Shikha Nangia

Professor and Interim Chair
Department of Biomedical and Chemical Engineering
College of Engineering and Computer Science
BioInspired Institute
343 Link Hall, Syracuse University, Syracuse NY 13244

(315) 443-0571 (o)
snangia@syr.edu
http://www.shikha.org

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

2024-present	Interim Chair, Department of Biomedical and Chemical Engineering *Syracuse University*
2023-present	Professor, Department of Biomedical and Chemical Engineering *Syracuse University*
2021-present	Associate Editor, ACS Applied Bio Materials *American Chemical Society*
2023-present	Member, ACS Board Standing Committee on the Petroleum Research Fund (PRF) *American Chemical Society*
2020-present	Director, Bioengineering Graduate Program, Department of Biomedical and Chemical Engineering, S*yracuse University*
2021-present	Director, NSF REU Site: *Interactive Biomaterials* *Syracuse University*
2022-present	Director, ESTEEMED LEADERS program *Syracuse University*
2019-present	Member, BioInspired Institute *Syracuse University*
2014-2023	Member, Interdisciplinary Neuroscience Studies *Syracuse University*
2018-2023	Associate Professor, Department of Biomedical and Chemical Engineering *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

2023 Winner, On My Own Time competition, *Syracuse University*
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 and Computer Science, 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 and Computer Science, Syracuse University*

2.1 Honors and Awards to Undergraduate and Graduate Mentees

2024 Chancellor's Award for Excellence in Student Research, J. Ji (G)
2024 All University Master's prize, Syracuse University, A. Wadurkar (G)
2024 Outstanding Graduate Student Award, Syracuse University, J. Ji (G)
2024 Graduate Dean's Award, Syracuse University, J. Ji (G)
2023 All University Master's prize, Syracuse University, B. Carpentier (G)
2022 All University Master's prize, Syracuse University, X. Qin (G)
2022 All University Doctoral prize, Syracuse University, N. Rajagopal (G)
2021 First place poster, 5th 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, 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, 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, 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, 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. Biophysics of claudin proteins in tight junction architecture: three decades of progress. P. Marsch, N. Rajagopal, and **S. Nangia**. Biophysical Journal (2024). https://doi.org/10.1016/j.bpj.2024.06.010
2. Lipidation alters the phase-separation of resilin-like polypeptides. Z. Zhang, J. Ji, MS Hossain, B. Bailey, S. Nangia, and D. Mozhdehi. Soft Matter, **20**, 4007-4014 (2024). https://doi.org/10.1016/j.bpj.2024.06.010
3. ZO-2 modulates JAM-A and γ-actin junctional recruitment, apical membrane and tight junction tension, and cell response to substrate stiffness and topography. D. C. Pinto-Dueñas, C. Hernández-Guzmán, P. Marsch, A. Wadurkar, D. Martín-Tapia, L. Alarcón, G. Vázquez-Victorio, J. V. Méndez-Méndez, J. J. Chanona-Pérez, **S. Nangia**, L. González-Mariscal. International Journal of Molecular Sciences, 25, 2453 (2024).

