACS Outstanding Junior Faculty Award*"- http://news.syr.edu/nangia-wins-acs-outstanding-junior-faculty-award-28186/

2015

- "*Nappi Research Competition Awards $650,000 to SU-Upstate Teams"*- http://news.syr.edu/nappi-research-competition-awards-650000-to-su-upstate-teams-73213/
- "Nangia's Bacteria Research Featured in Chemistry Journal"- http://news.syr.edu/nangias-bacteria-research-featured-in-chemistry-journal-13234/
- "*Better Cancer Treatment Through Nanotechnology*"- http://news.syr.edu/better-cancer-treatment-through-nanotechnology-48799/
- "*Nangia Awarded CAREER Grant to Break Barriers in Treating Alzheimer's*"- http://news.syr.edu/nangia-awarded-career-grant-to-break-barriers-in-treating-alzheimers-91343/
- "*@SyracuseU News Tips*"- http://news.syr.edu/syracuseu-news-tips-14251/
- "*Bioengineering Major Earns National Recognition for Research*"- http://news.syr.edu/bioengineering-major-earns-national-recognition-for-research-12813/
- Understanding Thermodynamics — There's an App for That - ""http://eng-cs.syr.edu/college-news/understanding-thermodynamics-theres-an-app-for-that/
- "*Shining a Light on Quantum Dots Measurement*"- http://news.syr.edu/shining-a-light-on-quantum-dots-measurement-79855/
- *"Computer Model Details QD Interaction with Protein,*" *Photonics.com*- http://www.photonics.com/Article.aspx?AID=57091
- *"Shining a light on quantum dots measurement"-phys.org*- http://phys.org/news/2015-01-quantum-dots.html

2013

- "Modifications of a nanoparticle can change chemical interactions with cell membranes"- http://news.syr.edu/modifications-of-a-nanoparticle-can-change-chemical-interactions-with-cell-membranes/
- NSF news- "Modifications of a Nanoparticle Can Change Chemical Interactions With Cell Membranes" https://www.nsf.gov/news/news_summ.jsp?cntn_id=126781

2011

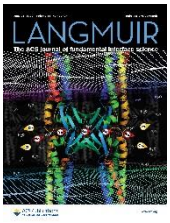
- "*Interdisciplinary team led by Syracuse University wins $2 million EFRI grant from NSF*"- http://news.syr.edu/bacterial-multicellular-systems/

2010

- "*SU researchers utilize computer simulations to explore biofilm fragmentation*"- http://news.syr.edu/biofilms/

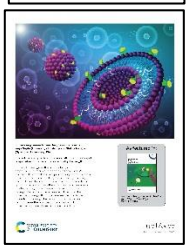
JOURNAL COVERS

2020 Ion transport through the tight junction pores formed by transmembrane claudin proteins between membranes of two adjacent cells. The ion conductance is regulated by the electrostatic environment created by the pore-lining amino acid residues
https://pubs.acs.org/toc/langd5/36/24



2020 Non-canonical lipoproteins with programmable assembly and architecture
https://pubs.rsc.org/en/content/articlelanding/2020/cc/d0cc90384a#!divAbstract

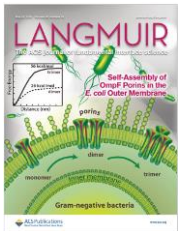
2020 A Tale of Two Tails: Photoactivity through amphiphilicity. We discovered that the liposomal permeability of the coumarin molecule depends on the length of its conjugated-alkyl chain. The short-chain coumarin molecules penetrate the liposomes less effectively than the long-chain molecules. The longer alkyl chains interact favorably with the hydrophobic lipids of the liposomal bilayer, and the molecule undergo flip-flops between the two leaflets. The efficacy of long-chain coumarins in liposomes demonstrates the promise of these amphiphilic molecules as fluorophores in cancer detection.
https://pubs.rsc.org/en/content/articlelanding/2020/cp/d0cp00696c#!divAbstract



