

# Shikha Nangia

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## EDUCATION

University of Minnesota, Twin Cities	Chemistry	PhD, 2006
Indian Institute of Technology, New Delhi, India	Chemistry	MS, 2000
University of Delhi, Delhi, India	Chemistry	BS, 1998

## 1 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 Director, Bioengineering Graduate Program, Department of Biomedical and Chemical Engineering, *Syracuse University*

2021-present Director, NSF REU Site: *Interactive Biomaterials*  
*Syracuse University*

2022-present Director, ESTEEMED LEADERS program  
*Syracuse University*

2014-present Member, Interdisciplinary Neuroscience Studies  
*Syracuse University*

2019-present Member, BioInspired Institute  
*Syracuse University*

2018-2021 Co-Director, NSF REU Site: *Interactive Biomaterials*  
*Syracuse University*

2012-2018 Assistant Professor, Department of Biomedical and Chemical Engineering  
*Syracuse University*

2009-2012 Research Professor, Department of Biomedical and Chemical Engineering  
*Syracuse University*

2006-2009 Postdoctoral Researcher, Department of Chemistry  
*Pennsylvania State University*

## 2 HONORS AND AWARDS

2022 Excellence in Graduate Education Faculty Recognition Award, *Syracuse University*

2022 Rising Star Award, *American Chemical Society (ACS) Women Chemist Committee*

2020 Scialog Fellow, *Research Corporation for Science Advancement*

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, *Nappi Family Foundation*  
 2015 CAREER Award, *National Science Foundation*  
 2015 Faculty Excellence Award, *College of Engineering, Syracuse University*

## **2.1 Honors and Awards to Undergraduate and Graduate Mentees**

2022 All University Master's prize, Syracuse University, X. Qin (G)  
 2021 All University Doctoral prize, Syracuse University, N. Rajagopal (G)  
 2021 First place poster, 5<sup>th</sup> Annual Neuroscience Day, Syracuse University, N. Rajagopal (G)  
 2021 Remembrance Scholar, Syracuse University, N. Murray (UG)  
 2021 All University Master's prize, Syracuse University, A. Karmazyn (G)  
 2021 Merck Research Award, Women Chemists Committee, ACS, N. Rajagopal (G)  
 2021 Bioengineering Graduate Student Award, Syracuse University, N. Rajagopal (G)  
 2021 Second place Research Talk, ECS Research Day, Syracuse University, N. Rajagopal (G)  
 2020 The Chemical Computing Group Excellence Award for Graduate Students, ACS, N. Rajagopal (G)  
 2020 First Place, ECS Research Day Pitch Competition, Syracuse University, K. Piston (G)  
 2020 Best poster, ECS Research Day, Syracuse University, K. Piston (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 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, 4<sup>th</sup> 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, N. 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, 3<sup>rd</sup> 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, ACS, 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 Biomedical & Chemical Engineering (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)

### 3 PUBLICATIONS

1. Unique structural features of claudin-5 and claudin-15 lead to functionally distinct tight junction strand architecture, N. Rajagopal and **S. Nangia**, *Annals of the New York Academy of Sciences* (2022). <https://doi.org/10.1111/nyas.14891>
2. Joint profile characteristics of long-latency transient evoked and distortion otoacoustic emissions, D. Pacheco, N. Rajagopal, B. Prieve, and **S. Nangia**, *American Journal of Audiology*, 31 (2022). [https://doi.org/10.1044/2022\\_AJA-21-00182](https://doi.org/10.1044/2022_AJA-21-00182)
3. Salt Destabilization of Cationic Colistin Complexation within Polyanionic Microgels, X. Xiao, J. Ji, W. Zhao, **S. Nangia**, and M. Libera, *Macromolecules* 55, 1736–1746 (2022). <https://doi.org/10.1021/acs.macromol.1c02157>
4. Adaptive Recombinant Nanoworms from Genetically Encodable Star Amphiphiles, Md. S. Hossain, J. Ji, C. Lynch, M. Guzman, **S. Nangia**, and D. Mozhdehi, *Biomacromolecules* 23, 3, 863-876 (2022). *Featured on the cover.* <https://doi.org/10.1021/acs.biomac.1c01314>
5. Persister control by leveraging dormancy associated reduction of antibiotic efflux, S. Roy, A. A. Bahar, H. Gu, **S. Nangia**, K. Sauer, D. Ren, *PLOS pathogens*, 17, e1010144 (2021). <https://doi.org/10.1371/journal.ppat.1010144>
6. 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>
7. High-Level Antibiotic Tolerance of a Clinically Isolated *Enterococcus faecalis* Strain, H. Gu, S. Roy, X. Zheng, T. Gao, H. Ma, Z. Sultana, C. Fortner, **S. Nangia**, D. Ren, *Chemical Communications Applied and Environmental Microbiology*, 87, 10281-10284 (2020). <https://doi.org/10.1128/AEM.02083-20>
8. Non-canonical lipoproteins with programmable assembly and architecture, Md S. Hossain, I. C. Maller, Y. Dai, **S. Nangia**, and D. Mozhdehi, *Chemical Communications*, 56, 10281-10284 (2020). *Featured on the cover.*