https://doi.org/10.3390/ijms25052453

4. Supramolecular Peptoid Structure Strengthens Complexation with Polyacrylic Acid Microgels. W. Zhao, J. Lin, J. Nielsen, K. Sorensen, A. Wadurkar, J. Ji, A. Barron, **S. Nangia**, M. Libera, Biomacromolecules, 25, 1274–1281 (2024). https://doi.org/10.1021/acs.biomac.3c01242
5. A combined computational-biochemical approach offers an accelerated path to membrane protein solubilization, M. Pierce, J. Ji, S. Novak, M. Sieburg, S. Nangia, **S. Nangia**, and J. Hougland, Journal of Chemical Information and Modeling, **63**, 7159–7170 (2023). https://doi.org/10.1021/acs.jcim.3c00917
6. Self-defensive antimicrobial shape memory polyurethanes with honey-based compounds, M. Ramezani, E. Labour, J. Ji, A. Vakil, C. Du, T. Orado, **S. Nangia**, M. B. Monroe, ACS Applied Materials & Interfaces, **15**, 56733–56748 (2023). https://doi.org/10.1021/acsami.3c12274
7. Claudin-23 reshapes epithelial tight junction architecture to regulate barrier function Scale. A. Rya-Sandino, K. M. Lozada-Soto, N. Rajagopal, V. Garcia-Hernandez, A. Luissint, J. C. Brazil, G. Cui, M. Koval, C. A. Parkos, **S. Nangia,** and A Nusrat, Nature Communications, **14**, 6214 (2023). https://doi.org/10.1038/s41467-023-41999-9
8. An Affordable Topography-Based Protocol for Assigning a Residue's Character on a Hydropathy (PARCH) Scale J Ji, B Carpentier, A Chakraborty, **S Nangia**, Journal of Chemical Theory and Computation **20***, 1656–1672* (2024). *Featured on the cover.* https://doi.org/10.1021/acs.jctc.3c00106
9. Lipidation Alters the Structure and Hydration of Myristoylated Intrinsically Disordered Proteins, J. Ji, Md S. Hossain, E. N Krueger, Z. Zhang, S. Nangia, B. Carpentier, M. Martel, S. Nangia, and D. Mozhdehi, Biomacromolecules, **24**, 1244–1257 (2023). *Featured on the cover.* https://doi.org/10.1021/acs.biomac.2c01309
10. Self-Defensive Antimicrobial Surfaces Using Polymyxin-Loaded Poly (styrene sulfonate) Microgels, X. Xiao, J. Ji, H. Wang, **S. Nangia**, H. Wang, M. Libera, ACS Biomaterials Science & Engineering 8, 4827-4837 (2022). https://doi.org/10.1021/acsbiomaterials.2c00783
11. 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
12. 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
13. 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
14. 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
15. 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
16. 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

17. 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
18. 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). *Featured on the cover.*
https://doi.org/10.1039/D0CC03271A
19. 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
20. 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
21. 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
22. 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
23. 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
24. 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
25. 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
26. 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
27. 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
28. 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
29. 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
30. 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

31. 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
32. 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
33. 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
34. 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
35. 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
36. 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
37. 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
38. 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
39. 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
40. 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
41. 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
42. 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
43. 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

44. 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
45. 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
46. 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
47. 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
48. 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
49. 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
50. 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
51. 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
52. 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
53. 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
54. 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
55. 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
56. 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
57. 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).
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58. 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,† 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

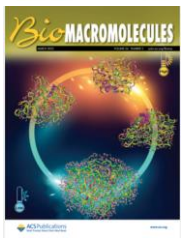
5 Journal Covers

2024

The PARCH scale is a tool for calculating the hydropathy of amino acid residues as a function of a protein's nanoscale topography, such as bumps, crevices, cavities, clefts, pockets, and channels. This computationally inexpensive method can compare hydropathies of the different protein surfaces and quantify the effect of point mutations.

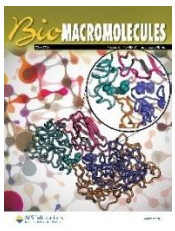
2023

Fat punching above its weight: Modification with lipids yields unexpected alterations in the proteins? structure and hydration. Fatty acid-modified elastin-like polypeptides combine the hierarchical assembly of lipids with the thermoresponsive character of elastins to form nanocarriers with temperature-dependent characteristics. By integrating computational and experimental techniques, we revealed the biophysical underpinnings of thermoresponsive behavior for this class of materials; temperature alters the structure, contact, and hydration of lipid, lipidation site, and protein. These findings enable the rational design of the biomaterials and therapeutics that rival the exquisite hierarchy and capabilities of biological systems.



