

SHIKHA NANGIA

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EDUCATION

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

PROFESSIONAL EXPERIENCE

2018-present	Associate Professor	Department of Biomedical and Chemical Engineering <i>Syracuse University</i>
2012-2018	Assistant Professor	Department of Biomedical and Chemical Engineering <i>Syracuse University</i>
2014-present	Member	Interdisciplinary Neuroscience Studies <i>Syracuse University</i>
2012-present	Member	Syracuse Biomaterials Institute <i>Syracuse University</i>
2009-2012	Research Assistant Professor	Department of Biomedical and Chemical Engineering <i>Syracuse University</i>
2009-2012	Research Assistant Professor	Department of Chemistry <i>Syracuse University</i>
2006-2009	Postdoctoral Researcher	Department of Chemistry <i>Pennsylvania State University</i>

HONORS AND AWARDS

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

HONORS AND AWARDS TO UNDERGRADUATE AND GRADUATE MENTEES

2019	Second place poster, Summer Research Symposium, Syracuse University, V. Bialczak (UG)
2019	Graduate Research Fellowship Program, National Science Foundation, K. Piston (G)
2019	University Scholar, Syracuse University, S. Ebangwese (UG)
2019	All University Doctoral prize, Syracuse University, H. Ma (G)
2019	2019 SBI Distinguished Student Research Award, Syracuse University, H. Ma (G)
2019	Outstanding Graduate Student in Bioengineering Award, Syracuse University, H. Ma (G)

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

PUBLICATIONS

1. 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. Houglund, JBC (accepted).
2. Obtaining Protein Association Energy Landscape (PANEL) for Integral Membrane Proteins, N. Rajagopal and **S. Nangia**, *Journal of Chemical Theory and Computation*, (under review).
3. 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 Biomater. Sci. Eng.* 4, 2370–2379 (2018).
<https://doi.org/10.1021/acsbiomaterials.9b00243>
4. 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. Houglund, *BioRxiv* (2019).
<https://doi.org/10.1101/556233>
5. 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>
6. 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>
 7. 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>
 8. 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 Biomater. Sci. Eng.* **4**, 2370–2379 (2018). <http://dx.doi.org/10.1021/acsbiomaterials.8b00486>
 9. 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>
 10. Architecture of the paracellular channels formed by Claudins of the blood-brain barrier tight junctions, F. J. Irudayanathan, N. Wang, X. Wang, and **S. Nangia**, *Annals of the New York Academy of Sciences*, **1–16** (2017). <http://dx.doi.org/10.1111/nyas.13378>
 11. 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>
 12. 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>
 13. 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>
 14. 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>
 15. 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>
 16. 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>
 17. 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>
 18. 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>
 19. 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>
20. 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>
 21. 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>
 22. 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>
 23. 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>
 24. 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>
 25. 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>
 26. 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>
 27. 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>
 28. 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>
 29. 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>
 30. A new form of MgTa₂O₆ 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>
 31. 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>
 32. 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>
 33. 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>
 34. 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).

CONFERENCE PAPERS AND OTHER INDEXED JOURNAL PUBLICATIONS

1. 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>
2. 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>
3. ChemXSeer digital library Gaussian search, S. Lahiri, J. P. Fernández-Ramírez, S. Nangia, P. Mitra, C. L. Giles, K. T Mueller, 2011. *arXiv:1104.4601*

CITATION METRICS

	Total Citations	h-index
Google Scholar	1206	16
Scopus	1156	16
Web of Science	1173	16