<https://doi.org/10.1039/D0CC03271A>

9. 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). *Featured on the cover.*  
<https://doi.org/10.1021/acs.langmuir.0c00877>
10. 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>
11. Rational identification and characterization of peptide ligands for targeting polysialic acid, D. G. Shastri, 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>
12. 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>
13. 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>
14. 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>
15. 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>
16. 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>
17. 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>
18. 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>
19. 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.jpcc.8b09535>
20. 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>
21. 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.jpcc.8b03842>

22. 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>
23. 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>
24. 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*, **1405**, 131–146 (2017). <http://dx.doi.org/10.1111/nyas.13378>
25. 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>
26. 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.jpcc.6b06070>
27. 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.jpcc.5b09977>
28. 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>
29. 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.jpcc.5b07122>
30. 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>
31. 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>
32. 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>
33. 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>
34. 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>
35. 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>

36. 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>
37. 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>
38. 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>
39. 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>
40. 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>
41. 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>
42. 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>
43. 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>
44. A new form of MgTa<sub>2</sub>O<sub>6</sub> 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>
45. 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>
46. 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>
47. 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>
48. 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>

#### 4 CONFERENCE PAPERS AND OTHER INDEXED JOURNAL PUBLICATIONS

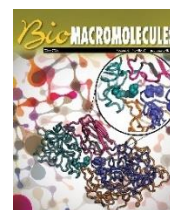
1. Peer mentoring for women in STEM, A. Rauh, M. Blum, N. Russo, M. A. Green, and **S. Nangia**, *ASEE Annual Conference and Exposition, Conference Proceedings*, 1087, (2020).
2. Multiscale simulations to characterize the blood brain barrier tight junctions, F.J. Irudayanathan, **S. Nangia** *Journal 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,<sup>†</sup> 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](https://arxiv.org/abs/1104.4601)

#### 5 JOURNAL COVERS

2022

Protein nanoworms are promising candidates for nanomedicine, biotechnology, and synthetic biology, but their promise is constrained by their narrow stability regimes. By integrating experiments, simulations, and data analytics, this study presents a new class of recombinant amphiphiles, post-translationally modified star-shaped lipoproteins, that form adaptive nanoworms with low polydispersity over a broad operational window and reveal their molecular design principles.

<https://pubs.acs.org/toc/bomaf6/23/3>



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

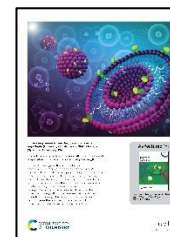
<https://pubs.rsc.org/en/content/articlelanding/2020/cc/d0cc90384a#!divAbstract>




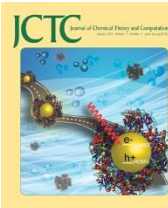




2020

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.  
<https://pubs.acs.org/toc/jpcbfc/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.  
<https://pubs.acs.org/toc/jpcbfc/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 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. The results indicate that the translocation rate can vary greatly based on the particle surface charge and shape.  
<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.  
<https://pubs.acs.org/toc/jpcck/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).