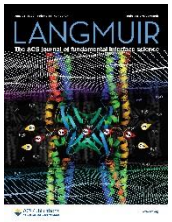
2022

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

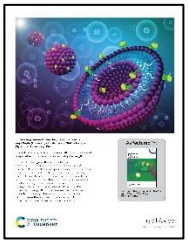


2020

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

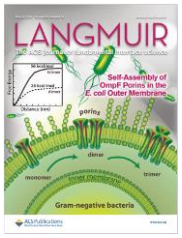
The protein association energy landscape (PANEL) method provides an extensive data set of membrane protein association in lipid milieu using a combination of stochastic sampling and equilibration simulations. The results are obtained in a fraction of the simulation cost compared to self-assembly simulations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

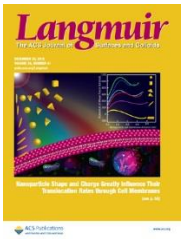
Molecular representation of multilayered Gram-negative bacterial membrane. The cell envelope of Gram-negative bacteria is a complex multilayered structure that, besides gatekeeping chemical transport in and out of the bacterial cell, protects the cell from hostile environments. The image shows an illustrative 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.
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 force field.
https://pubs.acs.org/toc/jctcce/11/1

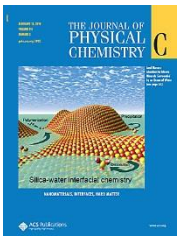
2012

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/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).

6 PRESENTATIONS

- (Oral, Invited) Bridging computational biology, biochemistry, biophysics, and biomedical engineering, Shikha Nangia, *IQ Biology*, University of Colorado, Denver CO (August 15, 2024).
- (Oral, Invited) Treating Alzheimer's Diseases: bridging scales from Angstroms to Microns, Shikha Nangia, *Lehigh University*, Bethlehem PA (April 17, 2024).
- (Oral, Invited) Bridging scales from Angstroms to Microns: What do we need to know to treat Alzheimer's disease? Shikha Nangia, *Johns Hopkins*, Baltimore MD (April 2, 2024).
- (Oral, Invited) Breaking the Barriers: Shaping a future without Alzheimer's disease, Shikha Nangia, *American Chemical Society (ACS) Science Talks*, ACS Virtual Lecture Series (March 22, 2024).
- (Oral, Invited) Challenges of treating Alzheimer's disease: Bridging scales from Angstroms to microns, Shikha Nangia, *American Chemical Society*, New Orleans, LA (March 12-21, 2024).
- (Oral, Invited) Quantifying hydropathy of self-assembling biomaterials, Shikha Nangia, *American Physical Society*, Minneapolis MN (March 3-8, 2024).
- (Oral, Invited) Beyond the basics: Unraveling the complexity of proteins in sickness and in health, Shikha Nangia, *Department of Chemistry*, Syracuse University, Syracuse NY (February 6, 2024).
- (Oral, Invited) Treating Alzheimer's disease: A molecular challenge, Shikha Nangia, *University of Washington*, Seattle WA (November 27, 2023).
- (Oral, Invited) Challenges of treating Alzheimer's disease, Shikha Nangia, *Korean Chemical Society Annual Meeting*, Gwangju, South Korea (October 25, 2023).

- (Oral, Invited) Challenges of treating Alzheimer's disease, Shikha Nangia, *Korea University*, Seoul, South Korea (October 23, 2023).
- (Oral, Invited, Virtual) Engineering pathways across the blood-brain barrier, Shikha Nangia, *University of Buffalo Medical School*, NY (October 11, 2023).
- (Oral, Invited) Engineering pathways across biological barriers: Treating Alzheimer's disease, Shikha Nangia, *University of Illinois at Urbana Champaign*, IL (September 26, 2023).
- (Oral, Invited, Keynote) Introduction to Molecular Dynamics of Proteins: *What can Jiggling and Wiggling of Molecules tell us?* Shikha Nangia, *MERCURY (The Molecular Education and Research Consortium in Undergraduate computational chemistry)* Conference, Greenville, SC (July 19-21, 2023)
- (Oral, Invited) Protein hydration, Shikha Nangia, *Molecular engineering of soft matter: Spanning small molecules to macromolecules*, Telluride, CO (June 20-24, 2023).
- (Oral, Invited) Computational Nanoscopy of the Tight Junction Architecture, Shikha Nangia, *Tight Junctions: from structure and Development to Therapeutics,* Leysin, Switzerland (June 19-21, 2023).
- (Oral, Invited) To touch or not to touch: mechanism of antibacterial contact transfer, Shikha Nangia, 6th *Stevens Conference,* Hoboken, NJ (May 31-June 1, 2023).
- (Oral, Invited) Undergraduate Powered Research: Are bacteria friends or foes? Shikha Nangia, *Slepecky Memorial Lecture*, Syracuse University (April 20, 2023).
- (Oral, Invited) Treating Alzheimer's Disease: A molecular challenge, Shikha Nangia, *Stevens Institute of Technology,* Hoboken, NJ (April 14, 2023).
- (Oral, Invited) Computational Nanoscopy of the Tight Junction Architecture, Shikha Nangia, *Tight Junction Club,* Virtual Presentation (March 21, 2023).
- (Oral, Invited) Engineering Pathways across Biological Barriers to treat Alzheimer's Disease, Shikha Nangia, *University of Notre Dame,* IN (January 31, 2023).
- (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, 21st 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) New Breakthrough in blood-brain barrier tight junctions, Shikha Nangia, 4th *International Tight Junction Conference*, Berlin, Germany (October 8-10, 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, 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, *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 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).

