

## 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

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

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, 3 <sup>rd</sup> Annual Neuroscience Day, F. J. Irudayanathan (G)
2017	Second place poster, Stevenson Biomaterials Day, Jerry Gomez (UG)
2017	Graduate Research Fellowship Program, National Science Foundation, Alexis Peña (UG)

- 2016 Meredith Symposium Finalist, Syracuse University, Aliza Khan (UG)
- 2016 Bioengineering Founder's Award, Syracuse University, Alexis Peña (UG)
- 2016 The Chemical Computing Group Excellence Award for Graduate Students, American Chemical Society, Wenjuan Jiang (G)
- 2016 First place poster, Stevenson Biomaterials Day, F. J. Irudayanathan (G)
- 2016 Syracuse Biomaterials Institute Graduate Fellowship, Wenjuan Jiang (G)
- 2016 Graduate School Master of Science Prize, Syracuse University, Xiaoyi Wang (G)
- 2015 First Place Poster, Emerging Researchers National Conference, Alexis Peña (UG)
- 2015 Graduate School Master of Science Prize, Syracuse University, Huilin Ma (G)
- 2015 Graduate Research Fellowship Program, National Science Foundation, Joshua Woods (UG)
- 2015 First place poster, Syracuse University Neuroscience Research Day, F. J. Irudayanathan (G)
- 2014 First place poster, Stevenson Biomaterials Day, F. Jerome Irudayanathan (G)
- 2014 Third place poster, Stevenson Biomaterials Poster Day, Wenjuan Jiang (G)
- 2014 Best poster, Biomedical Research Conference for Minority Students, Alexis Peña (UG)
- 2014 Third place, LSMCE Conference Roadmap to Action: LSAMP Principles for Broadening Minority Participation in STEM, Alexis Peña (UG)
- 2014 Best BMCE poster award, Nunan Research Day, F. Jerome Irudayanathan (G)
- 2014 Outstanding Graduate Student in Bioengineering Award, Haarika Kamani (G)
- 2014 Graduate School Master of Science Prize, Syracuse University, Haarika Kamani (G)

## PUBLICATIONS

1. 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*, **ASAP** (2018).
2. 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*, **ASAP** (2018). *Featured on the cover.*  
<http://dx.doi.org/10.1021/acs.jpcc.8b03842>
3. 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.* **ASAP** (2018).  
<http://dx.doi.org/10.1021/acsbiomaterials.8b00486>
4. 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>
5. 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>
6. 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>
7. 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>
8. 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>

9. 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>
10. 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>
11. 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>
12. 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>
13. 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>
14. 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>
15. 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>
16. 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>
17. 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>
18. 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>
19. 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>
20. 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>
21. 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>
22. 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>
23. 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>

24. 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>
25. A new form of MgTa<sub>2</sub>O<sub>6</sub> obtained by the molten salt method, A. K. Ganguly, **S. Nangia**, M. Thirumal, and P. L. Gai, *Journal of Chemical Science*, **118** 37–42 (2006).  
<http://dx.doi.org/10.1007/BF02708763>
26. 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>
27. 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>
28. 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>
29. Army ants algorithm for rare event sampling of delocalized nonadiabatic transitions by trajectory surface hopping and the estimation of sampling errors by the bootstrap method, **S. Nangia**, A. W. Jasper, T. F. Miller III, and D. G. Truhlar, *Journal of Chemical Physics* **120**, 3586–3597 (2004).  
<http://dx.doi.org/10.1063/1.1641019>

## CONFERENCE PAPERS AND OTHER INDEXED JOURNAL PUBLICATIONS

1. 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,<sup>†</sup> Y. Liu, **S. Nangia**, and R. Sureshkumar, *Bioengineering Conference (NEBEC), 2013 39th Annual Northeast*.  
<http://dx.doi.org/10.1109/NEBEC.2013.129>
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	1028	14
Scopus	954	14
Web of Science	919	14

## RESEARCH AWARDS

**Gerber Grant** \$10,000 (total)  
 PI \$10,000  
 Essential role of tight junctions in sound transduction 7/1/2018- 6/30/2019

**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

<b>NSF CBET Award (Award # 1706061)</b>	\$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
<b>NSF REU Site</b>	\$318,863 (total)
Co-PI	5/1/2018 - 4/30/2021
Interactive Biomaterials: REU Site	
<b>NIH R21</b>	\$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
<b>NSF CAREER</b>	\$530,000 (total)
PI	\$530,000
Enabling Transport Across the Blood-Brain Barrier by Engineering Thermodynamically Favorable Pathways	4/1/2015 - 3/31/2020
<b>NSF REU Site</b>	\$297,506 (total)
Senior Personal	5/1/2015 - 4/30/2018
Interactive Biomaterials: REU Site	
<b>NSF EFRI</b>	\$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