## 6 PRESENTATIONS

- (Oral, Invited) Engineering Pathways across Biological Barriers to treat Alzheimer's Disease, Shikha Nangia, *University of Notre Dame* (January 31, 2023).
- (Oral, Invited) Treating Alzheimer's Disease: A molecular challenge, Shikha Nangia, *Stevens Institute of Technology* (October 21, 2022).
- (Oral, Invited) Molecular challenges to treating Alzheimer's disease, Shikha Nangia, *Northeast Regional Meeting (NERM)* (October 2-5, 2022).
- (Oral, Invited) Treating Alzheimer's Disease: A molecular challenge, Shikha Nangia, *ACS Spring Meeting, San Diego* (March 22, 2022).
- (Oral, Invited, Keynote) Treating Alzheimer's Disease: A molecular challenge, Shikha Nangia, 21<sup>st</sup> annual MERCURY conference, July 19-21, 2023.
- (Oral, Invited) New Breakthrough in blood-brain barrier tight junctions, Shikha Nangia, *Foundations of Molecular Modeling and Simulation (FOMMS)*, Lake Lawn Resort in Delavan, WI (July 17-21, 2022).
- (Oral, Invited) Treating Alzheimer's Disease: A molecular challenge, Shikha Nangia, *ACS Spring Meeting, San Diego* (March 22, 2022).
- (Oral, Invited, Virtual) Antibiotics: Friend or Foes? Shikha Nangia, *Ramjas College, University of Delhi, India* (November 10, 2021).
- (Oral, Invited, Virtual) New Breakthrough in blood-brain barrier tight junctions, Shikha Nangia, *Eli Lilly* (March 3, 2021).
- (Oral, Invited, Virtual) Engineering Pathways across Biological Barriers, Shikha Nangia, *Ohio University* (October 18, 2021).
- (Oral, Invited, Virtual) Rags to Riches: Using Cancer's Secrets to Design Advanced Nanomaterials, Shikha Nangia, *BioInspired Institute for Materials and Living Systems, Syracuse, NY* (March 2, 2021).
- (Oral, Invited) New Breakthrough in blood-brain barrier tight junctions, Shikha Nangia, 4<sup>th</sup> *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 junction interface, Shikha Nangia, 256<sup>th</sup> *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, *250<sup>th</sup> ACS National Meeting, Boston MA* (August 16–20, 2015).
- (Oral) Molecular characterization of the blood brain barrier tight junctions, *Young Investigator Symposium*, Shikha Nangia, *250<sup>th</sup> 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, *250<sup>th</sup> 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 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 *243<sup>rd</sup> 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 *237<sup>th</sup> ACS National Meeting, Salt Lake City UT* (March 22–26, 2009).

## 7 CITATION METRICS - BASED ON GOOGLE SCHOLAR

Papers published	Total citations	h-index	i10-index
49	1971	21	32

## 8 RESEARCH AWARDS

<b>NIH NIBIB</b>	\$1,206,932
PI	Recommended
<i>ESTEEMED LEARNING and Discovery through Engineering Research at Syracuse (LEADERS)</i>	
<b>NSF REU Site</b>	\$354,683 (total)
PI	9/1/2021- 8/30/2024
<i>Interactive Biomaterials: REU Site</i>	
<b>NIH R01</b>	\$348,000 (total)
Co-Investigator	9/1/2019- 8/31/2022
<i>Defining the Molecular Architecture for Transmembrane Acylation by a Membrane Bound O-Acyltransferase</i>	
<b>NSF Engineering Research Center Planning Grant</b>	\$100,000 (total)
Co-PI	9/1/2019- 8/31/2020
<i>Planning Grant: Engineering Research Center for Innovative Materials and Processes for Antimicrobial Control Technologies (IMPACT)</i>	
<b>CUSE Grant</b>	20,000 (total)
PI	\$20,000
<i>Cancer epigenetics: Molecular and structural interplay of histone modifications</i>	3/1/2019- 4/31/2021
<b>CUSE Grant</b>	\$30,000 (total)
Co-PI	\$10,000
<i>Bringing a membrane enzyme into structural focus: Interdisciplinary computational-biochemical modeling of ghrelin O-acyltransferase</i>	5/1/2018- 4/31/2020
<b>NSF CBET Award</b>	\$321,000 (total)
Co-PI	\$62,769
<i>Integrating synthetic biology approaches with patterned biofilm formation to investigate bacterial persistence in heterogeneous</i>	7/15/2017- 7/14/2020
<b>NSF REU</b>	\$318,863 (total)
Co-PI	5/1/2018 - 4/30/2021
<i>Interactive Biomaterials: REU Site</i>	
<b>NIH R21</b>	\$213,000 (total)
Co-Investigator	\$74,000
<i>Rational Design and High Throughput Synthesis of Nanocarriers for Efficient Drug Delivery</i>	8/1/2015 - 7/31/2017
<b>NSF CAREER</b>	\$530,000 (total)
PI	\$530,000
<i>Enabling Transport Across the Blood-Brain Barrier by Engineering Thermodynamically Favorable Pathways</i>	4/1/2015 - 3/31/2020
<b>NSF REU Site</b>	\$297,506 (total)
Senior Personal	5/1/2015 - 4/30/2018
<i>Interactive Biomaterials: REU Site</i>	