7 RESEARCH AWARDS

Gerber Auditory Research Grant — $10,000.00
PI — 11/01/2023- 10/30/2024
Designing biomaterials for preventing ear infections

NSF MCB — $415,311.00
PI — 7/15/2022- 7/14/2025
Biophysical Effects of Reversible Lipid Modification of Integral Membrane Proteins

NIH NIBIB — $1,206,932
PI — 6/1/2022- 5/31/2026
ESTEEMED LEArning and Discovery through Engineering Research at Syracuse (LEADERS)

NSF REU Site — $354,683
PI — 9/1/2021- 8/30/2024
Interactive Biomaterials: REU Site

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

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

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

CUSE Grant — $30,000
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 — $321,000
Co-PI — $62,769
Integrating synthetic biology approaches with patterned biofilm formation to investigate bacterial persistence in heterogeneous — 7/15/2017- 7/14/2020

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

NIH R21 — $213,000
Co-Investigator — $74,000
Rational Design and High Throughput Synthesis of — 8/1/2015 - 7/31/2017

Nanocarriers for Efficient Drug Delivery

NSF CAREER $530,000
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
Senior Personal 5/1/2015 - 4/30/2018
Interactive Biomaterials: REU Site

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

7.1 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

Anton2 (PSCA17073P) 100,000 Units
PI 12/7/2017 –11/30/2018
Role of S-Palmitoylation on the Blood-Brain Barrier Tight Junction Interface

XSEDE Supercomputer Allocation MCB140216 (renewal) 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

XSEDE Supercomputer Allocation MCB140216 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

8 Research Advising and Mentoring

8.1 Graduate Students

2024-present	Anand Wadurkar
2023–present	Jumoke Omolola Ologun
2023–present	Felix Odhiambo Otenga
2023–present	Yu Liu
2022–present	Ratnakshi Mandal
2022–present	Xuyang Qin

2019–2024	Jingjing Ji, PhD *Investigation of Hydropathy of Proteins, Lipid-modified Proteins, and Self-defensive Biomaterials*
2022–2024	Anand Wadurkar, MS *Evaluating the clustering behavior of antimicrobial peptoids for application in implantable medical devices*
2023–2024	Steven Alexson, MS Systematically testing the clustering properties of peptoid for use in medical implants
2022–2023	Britnie Jean Carpentier, MS *Predicting the Hydration Properties of Anti-Freeze Proteins*
2020–2024	Patrick Marsch, PhD *Homomeric tight junction strand assembly of claudin proteins*
2021–2023	Faris Amer, MS *Computational Biophysics of the Lipidome*
2020–2022	Nelly Raissa Setchie-Tchato, MS *Discrepancy In the Biophysical Properties of Trophoblast Placental Plasma Membrane Between First and Third Trimester*
2019–2021	Allyson Karmazyn, MS *Computational investigation of biological membranes*
2020–2021	Xuyang Qin, MS *Depth of S-palmitoylated Cysteines on the Transmembrane protein governs palmitoylation-induced changes in protein-lipid interface*
2019-2020	Patrick Marsch, MS *Predicating Tight Junction Formation via Claudin Chimeras*
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*
2017–2022	Kathryn Marie Piston, Ph.D. *Atomistic investigation of nucleosomal h3 histone tail in unmodified and epigenetically modified states*
2017–2021	Yinghui Dai, Ph.D. *Computational Antibiotic screening platform*
2016–2021	Nandhini Rajagopal, Ph.D. *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