RESEARCH AWARDS

NSF Engineering Research Center Planning Grant	\$100,000 (total)
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 (total)
PI	\$20,000
Cancer epigenetics: Molecular and structural interplay of histone modifications	6/1/2019- 4/31/2021
CUSE Grant	\$30,000 (total)
Co-PI	\$10,000
Bringing a membrane enzyme into structural focus: Interdisciplinary computational-biochemical modeling of ghrelin O-acyltransferase	5/1/2018- 4/31/2020
NSF CBET Award (Award # 1706061)	\$321,000 (total)
Co-PI	\$62,769
Integrating synthetic biology approaches with patterned biofilm formation to investigate bacterial persistence in heterogeneous structures	7/15/2017- 7/14/2020
NSF REU Site	\$318,863 (total)
Co-PI	5/1/2018 - 4/30/2021
Interactive Biomaterials: REU Site	
NIH R21	\$213,000 (total)
Co-Investigator	\$74,000
Rational Design and High Throughput Synthesis of Nanocarriers for Efficient Drug Delivery	8/1/2015 - 7/31/2017

NSF CAREER	\$530,000 (total)
PI	\$530,000
Enabling Transport Across the Blood-Brain Barrier by Engineering Thermodynamically Favorable Pathways	4/1/2015 - 3/31/2020
NSF REU Site	\$297,506 (total)
Senior Personal	5/1/2015 - 4/30/2018
Interactive Biomaterials: REU Site	
NSF EFRI	\$2,000,000 (total)
Co-PI	\$ 253,750
Deciphering and Controlling the Signaling Processes in Bacterial Multicellular Systems and Bacteria-Host Interactions	1/01/2012 –12/31/2016

COMPUTER ALLOCATION AWARDS

XSEDE Supercomputer Allocation MCB140216 (renewal)	1.3 million hours
PI	(equivalent to \$27,052)
Multiscale Molecular Modeling of the Biomolecular Interfaces for Enhancing Drug Delivery and Designing Antimicrobial Peptides	7/1/2019 –6/30/2020
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

TEACHING AWARDS

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

PRESENTATIONS

- (Oral, Invited) Membrane Protein Structure Prediction using Co-evolutionary Analysis, Shikha Nangia, FASEB, PA (July 7-11, 2019).
- (Oral, Invited) Protein Crowding in Complex Lipid Environment, Shikha Nangia, Molecular engineering of soft matter: Spanning small molecules to macromolecules, Telluride, CO (June 15-20, 2019).