2019 The protein association energy landscape (PANEL) method provides an extensive data set of membrane protein association in lipid milieu using a combination of stochastic sampling and equilibration simulations. The results are obtained in a fraction of the simulation cost compared to self-assembly simulations
https://pubs.acs.org/toc/jctcce/15/11

2018 Molecular architecture of the claudin tight junction proteins. The claudin family of transmembrane proteins forms tight junctions between the adjacent cells in epithelial and endothelial tissues. These tight junctions control the transport and permeability of ions and small molecules through the paracellular space. The tight junction permeability is critical in understanding physiological processes such as the blood–brain barrier, renal filtration, ionic hemostasis, and drug transport across tissue barriers. This multiscale dynamics study of classic claudins provides the molecular architecture of the tight junction pores as well as the putative conformation of claudin proteins that acts as a receptor for the Clostridium perfringens enterotoxin.
https://pubs.acs.org/toc/jpcbfk/122/30

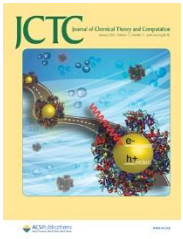
2018 The channel-forming protein OmpF porin from Escherichia coli spans the bacterial outer membrane and facilitates the diffusion-mediated influx of nutrients into the cell. Using molecular dynamics approach, we explore the thermodynamics of OmpF assembly over microsecond timescale simulations, enabled by the newly developed coarse-grain force field parameter set for *E. coli* outer membrane lipids.
https://pubs.acs.org/toc/langd5/34/19



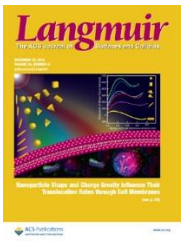
2015 Molecular representation of multilayered Gram-negative bacterial membrane. The cell envelope of Gram-negative bacteria is a complex multilayered structure that, besides gatekeeping chemical transport in and out of the bacterial cell, protects the cell from hostile environments. The image shows an illustrative model of the Gram-negative bacterial membrane with lipopolysaccharide enriched outer membrane, containing O-antigen domains (pink), outer membrane proteins (in green, red, purple, yellow cartoon representation), and the phospholipid (orange and white) inner membrane. Until now, molecular level understanding of the bacterial

membrane, especially over long time scales, has been challenging due to the enormous computational cost associated with molecular simulations of such complex structures. Here, we have developed and benchmarked a coarse grained force field for the lipopolysaccharide macromolecule with O-antigen domain that will enable long timescale molecular simulations of bacterial membranes with fractional computational cost.
https://pubs.acs.org/toc/jpcbfk/119/46

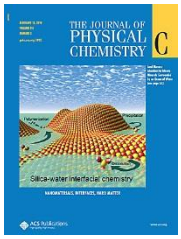
2015 The optical properties of quantum dots are influenced by the presence of surface ligands. Here we investigate the effect of protein corona formation on the optical properties of the firefly Luciferase-CdSe quantum dot complex. To make the computational cost tractable for a large protein-quantum dot system, a multilevel approach was developed where the electronically excited quantum dot was treated quantum mechanically (QM) using electron-hole quasiparticle representation and the protein corona was represented using the molecular mechanics (MM) force field.
https://pubs.acs.org/toc/jctcce/11/1



2012 Concerns of nanotoxicity caused by nanoparticle-cell interactions are becoming increasingly important as the applications of nanoparticles continue to grow. The cover illustrates the interaction of charged cone-, cube-, rod-, rice-, pyramid-, and sphere-shaped nanoparticles with a model cell membrane. High-performance molecular dynamics simulations were employed to calculate the potential of mean force associated with nanoparticle translocation as well as translocation rate constants. The results indicate that the translocation rate can vary greatly based on the particle surface charge and shape. The simulations also unravel a fascinating electrostatics-driven reorientation mechanism of faceted nanoparticles that facilitates instantaneous transport resulting in the disruption of the self-assembly of the membrane lipids
https://pubs.acs.org/toc/langd5/28/51