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

### **8.1 Computer Allocation Awards**

<b>XSEDE Supercomputer Allocation MCB140216 (renewal)</b>	1.3 million hours
PI	(equivalent to \$27,052)

Multiscale Molecular Modeling of the Biomolecular Interfaces for Enhancing Drug Delivery and Designing Antimicrobial Peptides

<b>Anton2 (PSCA18067P)</b>	120,000 Units
PI	12/7/2018 –11/30/2019

Role of S-Palmitoylation on the Blood-Brain Barrier Tight Junction Interface

<b>Anton2 (PSCA17073P)</b>	100,000 Units
PI	12/7/2017 –11/30/2018

Role of S-Palmitoylation on the Blood-Brain Barrier Tight Junction Interface

<b>XSEDE Supercomputer Allocation MCB140216 (renewal)</b>	2.9 million hours
PI	(equivalent to \$65,006)

Multiscale Molecular Modeling of the Biomolecular Interfaces for Enhancing Drug Delivery and Designing Antimicrobial Peptides

7/1/2017 –6/30/2018

<b>XSEDE Supercomputer Allocation MCB140216</b>	1.3 million hours
PI	(equivalent to 46,267.71)

Multiscale Molecular Modeling of the Biomolecular Interfaces for Enhancing Drug Delivery and Designing Antimicrobial Peptides

10/01/2015 –09/30/2016

## **9 RESEARCH ADVISING AND MENTORING**

### **9.1 Graduate Students**

2022–	Britnie Jean Carpentier
2022–	Xuyang Qin
2021–	Faris Amer
2020–2022	Nelly Raissa Setchie-Tchato, MS <i>Discrepancy In the Biophysical Properties of Trophoblast Placental Plasma Membrane Between First and Third Trimester</i>
2020–	Patrick Marsch
2019–	Jingjing Ji
2019–2021	Allyson Karmazyn, MS <i>Computational investigation of biological membranes</i>
2020–2021	Xuyang Qin, MS <i>Depth of S-palmitoylated Cysteines on the Transmembrane protein governs palmitoylation-induced changes in protein-lipid interface</i>
2019–2020	Zhenyu Qiu, MS

2019–2020	<i>Effect of palmitoylation on claudin-5 dimerization</i> Patrick Marsch, MS
2019–2020	<i>Predicating Tight Junction Formation via Claudin Chimeras</i> Santita Ebangwese, MS
2018–2020	<i>Molecular investigation of tight junction proteins related to the small intestines</i> Zhenqi Li, MS
2017–2022	<i>Computational models of mitochondrial membrane</i> Kathryn Marie Piston, Ph.D.
2017–2021	<i>Atomistic investigation of nucleosomal h3 histone tail in unmodified and epigenetically modified states</i> Yinghui Dai, Ph.D.
2016–2021	<i>Computational Antibiotic screening platform</i> Nandhini Rajagopal, Ph.D.
2013–2020	<i>Molecular architecture of tight junctions</i> Flaviyan Jerome Irudayanathan, Ph.D.
2015–2019	<i>Molecular structure of Claudin-5 tight junctions responsible for the blood-brain barrier</i> Huilin Ma, Ph.D.
2012–2016	<i>Computational modeling of bacterial outer membranes and development of high-throughput screening platform for antibiotics</i> Wenjuan Jiang, Ph.D.
2017–2019	<i>Stochastic simulations of transport of molecules across the blood-brain barrier</i> Xichen Xu, MS
2017–2018	<i>Coarse grained parameterization of Gram-positive bacteria cell wall</i> Lisa Danielle Nguyen, MS
2017–2018	<i>Homotypic and heterotypic self-assembly of Claudin family of tight junction proteins</i> Amogh Srihari, MS
2015–2016	<i>Statistical Mechanical Treatments of the Optical Properties of CdSe Quantum Dots</i> Nan Wang, MS
2014–2016	<i>Self-assembly of Claudin Family of Membrane Proteins</i> Xiaoyi Wang, MS
2014–2016	<i>Designing of anticancer drug delivery nanocarriers using multiscale modeling</i> Huilin Ma, MS
2012–2013	<i>Coarse grained parameterization of Gram-negative bacteria outer membrane</i> Haarika Kamani, MS
	<i>Effects of protein corona on gold nanoparticle cellular uptake</i>