<b>Anton2 (PSCA17073P)</b>	100,000 Units
PI	12/7/2017 –11/30/2018
Role of S-Palmitoylation on the Blood-Brain Barrier Tight Junction Interface	
<b>XSEDE Supercomputer Allocation MCB140216 (renewal)</b>	2.9 million hours
PI	(equivalent to \$65,006)
Multiscale Molecular Modeling of the Biomolecular Interfaces for Enhancing Drug Delivery and Designing Antimicrobial Peptides	7/1/2017 –6/30/2018
<b>XSEDE Supercomputer Allocation MCB140216</b>	1.3 million hours
PI	(equivalent to 46,267.71)
Multiscale Molecular Modeling of the Biomolecular Interfaces for Enhancing Drug Delivery and Designing Antimicrobial Peptides	10/01/2015 –09/30/2016

## TEACHING AWARDS

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

## PRESENTATIONS

- (Oral, Invited) Engineering pathways across biological barriers, Shikha Nangia, *Tulane University*, Minneapolis (January 25-26, 2018).

- (Oral, Invited) Modeling the protein-protein interactions at the blood-brain barrier interface, Shikha Nangia, *Application of Molecular Modeling to Study Interfacial Phenomena, AIChE Annual Meeting*, Minneapolis (October 29-November 2, 2017).
- (Oral, Invited) Multiscale modeling of complex biological interfaces, Shikha Nangia, *Molecular engineering of soft matter: Spanning small molecules to macromolecules*, Telluride, CO (June 19-23, 2017).
- (Oral, Invited) Breaking through the blood-brain barrier, Shikha Nangia, *Material Science and Engineering, University of Michigan*, Ann Arbor, MI (December 4, 2016).
- (Oral, Invited) Breaking through the blood-brain barrier, Shikha Nangia, *Chemical and Biological Engineering, Rensselaer Polytechnic Institute*, Troy, NY (October 19, 2016).
- (Oral, Invited) Breaking through the blood-brain barrier, Shikha Nangia, *Research Colloquy, Information Technology Services and Research Computing Advisory Council (RCAC)*, Syracuse University, Syracuse, NY (October 24, 2016).
- (Oral, Invited) Breaking through the blood-brain barrier, Shikha Nangia, *Syracuse Biomaterials Seminar Series, SBI, Syracuse University*, Syracuse, NY (October 4, 2016).
- (Oral, Invited) Breaking through the blood-brain barrier, Shikha Nangia, *School of Chemical and Biomolecular Engineering, Cornell University*, Ithaca, NY (September 26, 2016).
- (Oral, Invited) Breaking through the blood-brain barrier, Shikha Nangia, *SyracuseCoE Symposium, Syracuse University*, Syracuse, NY (September 22, 2016).
- (Oral, Invited) Breaking through the blood-brain barrier, Shikha Nangia, *Biomedical Engineering, Binghamton University*, Binghamton, NY (September 20, 2016).
- (Oral, Invited) Breaking through the blood-brain barrier, Shikha Nangia, *Chemical and Biomolecular Engineering, Clemson University*, Clemson, SC (September 15, 2016).
- (Oral, Invited) Multiscale simulations to characterize the blood-brain barrier tight junctions, Shikha Nangia, *2016 Middle Atlantic Regional Meeting MARM, Riverdale, NY* (June 9–12, 2016).
- (Oral, Invited) Engineering nanocarriers for brain tumor treatment, Shikha Nangia and Juntao Luo, *Nappi Research Award Competition, Syracuse University*, Syracuse, NY (December 11, 2015).
- (Oral) Coarse grained parameterization of gram-negative bacterial outer membrane, Shikha Nangia, *AIChE Annual Meeting, Salt Lake City, UT* (November 8–13, 2015).
- (Oral) Multiscale simulations to characterize the blood brain barrier tight junctions, Shikha Nangia, *AIChE Annual Meeting, Salt Lake City, UT* (November 8–13, 2015).
- (Oral, Invited) Insights into the blood brain barrier tight junctions for treatment of Alzheimer's disease, Shikha Nangia, *2015 West Virginia University*, Morgantown, WV (August 28, 2015).
- (Oral, Invited) Synergistic experimental and multiscale modeling approaches for optimizing anticancer drug nanocarriers, Shikha Nangia, *250<sup>th</sup> ACS National Meeting, Boston MA* (August 16–20, 2015).
- (Oral) Molecular characterization of the blood brain barrier tight junctions, *Young Investigator Symposium, Shikha Nangia, 250<sup>th</sup> ACS National Meeting, Boston MA* (August 16–20, 2015).
- (Oral) Spectroscopic properties of semiconductor quantum dots embedded in biological medium, B. Ellis, W. Jiang, J. Elward, F. J. Irudayanathan, Shikha Nangia, A. Chakraborty, *250<sup>th</sup> ACS National Meeting, Boston MA* (August 16–20, 2015).
- (Oral, Invited) Multiscale simulations to characterize the blood brain barrier tight junctions, Shikha Nangia, *Neuroscience Research Day, Syracuse, NY* (April 3, 2015).
- (Oral, Invited) Multiscale simulations to characterize the blood brain barrier tight junctions, Shikha Nangia, *Albany 2015: Conversation 19, Albany, NY* (June 9-13, 2015).
- (Oral) Introduction of computational simulations to high school students will increase their STEM knowledge and interest, Suzanne DeTore and Shikha Nangia, *2015 Emerging Researchers National (ERN) Conference in STEM*, Washington, D.C. (February 19-21, 2015).
- (Oral, Invited) Multiscale modeling approach to determine the role of amphiphilic building block in the stability of paclitaxel drug delivery nanocarriers, at *AIChE Annual Meeting, Atlanta, GA* (Nov. 16–22, 2014).