2010 Land masses abundant in silicate minerals surrounded by an ocean of water. Interfacial silica–water chemistry involves competing dissolution, precipitation, and polymerization reactions. These reactions are ubiquitous on Earth's surface and occur over geological time scales. A new time-independent advanced Monte Carlo algorithm has been developed that provides insight into reaction mechanisms, equilibrium properties, and surface topography. In the present application of this method, the role of intrasurface hydrogen bonding in the dissolution process is explored.
https://pubs.acs.org/toc/jpccck/114/5



2006 Potential Energy Surfaces for Photodissociation of Ammonia through a Conical Intersection Special Issue honoring Donald G. Truhlar, *J. Physical Chemistry A* **110**, (2006).

PEER REVIEW & EDITORIAL ACTIVITIES FOR SCIENTIFIC JOURNALS & FUNDING AGENCIES

2016-2019 Scientific American, Editorial Board Member
2016-2017 PLOS Computational Biology, Guest Editor
2021-present ACS Applied Bio Materials, Associate Editor

Ad hoc review for scientific journals

Annals of New York Academy of Sciences
ACS Nano
ACS Central Science
ACS Macro Letters
Biochemistry
Biomacromolecules
Journal of American Chemical Society
Journal of Chemical Physics
Journal of Physical Chemistry A
Journal of Physical Chemistry B
Journal of Physical Chemistry C
Journal of Chemical Theory and Computation
Journal of Biomolecular Structure & Dynamics
Journal of Nanotechnology
Macromolecules
Molecular Systems Design & Engineering
Nature Nanotechnology
Nanoletters
Langmuir
Scientific American
Plos Computational Biology
Plos ONE

Ad hoc review for funding agencies

2014-2019 Ad-hoc reviewer, ACS PRF program
2014-2020 NSF Panelist
2014-2020 NSF GRFP Panelist

MENTORING AND SUPERVISION OF RESEARCH ACTIVITIES

Graduate Students

2021-persent Faris Amer
2021-persent Simran Karamchandani
2020-present Nelly Raissa Setchie-Tchato
2019-present Mario Pietra
Biocompatibility of Ionic liquids
2019-present Jingjing Ji
Claudin cis and trans assembly
2020-present Patrick Marsch
2020-present Allyson Karmazyn
2019-present Zhenyu Qiu
Effect of palmitoylation on claudin-5 dimerization
2019-2020 Santita Ebangwese, MS
Molecular investigation of tight junction proteins related to the small intestines
2018-2020 Zhenqi Li, MS
Computational models of mitochondrial membrane
2017-present Yinghui Dai
Computational Antibiotic screening platform
2017-present Kathryn Marie Piston
Cancer epigenetics
2016-present Nandhini Rajagopal
Molecular architecture of tight junctions
2013-2020 Flaviyan Jerome Irudayanathan, Ph.D.
Molecular structure of Claudin-5 tight junctions responsible for the blood-brain barrier
2015-2019 Huilin Ma, Ph.D.
Computational modeling of bacterial outer membranes and development of high-throughput screening platform for antibiotics
2012-2016 Wenjuan Jiang, Ph.D.
Stochastic simulations of transport of molecules across the blood-brain barrier
2017-2019 Xichen Xu, MS

Coarse grained parameterization of Gram-positive bacteria cell wall

2017-2018 Lisa Danielle Nguyen, MS

Homotypic and heterotypic self-assembly of Claudin family of tight junction proteins