- (Oral, Invited) Engineering Pathways across Biological Barriers, Shikha Nangia, *AICHE Annual Meeting*, Pittsburgh, PA (October 29-November 3, 2018).
- (Oral, Invited) Molecular perspective on protein-protein interactions at the tight junctions interface, Shikha Nangia, *256th ACS National Meeting*, Boston, MA (August 19-23, 2018).
- (Oral, Invited) Engineering pathways across biological barriers, Shikha Nangia, *Tulane University*, New Orleans, LA (January 25-26, 2018).
- (Oral, Invited) Modeling the protein-protein interactions at the blood-brain barrier interface, Shikha Nangia, *Application of Molecular Modeling to Study Interfacial Phenomena, AICHE Annual Meeting*, Minneapolis (October 29-November 2, 2017).
- (Oral, Invited) Multiscale modeling of complex biological interfaces, Shikha Nangia, *Molecular engineering of soft matter: Spanning small molecules to macromolecules*, Telluride, CO (June 19-23, 2017).
- (Oral, Invited) Breaking through the blood-brain barrier, Shikha Nangia, *Material Science and Engineering, University of Michigan*, Ann Arbor, MI (December 4, 2016).
- (Oral, Invited) Breaking through the blood-brain barrier, Shikha Nangia, *Chemical and Biological Engineering, Rensselaer Polytechnic Institute*, Troy, NY (October 19, 2016).
- (Oral, Invited) Breaking through the blood-brain barrier, Shikha Nangia, *Research Colloquy, Information Technology Services and Research Computing Advisory Council (RCAC)*, Syracuse University, Syracuse, NY (October 24, 2016).
- (Oral, Invited) Breaking through the blood-brain barrier, Shikha Nangia, *Syracuse Biomaterials Seminar Series, SBI, Syracuse University*, Syracuse, NY (October 4, 2016).
- (Oral, Invited) Breaking through the blood-brain barrier, Shikha Nangia, *School of Chemical and Biomolecular Engineering, Cornell University*, Ithaca, NY (September 26, 2016).
- (Oral, Invited) Breaking through the blood-brain barrier, Shikha Nangia, *SyracuseCoE Symposium, Syracuse University*, Syracuse, NY (September 22, 2016).
- (Oral, Invited) Breaking through the blood-brain barrier, Shikha Nangia, *Biomedical Engineering, Binghamton University*, Binghamton, NY (September 20, 2016).
- (Oral, Invited) Breaking through the blood-brain barrier, Shikha Nangia, *Chemical and Biomolecular Engineering, Clemson University*, Clemson, SC (September 15, 2016).
- (Oral, Invited) Multiscale simulations to characterize the blood-brain barrier tight junctions, Shikha Nangia, *2016 Middle Atlantic Regional Meeting MARM, Riverdale, NY* (June 9–12, 2016).
- (Oral, Invited) Engineering nanocarriers for brain tumor treatment, Shikha Nangia and Juntao Luo, *Nappi Research Award Competition, Syracuse University*, Syracuse, NY (December 11, 2015).
- (Oral) Coarse grained parameterization of gram-negative bacterial outer membrane, Shikha Nangia, *AICHE Annual Meeting, Salt Lake City, UT* (November 8–13, 2015).
- (Oral) Multiscale simulations to characterize the blood brain barrier tight junctions, Shikha Nangia, *AICHE Annual Meeting, Salt Lake City, UT* (November 8–13, 2015).
- (Oral, Invited) Insights into the blood brain barrier tight junctions for treatment of Alzheimer's disease, Shikha Nangia, *2015 West Virginia University*, Morgantown, WV (August 28, 2015).
- (Oral, Invited) Synergistic experimental and multiscale modeling approaches for optimizing anticancer drug nanocarriers, Shikha Nangia, *250th ACS National Meeting, Boston MA* (August 16–20, 2015).
- (Oral) Molecular characterization of the blood brain barrier tight junctions, *Young Investigator Symposium*, Shikha Nangia, *250th ACS National Meeting, Boston MA* (August 16–20, 2015).
- (Oral) Spectroscopic properties of semiconductor quantum dots embedded in biological medium, B. Ellis, W. Jiang, J. Elward, F. J. Irudayanathan, Shikha Nangia, A. Chakraborty, *250th ACS National Meeting, Boston MA* (August 16–20, 2015).
- (Oral, Invited) Multiscale simulations to characterize the blood brain barrier tight junctions, Shikha Nangia, *Neuroscience Research Day*, Syracuse, NY (April 3, 2015).
- (Oral, Invited) Multiscale simulations to characterize the blood brain barrier tight junctions, Shikha Nangia, *Albany 2015: Conversation 19*, Albany, NY (June 9-13, 2015).