8.2 Undergraduate Students

2024 Claire Sheridan (REU Student, Bioengineering)
2024 Faith Nwando ((REU Student, Bioengineering)
2024-present Khuong Pham (Biomedical Engineering)
2024-present Alem Yirefu (Neuroscience)
2023-present Wafiq Ibsan Khondkar (Biotechnology)
2023-2024 Caitlin Mehl (Biomedical Engineering)
2021–2022 Britnie Jean Carpentier (Bioengineering)
2021–2022 Nathena Murray (Neuroscience)
2021 Isabelle Tawyer (Biotechnology)
2021 Mae Martel (REU Student, Bioengineering)
2020 Alexis Rose Aquilino (REU Student, Bioengineering)
2020 Amelia Gilbert (REU Student, Bioengineering)
2020 Ivan Sarbinov (Chemical Engineering)
2020 Faris Amer (Chemistry)
2019 Aria Atwal (Biology)
2019 Laurie Mouk (Bioengineering)
2019 Victoria Bialczak (ECS Scholar, Bioengineering)
2019 Patrick Matthew Marsch (Chemical Engineering)
2019 Caroline Almonte (Syracuse Biomaterials Institute, REU student)
2019 Andreea C Merloiu (Bioengineering)
2019 Alina Zdebska (ECS Scholar)
2018–2019 Jingzhi Liu (Chemical Engineering)
2018–2019 Wenlin He (Chemical Engineering)
2018–2021 Allyson Karmazyn (ECS Scholar, Bioengineering)
2018 Naomi Brandt (Syracuse Biomaterials Institute, REU student)
2018 Natalie Marie Petryk (ECS Scholar)
2018 Bailey M Felix (ECS Scholar, Bioengineering)
2018 Alejandro J Durand (ECS Scholar, Bioengineering)
2018 Priya S Ganesh (ECS Scholar, Bioengineering)
2017–2018 Santita Ebangwese (Bioengineering)
2018 Austin Freer (Chemical Engineering)

2018	Meishan Wu (Chemical Engineering)
2017	Prakash Khare (Bioengineering)
2017	Soor Vora (REU student, Chemical Engineering)
2017	Tory Welch (Syracuse Biomaterials Institute, REU student, Bioengineering)
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)

8.3 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 l, Syracuse School District, Syracuse NY
2013	Sally Mitchell (teacher), East Syracuse-Minoa High School, East Syracuse NY

8.4 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

9 TEACHING

2023	ECS 326- Engineering Materials, Properties, and Processing, *Instructor*
2022	CEN 451/651-Chemical Engineering Thermodynamics, *Instructor*

	ECS 326- Engineering Materials, Properties, and Processing, *Instructor*
2021	ECS 326- Engineering Materials, Properties, and Processing, *Instructor*
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*

9.1 Professional Development in Teaching

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)
2017	*Participant,* Summer Institute for Technology-Enhanced Teaching & Learning (SITETL), training program for faculty members to incorporate technology in their classes
2017	*Participant,* Gateway Redesign Working Group, a group to redesign the College of engineering gateway classes to enhance active learning.
2014	*Participant*, "How to Engineer Engineering Education," a 3-day hands-on summer workshop to obtain formal training in educational theory and pedagogical practices
2014	*Participant*, "Intro to Process-Oriented Guided Inquiry Learning (POGIL) Workshop" aimed to explore the benefits of this approach to active learning in the classroom