## 9.2 Undergraduate Students

2021–2022	Britnie Jean Carpentier
2021–2022	Nathena Murray
2021	Isabelle Tawyer
2021	Mae Martel
2020	Alexis Rose Aquilino
2020	Amelia Gilbert
2020	Ivan Sarbinov

2020	Faris Amer
2019	Aria Atwal
2019	Laurie Mouk
2019	Victoria Bialczak (ECS Scholar)
2019	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
2018–2021	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	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	Tory 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 (Research Experience and Mentoring (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)

### **9.3 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 I, Syracuse School District, Syracuse NY
2013	Sally Mitchell (teacher), East Syracuse-Minoa High School, East Syracuse NY

#### 9.4 Broader Impacts 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 students on hands-on multiscale molecular dynamics simulations
2014	Mentored, high school teacher as part of the REM program
2013	Mentored, high school teacher as part of the EFRI-REM program
2011-2012	Organized 3-day workshop for local high school students and teachers training on computers in chemistry

#### 10 TEACHING

2022	CEN 451/651-Chemical Engineering Thermodynamics, <i>Instructor</i> ECS 326- Engineering Materials, Properties, and Processing, <i>Instructor</i>
2021	ECS 326- Engineering Materials, Properties, and Processing, <i>Instructor</i>
2020	CEN 451/651-Chemical Engineering Thermodynamics, <i>Instructor</i> CEN 353- Chemical Thermodynamics II, <i>Instructor</i>
2019	CEN 451/651-Chemical Engineering Thermodynamics, <i>Instructor</i> CEN 353- Chemical Thermodynamics II, <i>Instructor</i>
2018	ECS 326- Engineering Materials, Properties, and Processing, <i>Instructor</i>
2017	CEN 353- Chemical Thermodynamics II, <i>Instructor</i>
2015-2017	CEN 651-Chemical Engineering Thermodynamics, <i>Instructor</i>
2016	CEN 601- BMCE Seminar, <i>Coordinator</i> CEN 353- Chemical Thermodynamics II, <i>Instructor</i>
2015	CEN 651-Chemical Engineering Thermodynamics, <i>Instructor</i> CEN 353- Chemical Thermodynamics II, <i>Instructor</i>
2014	CEN 651-Chemical Engineering Thermodynamics, <i>Instructor</i> CEN 353- Chemical Thermodynamics II, <i>Instructor</i> CEN 600- Multiscale computation methods, <i>Co-instructor</i>
2013	CEN 651-Chemical Engineering Thermodynamics, <i>Instructor</i> CEN 353- Chemical Thermodynamics II, <i>Instructor</i>
2012	CEN 651-Chemical Engineering Thermodynamics, <i>Instructor</i> CHE 106- General Chemistry Lecture I, <i>Instructor</i> CHE 107- General Chemistry Laboratory I, <i>Instructor</i> CHE 116- General Chemistry Lecture II, <i>Instructor</i> CHE 117- General Chemistry Laboratory II, <i>Instructor</i>
2011	CEN 600- Multiscale computation methods, <i>Co-instructor</i> CHE 106- General Chemistry Lecture I, <i>Instructor</i> CHE 107- General Chemistry Laboratory I, <i>Instructor</i> CHE 116- General Chemistry Lecture II, <i>Instructor</i>
2010	CHE 117- General Chemistry Laboratory II, <i>Instructor</i> CHE 106- General Chemistry Lecture I, <i>Instructor</i> CHE 107- General Chemistry Laboratory I, <i>Instructor</i>



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

### 10.1 Professional Development in Teaching

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

## 11 TEACHING AWARDS

<b>Faculty Excellence Award, Syracuse University</b>	\$17,000
Enhancing the Teaching and Learning of Chemical Thermodynamics using Active-Learning Pedagogies	5/1/2015 –4/31/2016
<b>Teaching Recognition Award, Meredith Professors</b>	\$3,000
	8/1/2017 –5/15/2018