- (Oral) Introduction of computational simulations to high school students will increase their STEM knowledge and interest, Suzanne DeTore and Shikha Nangia, *2015 Emerging Researchers National (ERN) Conference in STEM*, Washington, D.C. (February 19-21, 2015).
- (Oral, Invited) Multiscale modeling approach to determine the role of amphiphilic building block in the stability of paclitaxel drug delivery nanocarriers, at *AIChE Annual Meeting, Atlanta, GA* (Nov. 16–22, 2014).
- (Oral), Cellular uptake of nanoparticles with protein coronas: A coarse-grained molecular dynamics simulations study, Ayten Ay, Haarika Kamani, Sydney Mendez, and Shikha Nangia, *2014 Emerging Researchers National (ERN) Conference in STEM*, Washington, D.C. February 20-22, 2014.
- (Oral, Invited) Effect of protein corona on nanoparticle cellular uptake, at *AIChE Annual Meeting, San Francisco* (Nov. 2-8, 2013).
- (Oral) Effect of nanoparticle shape and charge on cytotoxicity, at *AIChE Annual Meeting, Pittsburgh PA* (October 28– Nov. 2, 2012).
- (Oral) Effect of nanoparticle shape and charge on cytotoxicity, at *243rd ACS National Meeting, San Diego CA* (March 25–29, 2012).
- (Oral) Viscoelastic properties of bacterial biofilms using coarse-grained molecular dynamics simulations, at *AIChE Annual Meeting, Minneapolis MN* (October 16–21, 2011).
- (Oral) Coarse-grained molecular dynamics simulations of bacterial polysaccharides for studying flow-induced fragmentation mechanisms, at *241 ACS National Meeting, Anaheim CA* (March 27–31, 2011).
- (Oral, Invited) Theoretical and Computational Modeling of Dissolution Processes, at *SUNY-ESF, Syracuse, NY* (March 11, 2011)
- (Oral, Invited) Computational approaches of modeling dissolution of rocks and evolution of Earth surface, at *Rensselaer Polytechnic Institute, Troy, NY* (Feb. 8–9, 2010)
- (Oral) Dissolution studies of mineral-water interfaces using newly developed Monte Carlo algorithm, at *237th ACS National Meeting, Salt Lake City UT* (March 22–26, 2009).

NEWS AND MEDIA

2019

- “How Research Enhances Students’ Educational Experience”- <https://news.syr.edu/blog/2019/07/25/how-research-enhances-students-educational-experience/>

2017

- “Professors Honored with Prestigious Meredith, Teaching Recognition, Scholar and Teacher Awards” <https://news.syr.edu/2017/05/professors-honored-with-prestigious-meredith-teaching-recognition-and-scholar-and-teacher-awards/>
- “Teaching Awards Program to Honor 10 Faculty” <https://news.syr.edu/2017/04/teaching-awards-program-to-honor-10-faculty/>

2016

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

2015

- “Nappi Research Competition Awards \$650,000 to SU-Upstate Teams”- <http://news.syr.edu/nappi-research-competition-awards-650000-to-su-upstate-teams-73213/>
- “Nangia’s Bacteria Research Featured in Chemistry Journal”- <http://news.syr.edu/nangias-bacteria-research-featured-in-chemistry-journal-13234/>

- “Better Cancer Treatment Through Nanotechnology”- <http://news.syr.edu/better-cancer-treatment-through-nanotechnology-48799/>
- “Nangia Awarded CAREER Grant to Break Barriers in Treating Alzheimer’s”- <http://news.syr.edu/nangia-awarded-career-grant-to-break-barriers-in-treating-alzheimers-91343/>
- “@SyracuseU News Tips”- <http://news.syr.edu/syracuseu-news-tips-14251/>
- “Bioengineering Major Earns National Recognition for Research”- <http://news.syr.edu/bioengineering-major-earns-national-recognition-for-research-12813/>
- Understanding Thermodynamics — There’s an App for That - “<http://eng-cs.syr.edu/college-news/understanding-thermodynamics-theres-an-app-for-that/>
- “Shining a Light on Quantum Dots Measurement”- <http://news.syr.edu/shining-a-light-on-quantum-dots-measurement-79855/>
- “Computer Model Details QD Interaction with Protein,” *Photonics.com*- <http://www.photonics.com/Article.aspx?AID=57091>
- “Shining a light on quantum dots measurement”-*phys.org*- <http://phys.org/news/2015-01-quantum-dots.html>

2013

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

2011

- “Interdisciplinary team led by Syracuse University wins \$2 million EFRI grant from NSF”- <http://news.syr.edu/bacterial-multicellular-systems/>

2010

- “SU researchers utilize computer simulations to explore biofilm fragmentation”- <http://news.syr.edu/biofilms/>

JOURNAL COVERS

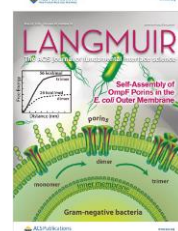
2018

Self-Assembly Simulations of Classic Claudins—
Insights into the Pore Structure, Selectivity, and Higher
Order Complexes



2018

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).