2017-2018 Amogh Srihari, MS

Statistical Mechanical Treatments of the Optical Properties of CdSe Quantum Dots

2015-2016 Nan Wang, MS

Self-assembly of Claudin Family of Membrane Proteins

2014-2016 Xiaoyi Wang, MS

Designing of anticancer drug delivery nanocarriers using multiscale modeling

2014-2016 Huilin Ma, MS

Coarse grained parameterization of Gram-negative bacteria outer membrane

2012-2013 Haarika Kamani, MS

Effects of protein corona on gold nanoparticle cellular uptake

Undergraduate Students

2021 Nathena Murray
2021 Isabelle Tawyer
2020 Alexis Rose Aquilino
2020 Amelia Gilbert
2020 Ivan Sarbinov
2020 Faris Amer
2019 Aria Atwal
2019 Laurie Mouk
2019-present Victoria Bialczak (ECS Scholar)
2019-present Patrick Matthew Marsch
2019 Caroline Almonte (Syracuse Biomaterials Institute, REU student)
2019 Andreea C Merloiu
2019 Alina Zdebska (ECS Scholar)
2018-2019 Jingzhi Liu
2018-2019 Wenlin He
2018-present Allyson Karmazyn (ECS Scholar)
2018 Naomi Brandt (Syracuse Biomaterials Institute, REU student)
2018 Natalie Marie Petryk (ECS Scholar)
2018 Bailey M Felix (ECS Scholar)
2018-present Alejandro J Durand (ECS Scholar)
2018 Priya S Ganesh (ECS Scholar)
2017-2018 Santita Ebangwese (Bioengineering)
2018 Austin Freer (Chemical Engineering)
2018 Meishan Wu (Chemical Engineering)
2017 Prakash Khare (Bioengineering)
2017 Soor Vora (REU student)
2017 Tori Welch (Syracuse Biomaterials Institute, REU student)
2017 Colleen Marie Cassidy (Bioengineering)
2016 Daniel Cummins (Syracuse Biomaterials Institute, REU student)
2016 Tara Picudella (Chemical Engineering)
2016 Masud Dikita Llewellyn (Chemical Engineering)
2016-2018 Jerry Gomez (Chemical Engineering)

2016	Natalie Edelstein (Bioengineering)(Dean's Leadership Award)
2015-2017	Aliza Khan (Bioengineering)
2014-2016	Sarah R. Willsey (Dean's Leadership Award)
2015	Ian Seddon (Syracuse Biomaterials Institute, REU student)
2014-2015	Alexis N. Peña (REM participant, LSAMP student)
2014	Benjamin Yue (Syracuse Biomaterials Institute, REU student)
2013-2014	Yee-Pien Cheng (Chemical Engineering)
2013-2014	Julie Theresa Hess (REM participant)

High School Students and Teachers

2019	Jamison Jones (student), Oneida High School, Oneida, NY
2018	Jenna Ruzekowicz (student), Fulton High School, Fulton, NY
2018	Alexys Gayne (student), South Jefferson Central School, Jefferson, NY
2016	Yatin Zirath (student), Christian Brothers Academy, DeWitt, NY
2015	Dhruv Thota (student), Jamesville-DeWitt High School, Jamesville, NY
2014	Phillip Falcone (student), East Syracuse-Minoa High School, East Syracuse NY
2014	Suzanne DeTore (teacher) Fowler High School, Syracuse School District, Syracuse NY
2013	Ayten Ay (teacher), Syracuse Academy of Science Charter School, Syracuse NY
2013	Sydney Mendez (teacher), Lincoln Middle l, Syracuse School District, Syracuse NY
2013	Sally Mitchell (teacher), East Syracuse-Minoa High School, East Syracuse NY