10 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

11 Academic Service

2024-present	*Member,* Advisory board BOREALIS (NIH ESTEEMED) program at Clarkson University
2024	*Member,* Chemistry Faculty Search Committee
2024	*Member*, ECS Faculty Recruitment Committee
2023-present	*Member,* Research Advisory Committee, College of Engineering and Computer Science
2021-2024	*Member,* WiSE Women of Color in STEM (WWoCS)
2023-2024	*Member,* BMCE Faculty Search Committee (Chemical Engineering)
2024	*Co-chair,* 2024 Foundations of Molecular Modeling and Simulation (FOMMS) meeting, Snowbird, UT (July 28-Aug 1, 2024).
2022-present	*Co-chair,* Spotlights in Thermodynamics and Computational Molecular Science, *AIChE Annual Meeting*
2022-2023	*Chair,* College Academic Strategic Committee, College of Engineering and Computer Science
2022-2023	*Member,* University Academic Strategic Committee, DEIA Committee
2021-2023	*Chair,* Frontiers of Molecular Thermodynamics, AIChE Annual Meeting
2022-2023	*Chair,* BMCE Faculty Search Committee (BioInspired Positions)
2021	*Team Leader,* Remembrance Scholar Program Committee, Syracuse University
2020	*Member,* Search Committee for the Associate Dean of Student Affairs, College of Engineering and Computer Science
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
2019-2021	*Member,* Financial Conflict of Interest Committee, 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 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*, 4th 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-Novermber 3)
2017	*Organize*r, 3rd 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	*Presente*r, workshop sponsored by Women in Science and Engineering (WiSE)
2012-2016	*Member*, 39th 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	*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
2013	*Member*, Department of Chemistry Faculty Search Committee

12 Professional Service

12.1 Editorial Activities

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

12.2 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

12.3 Ad hoc Merit Reviewer for Funding Agencies

2014-2023	NSF Panelist
2014-2023	NSF GRFP Panelist
2014-2020	Ad hoc reviewer, ACS PRF program

13 News And Media

2010	"SU researchers utilize computer simulations to explore biofilm fragmentation"- https://news.syr.edu/blog/2010/09/20/biofilms/
2011	*"Interdisciplinary team led by Syracuse University wins $2 million EFRI grant from NSF"*- http://news.syr.edu/bacterial-multicellular-systems/
2013	NSF news- "Modifications of a Nanoparticle Can Change Chemical Interactions with Cell Membranes" https://www.nsf.gov/news/news_summ.jsp?cntn_id=126781
2015	"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/ "*Bioengineering Major Earns National Recognition for Research*"- http://news.syr.edu/bioengineering-major-earns-national-recognition-for-research-12813/ "*@SyracuseU News Tips*"- http://news.syr.edu/syracuseu-news-tips-14251/ "*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/ "*Better Cancer Treatment Through Nanotechnology*"- http://news.syr.edu/better-cancer-treatment-through-nanotechnology-48799/ "Nangia's Bacteria Research Featured in Chemistry Journal"- http://news.syr.edu/nangias-bacteria-research-featured-in-chemistry-journal-13234/ "*Nappi Research Competition Awards $650,000 to SU-Upstate Teams"-* http://news.syr.edu/nappi-research-competition-awards-650000-to-su-upstate-teams-73213/
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/
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/
2018	*"Nangia's Research Featured on Journal of Physical Chemistry Cover"* *https://news.syr.edu/blog/2018/08/13/nangias-research-featured-on-journal-of-physical-chemistry-cover/* *"Dr Shikha Nangia – The Blood-Brain Barrier: More than Just a Barrier"* https://www.scientia.global/dr-shikha-nangia-the-blood-brain-barrier-more-than-just-a-barrier/
2019	*"How Research Enhances Students' Educational Experience"-* *https://news.syr.edu/blog/2019/07/25/how-research-enhances-students-educational-experience/*
2021	*Professor Shikha Nangia Selected as Associate Editor for ACS Applied Bio Materials Journal"* *https://news.syr.edu/blog/2021/01/06/professor-shikha-nangia-selected-as-associate-editor-for-acs-applied-bio-materials-journal/* *"Professor Shikha Nangia Selected as Rising Star by American Chemical Society"* https://news.syr.edu/blog/2021/10/11/professor-shikha-nangia-selected-as-rising-star-by-american-chemical-society/
2022	*"Molecular Mystery"*

	https://www.syracuse.edu/stories/shikha-nangia-molecular-mystery/
2023	https://spectrumlocalnews.com/nys/central-ny/news/2023/03/02/su-professor-making-progress-to-advance-potential-treatment-paths-for-alzheimer-s#