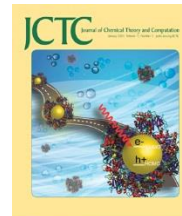


2015

Simulating Gram-Negative Bacterial Outer Membrane:
A Coarse Grain Model, H. Ma, Huilin, F. J.
Irudayanathan, W. Jiang, and S. Nangia, *Journal of
Physical Chemistry B*, **119** (2015).



- 2015 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).
- 2012 Effect of nanoparticle charge and shape anisotropy on translocation through cell membranes, **S. Nangia** and R. Sureshkumar, *Langmuir*, **28**, 17666-17671 (2012).
- 2010 Role of intrasurface hydrogen bonding on dissolution of silica, **S. Nangia** and B. J. Garrison, *J. Physical Chemistry C* **114**, 2267-2272 (2010).
- 2006 Potential Energy Surfaces for Photodissociation of Ammonia through a Conical Intersection Special Issue honoring Donald G. Truhlar, *J. Physical Chemistry A* **110**, (2006).



PEER REVIEW & EDITORIAL ACTIVITIES FOR SCIENTIFIC JOURNALS & FUNDING AGENCIES

- 2016-2019 Scientific American, Editorial Board Member
 2016-2017 PLOS Computational Biology, Guest Editor

Ad hoc review for scientific journals

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

Ad hoc review for funding agencies

- 2014-2019 Ad-hoc reviewer, ACS PRF program
 2014-2019 NSF Panelist
 2014-2015 NSF GRFP Panelist

MENTORING AND SUPERVISION OF RESEARCH ACTIVITIES

Graduate Students

2019-present	Zhenyu Qiu <i>Effect of palmitoylation on claudin-5 dimerization</i>
2018-present	Zhenqi Li <i>Computational models of mitochondrial membrane</i>
2017-present	Yinghui Dai <i>Computational Antibiotic screening platform</i>
2017-present	Kathryn Marie Piston <i>Cancer epigenetics</i>
2016-present	Nandhini Rajagopal, Ph.D <i>Molecular architecture of tight junctions</i>
2015-2019	Huilin Ma, Ph.D <i>Computational modeling of bacterial outer membranes and development of high-throughput screening platform for antibiotics</i>
2013-2019	Flaviyan Jerome Irudayanathan, Ph.D <i>Molecular structure of Claudin-5 tight junctions responsible for the blood-brain barrier</i>
2012-2016	Wenjuan Jiang, Ph.D <i>Stochastic simulations of transport of molecules across the blood-brain barrier</i>
2017-2019	Xichen Xu, MS <i>Coarse grained parameterization of Gram-positive bacteria cell wall</i>
2017-2018	Lisa Danielle Nguyen, MS <i>Homotypic and heterotypic self-assembly of Claudin family of tight junction proteins</i>
2017-2018	Amogh Srihari, MS <i>Statistical Mechanical Treatments of the Optical Properties of CdSe Quantum Dots</i>
2015-2016	Nan Wang, MS <i>Self-assembly of Claudin Family of Membrane Proteins</i>
2014-2016	Xiaoyi Wang, MS <i>Designing of anticancer drug delivery nanocarriers using multiscale modeling</i>
2014-2016	Huilin Ma, MS <i>Coarse grained parameterization of Gram-negative bacteria outer membrane</i>
2012-2013	Haarika Kamani, MS <i>Effects of protein corona on gold nanoparticle cellular uptake</i>

Undergraduate Students

2019	Aria Atwal
2019	Laurie Mouk
2019-present	Victoria Bialczak
2019-present	Patrick Matthew Marsch
2019	Caroline Almonte (Syracuse Biomaterials Institute, REU student)
2019	Andreea C Merloiu
2019	Alina Zdebska (ECS Scholar)
2018-2019	Jingzhi Liu
2018-2019	Wenlin He
2018-present	Allyson Karmazyn (ECS Scholar)
2018	Naomi Brandt (Syracuse Biomaterials Institute, REU student)