TEACHING

2020	CEN 451/651-Chemical Engineering Thermodynamics, *Instructor*
	CEN 353- Chemical Thermodynamics II, *Instructor*
2019	CEN 451/651-Chemical Engineering Thermodynamics, *Instructor*
	CEN 353- Chemical Thermodynamics II, *Instructor*
2018	ECS 326- Engineering Materials, Properties, and Processing, *Instructor*
2017	CEN 353- Chemical Thermodynamics II, *Instructor*
2015-2017	CEN 651-Chemical Engineering Thermodynamics, *Instructor*
2016	CEN 601- BMCE Seminar, *Coordinator*
	CEN 353- Chemical Thermodynamics II, *Instructor*
2015	CEN 651-Chemical Engineering Thermodynamics, *Instructor*
	CEN 353- Chemical Thermodynamics II, *Instructor*
2014	CEN 651-Chemical Engineering Thermodynamics, *Instructor*
	CEN 353- Chemical Thermodynamics II, *Instructor*
	CEN 600- Multiscale computation methods, *Co-instructor*
2013	CEN 651-Chemical Engineering Thermodynamics, *Instructor*
	CEN 353- Chemical Thermodynamics II, *Instructor*
2012	CEN 651-Chemical Engineering Thermodynamics, *Instructor*
	CHE 106- General Chemistry Lecture I, *Instructor*
	CHE 107- General Chemistry Laboratory I, *Instructor*
	CHE 116- General Chemistry Lecture II, *Instructor*
	CHE 117- General Chemistry Laboratory II, *Instructor*
2011	CEN 600- Multiscale computation methods, *Co-instructor*
	CHE 106- General Chemistry Lecture I, *Instructor*
	CHE 107- General Chemistry Laboratory I, *Instructor*
	CHE 116- General Chemistry Lecture II, *Instructor*
2010	CHE 117- General Chemistry Laboratory II, *Instructor*

CHE 106- General Chemistry Lecture I, *Instructor*
CHE 107- General Chemistry Laboratory I, *Instructor*
CHE 116- General Chemistry Lecture II, *Instructor*
CHE 117- General Chemistry Laboratory II, *Instructor*

ADDITIONAL TEACHING TRAINING

2019 *Participant*, Course Redesign Working Group, a group to redesign the College of engineering
2018 *Participant*, Inclusive Teaching Workshop, College of ECS, Syracuse University
2018 *Participant*, Inclusive Excellence Training, College of ECS, Syracuse University
2017 *Participant*, ASEE Summer School for Chemical Engineering Faculty, *Raleigh*, NC State University (July 29-Aug. 3)
Participant, Summer Institute for Technology-Enhanced Teaching & Learning (SITETL), training program for faculty members to incorporate technology in their
2017 classes
Participant, Gateway Redesign Working Group, a group to redesign the College of
2017 engineering gateway classes to enhance active learning.
Participant, "How to Engineer Engineering Education", a 3-day hands-on summer
2014 workshop to obtain formal training in educational theory and pedagogical practices
Participant, "Intro to Process-Oriented Guided Inquiry Learning (POGIL) Workshop"
2014 aimed to explore the benefits of this approach to active learning in the classroom

ACADEMIC SERVICE

2020 *Panelist*, NSF and NSF GRFP
2020 *Chair*, Modeling of Lipid Membranes and Membrane Proteins, 2020 Virtual AIChE Annual Meeting (November 16-20)
2020 *Member*, Committee on Export Control, Syracuse University
2019 *Chair*, Modeling of Lipid Membranes and Membrane Proteins, 2019 AIChE Annual Meeting, Orlando (November 10-15)
2019 *Executive Committee Member*, BioInspired Syracuse: Institute for Material and Living Systems
2019 *Member*, Chemistry Faculty Search Committee
2019 *Member*, College of Engineering and Computer Science Dean's Search Committee
2019 *Organizer*, Molecular engineering of soft matter: Spanning small molecules to
2019 macromolecules, Telluride Science Research Center, Telluride, CO (June 16-June 21)
2019 *Chair*, Non-tenured Faculty Review Committee, BMCE, Syracuse University
2018 *Member*, Meredith Teaching Award Selection Committee, Syracuse University
2018 *Member*, BMCE Faculty Search Committee
2018 *Member*, WiSE FPP Advisory Board, Syracuse University
2018 *Member*, Committee on Export Control, Syracuse University
2018 *Panelist*, NSF Biological and Environmental Interactions of Nanoscale Materials
2018 *Panelist*, NSF Interfacial transport
2018 *Chair*, Modeling of Lipid Membranes and Membrane Proteins, 2018 AIChE Annual
2018 Meeting, Minneapolis (October 28-November 2)
2017 *Chair*, 4th Annual Neuroscience Day, Syracuse University, Syracuse (April 6, 2018)
Organizer, Molecular engineering of soft matter: Spanning small molecules to
2017 macromolecules, Telluride Science Research Center, Telluride, CO (June 20-June 24)
2017 *Chair*, Modeling of Lipid Membranes and Membrane Proteins, 2017 AIChE Annual Meeting, Minneapolis (October 29-Novermber 3)
2017 *Organizer*, 3rd Annual Neuroscience Day, Syracuse University, Syracuse (April 7, 2017)
2016-2018 *Member*, ECS Faculty Council, Syracuse University
2016