## 12 ACADEMIC SERVICE

2022	<i>Co-chair</i> , 2024 Foundations of Molecular Modeling and Simulation (FOMMS) meeting. TBA
2022	<i>Co-chair</i> , Spotlights in Thermodynamics and Computational Molecular Science, <i>AIChE Annual Meeting</i>
2021-present	<i>Chair</i> , Frontiers of Molecular Thermodynamics, 2021 <i>AIChE Annual Meeting</i> , Boston, MA
2021	<i>Team Leader</i> , Remembrance Scholar Program Committee, Syracuse University
2020	<i>Member</i> , Search Committee for the Associate Dean of Student Affairs, College of Engineering and Computer Science
2020	<i>Panelist</i> , NSF and NSF GRFP
2020	<i>Chair</i> , Modeling of Lipid Membranes and Membrane Proteins, 2020 Virtual <i>AIChE Annual Meeting</i> (November 16-20)
2020	<i>Member</i> , <i>Committee on Export Control</i> , Syracuse University
2019-2021	<i>Member</i> , Financial Conflict of Interest Committee, Syracuse University
2019	<i>Chair</i> , Modeling of Lipid Membranes and Membrane Proteins, 2019 <i>AIChE Annual Meeting</i> , Orlando (November 10-15)
2019	<i>Executive Committee Member</i> , BioInspired Syracuse: Institute for Material and Living Systems
2019	<i>Member</i> , Chemistry Faculty Search Committee
2019	<i>Member</i> , College of Engineering and Computer Science Dean's Search Committee

2019 *Organizer*, Molecular engineering of soft matter: Spanning small molecules to macromolecules, Telluride Science Research Center, Telluride, CO (June 16-June 21)

2019 *Chair*, Non-tenured Faculty Review Committee, BMCE, Syracuse University

2019 *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 Meeting, Minneapolis (October 28-November 2)

2018 *Chair*, 4<sup>th</sup> Annual Neuroscience Day, Syracuse University, Syracuse

2018 *Organizer*, Molecular engineering of soft matter: Spanning small molecules to 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-November 3)

2017 *Organizer*, 3<sup>rd</sup> Annual Neuroscience Day, Syracuse University, Syracuse (April 7, 2017)

2017 *Member*, ECS Faculty Council, Syracuse University

2016 *Chair*, Development of Intermolecular Potential Models, 2016 AIChE Annual Meeting, San Francisco (November 13-18).

2016 *Chair*, Biomimetic and Biohybrid Materials and Devices, 2016 AIChE Annual Meeting, San Francisco (November 13-18)

2016 *Panelist*, New Faculty Orientation Program, Syracuse University

2016 *Panelist*, NSF Particulate and Multiphase Processes panel on interfacial phenomena (February 9-10)

2016 *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 *Member*, Department of Psychology Faculty Search Committee

2015 *Coordinator*, Biomedical and Chemical Engineering Department Seminar Series

2015 *Presenter*, workshop sponsored by Women in Science and Engineering (WiSE)

2015 *Member*, Neuroscience Executive Committee

2015-2017 *Member*, Department of Physics Faculty Search Committee. *Emphasis on Experimental soft matter physics*

2014 *Member*, Graduate Admissions Committee, Department of Biomedical and Chemical Engineering

2014 *Member*, BMCE faculty representative for College of engineering and computer science website committee

2014 *Member*, Soft Interfaces IGERT @ SU Graduate Recruitment Committee

2014-2018 *Website coordinator*, Department of Biomedical and Chemical Engineering

2013-2017 *Co-chair*, Biomimetic and Biohybrid Materials and Devices I and II, 2014 AIChE Annual Meeting, Atlanta, GA

2012 *Presenter*, workshop sponsored by Women in Science and Engineering (WiSE)

2012-2016 *Member*, 39<sup>th</sup> Annual Northeast Bioengineering Conference Program Committee

2014 *Reviewer*, Women in Science and Engineering–Future Professoriate Program (WiSE–FPP)

2014	Soft Interfaces IGERT @ SU Graduate Admissions Committee
2013	<i>Member</i> , Department of Biomedical and Chemical Engineering Faculty Search Committee,
2013	<i>Member</i> , Department of Biology and Chemistry Faculty Search Committee
2013	<i>Co-chair</i> , Biomimetic and Biohybrid Materials and Devices I and II, 2013 AIChE Annual Meeting, San Francisco, CA
2013	<i>Session chair</i> , 39th Annual Northeast Bioengineering Conference, Syracuse
2013	<i>Member</i> , Department of Chemistry Faculty Search Committee

## 13 PROFESSIONAL SERVICE

### 13.1 Editorial Activities

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

### 13.2 Ad hoc Reviewer for Scientific Journals

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

### 13.3 Ad hoc Merit Reviewer for Funding Agencies

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

## 14 NEWS AND MEDIA

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2010	“SU researchers utilize computer simulations to explore biofilm fragmentation” - <a href="https://news.syr.edu/blog/2010/09/20/biofilms/">https://news.syr.edu/blog/2010/09/20/biofilms/</a>
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