2018	Natalie Marie Petryk (ECS Scholar)
2018	Bailey M Felix (ECS Scholar)
2018-present	Alejandro J Durand (ECS Scholar)
2018	Priya S Ganesh (ECS Scholar)
2017-2018	Santita Ebangwese (Bioengineering)
2018	Austin Freer (Chemical Engineering)
2018	Meishan Wu (Chemical Engineering)
2017	Prakash Khare (Bioengineering)
2017	Soor Vora (REU student)
2017	Tori Welch (Syracuse Biomaterials Institute, REU student)
2017	Colleen Marie Cassidy (Bioengineering)
2016	Daniel Cummins (Syracuse Biomaterials Institute, REU student)
2016	Tara Picudella (Chemical Engineering)
2016	Masud Dikita Llewellyn (Chemical Engineering)
2016-2018	Jerry Gomez (Chemical Engineering)
2016	Natalie Edelstein (Bioengineering)(Dean's Leadership Award)
2015-2017	Aliza Khan (Bioengineering)
2014-2016	Sarah R. Willsey (Dean's Leadership Award)
2015	Ian Seddon (Syracuse Biomaterials Institute, REU student)
2014-2015	Alexis N. Peña (REM participant, LSAMP student)
2014	Benjamin Yue (Syracuse Biomaterials Institute, REU student)
2013-2014	Yee-Pien Cheng (Chemical Engineering)
2013-2014	Julie Theresa Hess (REM participant)

High School Students and Teachers

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

TEACHING

2019	CEN 451/651-Chemical Engineering Thermodynamics, <i>Instructor</i>
2018	CEN 353- Chemical Thermodynamics II, <i>Instructor</i>
2017	CEN 353- Chemical Thermodynamics II, <i>Instructor</i> ECS 326- Engineering Materials, Properties, and Processing, <i>Instructor</i>
2017	CEN 651-Chemical Engineering Thermodynamics, <i>Instructor</i>
2015-2017	CEN 601- BMCE Seminar, <i>Coordinator</i>
2016	CEN 353- Chemical Thermodynamics II, <i>Instructor</i> CEN 651-Chemical Engineering Thermodynamics, <i>Instructor</i>
2015	CEN 353- Chemical Thermodynamics II, <i>Instructor</i> CEN 651-Chemical Engineering Thermodynamics, <i>Instructor</i>
2014	CEN 353- Chemical Thermodynamics II, <i>Instructor</i>

	CEN 600- Multiscale computation methods, <i>Co-instructor</i>
	CEN 651-Chemical Engineering Thermodynamics, <i>Instructor</i>
2013	CEN 353- Chemical Thermodynamics II, <i>Instructor</i>
	CEN 651-Chemical Engineering Thermodynamics, <i>Instructor</i>
2012	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>
	CEN 600- Multiscale computation methods, <i>Co-instructor</i>
2011	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>
2010	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>

ADDITIONAL TEACHING TRAINING

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

ACADEMIC SERVICE

2019	<i>Chair</i> , Modeling of Lipid Membranes and Membrane Proteins, 2019 AIChE Annual Meeting, Orlando (November 10-15)
2019-present	<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	<i>Organizer</i> , Molecular engineering of soft matter: Spanning small molecules to macromolecules, Telluride Science Research Center, Telluride, CO (June 16-June 21)
2019	<i>Chair</i> , Non-tenured Faculty Review Committee, BMCE, Syracuse University
2019	<i>Member</i> , Meredith Teaching Award Selection Committee, Syracuse University
2019	<i>Member</i> , BMCE Faculty Search Committee
2018	<i>Member</i> , WiSE FPP Advisory Board, Syracuse University
2018	<i>Member</i> , Committee on Export Control, Syracuse University
2018	<i>Panelist</i> , NSF Biological and Environmental Interactions of Nanoscale Materials
2018	<i>Panelist</i> , NSF Interfacial transport
2018	<i>Chair</i> , Modeling of Lipid Membranes and Membrane Proteins, 2018 AIChE Annual Meeting, Minneapolis (October 28-November 2)