2016	*Chair*, Development of Intermolecular Potential Models, 2016 AIChE Annual Meeting,
2016	San Francisco (November 13-18).
2016	*Chair*, Biomimetic and Biohybrid Materials and Devices, 2016 AIChE Annual Meeting, San Francisco (November 13-18)
2015	*Panelist*, New Faculty Orientation Program, Syracuse University
2015	*Panelist*, NSF Particulate and Multiphase Processes panel on interfacial phenomena (February 9-10)
2015	*Member*, Department of Biomedical and Chemical Engineering Faculty Search Committee
2015	*Co-chair*, Biomimetic and Biohybrid Materials and Devices, 2015 AIChE Annual Meeting, Salt Lake City, UT
2015	*Panelist*, New Faculty Orientation Program, Syracuse University
2015-2017	*Member*, Department of Psychology Faculty Search Committee
2014-present	*Coordinator*, Biomedical and Chemical Engineering Department Seminar Series
2014	*Presenter*, workshop sponsored by Women in Science and Engineering (WiSE)
2014	*Member*, Neuroscience Executive Committee
2014-2018	*Member*, Department of Physics Faculty Search Committee. *Emphasis on Experimental soft matter physics*
2013-2017	*Member*, Graduate Admissions Committee, Department of Biomedical and Chemical Engineering
2012	*Member*, BMCE faculty representative for College of engineering and computer science website committee
2012-2016	*Member*, Soft Interfaces IGERT @ SU Graduate Recruitment Committee
2014	*Website coordinator*, Department of Biomedical and Chemical Engineering
2014	*Co-chair*, Biomimetic and Biohybrid Materials and Devices I and II, 2014 AIChE Annual Meeting, Atlanta, GA
2013	*Presente*r, workshop sponsored by Women in Science and Engineering (WiSE)
2013	*Member*, 39th Annual Northeast Bioengineering Conference Program Committee
2013	*Reviewer*, Women in Science and Engineering–Future Professoriate Program (WiSE–FPP)
2012-2013	Soft Interfaces IGERT @ SU Graduate Admissions Committee
2013	*Member*, Department of Biomedical and Chemical Engineering Faculty Search Committee,
2013	*Member*, Department of Biology and Chemistry Faculty Search Committee
2013	*Co-chair*, Biomimetic and Biohybrid Materials and Devices I and II, 2013 AIChE Annual Meeting, San Francisco, CA
2013	*Session chair*, 39th Annual Northeast Bioengineering Conference, Syracuse
	Member, Department of Chemistry Faculty Search Committee

BROADER IMPACT AND OUTREACH

2020	Virtual Cohort-based Research Experience for 7 undergraduate students
2019	Mentored high school student- ECS High School Research Internship Program
2018	Mentored high school student- ECS High School Research Internship Program
2016	Mentored two high school females in computational modeling-ECS Research Internship Program
2015	Mentored one high school student on computational modeling
2014-2015	Project ENGAGE Instructor, Syracuse University
2014	Mentored three high school student on hands-on multiscale molecular dynamics simulations
2013	Mentored, high-school teacher as part of the Research Experience and Mentoring (REM) program
2011-2012	Mentored, high-school teacher as part of the EFRI-REM program

Organized 3-day workshop for local high school students and teachers training on computers in chemistry