2018	<i>Chair</i> , 4 th Annual Neuroscience Day, Syracuse University, Syracuse (April 6, 2018)
2017	<i>Organizer</i> , Molecular engineering of soft matter: Spanning small molecules to macromolecules, Telluride Science Research Center, Telluride, CO (June 20-June 24)
2017	<i>Chair</i> , Modeling of Lipid Membranes and Membrane Proteins, 2017 AIChE Annual Meeting, Minneapolis (October 29-November 3)
2017	<i>Organizer</i> , 3 rd Annual Neuroscience Day, Syracuse University, Syracuse (April 7, 2017)
2016-2018	<i>Member</i> , ECS Faculty Council, Syracuse University
2016	<i>Chair</i> , Development of Intermolecular Potential Models, 2016 AIChE Annual Meeting, San Francisco (November 13-18).
2016	<i>Chair</i> , Biomimetic and Biohybrid Materials and Devices, 2016 AIChE Annual Meeting, San Francisco (November 13-18)
2016	<i>Panelist</i> , New Faculty Orientation Program, Syracuse University
2016	<i>Panelist</i> , NSF Particulate and Multiphase Processes panel on interfacial phenomena
2016	(February 9-10)
2015	<i>Member</i> , Department of Biomedical and Chemical Engineering Faculty Search Committee
2015	<i>Co-chair</i> , Biomimetic and Biohybrid Materials and Devices, 2015 AIChE Annual Meeting, Salt Lake City, UT
2015	<i>Panelist</i> , New Faculty Orientation Program, Syracuse University
2015	<i>Member</i> , Department of Psychology Faculty Search Committee
2015	<i>Coordinator</i> , Biomedical and Chemical Engineering Department Seminar Series
2015-2017	<i>Presenter</i> , workshop sponsored by Women in Science and Engineering (WiSE)
2014-present	<i>Member</i> , Neuroscience Executive Committee
2014	<i>Member</i> , Department of Physics Faculty Search Committee. <i>Emphasis on Experimental soft matter physics</i>
2014	
2014-2018	<i>Member</i> , Graduate Admissions Committee, Department of Biomedical and Chemical Engineering
2013-2017	<i>Member</i> , BMCE faculty representative for College of engineering and computer science website committee
2012	<i>Member</i> , Soft Interfaces IGERT @ SU Graduate Recruitment Committee
2012-2016	<i>Website coordinator</i> , Department of Biomedical and Chemical Engineering
2014	<i>Co-chair</i> , Biomimetic and Biohybrid Materials and Devices I and II, 2014 AIChE Annual Meeting, Atlanta, GA
2014	<i>Presenter</i> , workshop sponsored by Women in Science and Engineering (WiSE)
2013	<i>Member</i> , 39 th Annual Northeast Bioengineering Conference Program Committee
2013	<i>Reviewer</i> , Women in Science and Engineering–Future Professoriate Program (WiSE–FPP)
	Soft Interfaces IGERT @ SU Graduate Admissions Committee
2013	<i>Member</i> , Department of Biomedical and Chemical Engineering Faculty Search Committee,
	<i>Member</i> , Department of Biology and Chemistry Faculty Search Committee
2012-2013	<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> , 39 th Annual Northeast Bioengineering Conference, Syracuse
2013	<i>Member</i> , Department of Chemistry Faculty Search Committee

BROADER IMPACT AND OUTREACH

2019	Mentored high school student- ECS High School Research Internship Program
2018	Mentored two high school females in computational modeling-ECS Research Internship Program
2016	Mentored one high school student on computational modeling
2015	Project ENGAGE Instructor, Syracuse University
2014-2015	Mentored three high school student on hands-on multiscale molecular dynamics simulations
2014	Mentored, high-school teacher as part of the Research Experience and Mentoring (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