- (Oral), Cellular uptake of nanoparticles with protein coronas: A coarse-grained molecular dynamics simulations study, Aytan 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 *243<sup>rd</sup> ACS National Meeting, San Diego CA* (March 25–29, 2012).
- (Oral) Viscoelastic properties of bacterial biofilms using coarse-grained molecular dynamics simulations, at *AICHE Annual Meeting, Minneapolis MN* (October 16–21, 2011).
- (Oral) Coarse-grained molecular dynamics simulations of bacterial polysaccharides for studying flow-induced fragmentation mechanisms, at *241 ACS National Meeting, Anaheim CA* (March 27–31, 2011).
- (Oral, Invited) Theoretical and Computational Modeling of Dissolution Processes, at *SUNY-ESF, Syracuse, NY* (March 11, 2011)
- (Oral, Invited) Computational approaches of modeling dissolution of rocks and evolution of Earth surface, at *Rensselaer Polytechnic Institute, Troy, NY* (Feb. 8–9, 2010)
- (Oral) Dissolution studies of mineral-water interfaces using newly developed Monte Carlo algorithm, at *237th ACS National Meeting, Salt Lake City UT* (March 22–26, 2009).

## NEWS AND MEDIA

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](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

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).



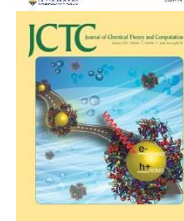
2015

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).



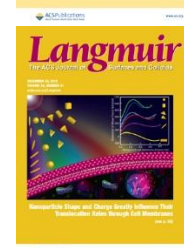
2015

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).



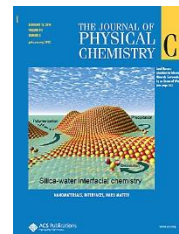
2012

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

### Ad hoc review for funding agencies

2014-2016 Ad-hoc reviewer, ACS PRF program  
2014-2016 NSF Panelist  
2014-2015 NSF GRFP Panelist

## MENTORING AND SUPERVISION OF RESEARCH ACTIVITIES

### Graduate Students

2017-present	Xichen Xu <i>Coarse grained parameterization of Gram-positive bacteria cell wall</i>
2016-present	Nandhini Rajagopal, Ph.D <i>Molecular architecture of tight junctions</i>
2015-present	Huilin Ma, Ph.D <i>Designing antimicrobial peptides effective against Gram-negative bacteria</i>
2013-present	Flaviyan Jerome Irudayanathan, Ph.D. student <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>
2017-2018	Lisa Danielle Nguyen, MS <i>Homotypic and heterotypic self-assembly of Claudin family of tight junction proteins</i>
2015-2016	Amogh Srihari, MS <i>Statistical Mechanical Treatments of the Optical Properties of CdSe Quantum Dots</i>
2014-2016	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>
2014-2015	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

2018-present	Naomi Brandt (Syracuse Biomaterials Institute, REU student)
2018-present	Natalie Marie Petryk (ECS Scholar)
2018-present	Bailey M Felix (ECS Scholar)
2018-present	Alejandro J Durand (ECS Scholar)
2018-present	Priya S Ganesh (ECS Scholar)
2018-present	Santita Ebangwese (Bioengineering)
2018-present	Austin Freer (Chemical Engineering)
2018-present	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

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

### ADDITIONAL TEACHING TRAINING

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

## ACADEMIC SERVICE

- 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, 2017 AIChE Annual Meeting, Minneapolis (October 28-November 2)
- 2018 *Chair*, 4<sup>th</sup> Annual Neuroscience Day, Syracuse University, Syracuse (April 6, 2018)
- 2017 *Organizer*, Molecular engineering of soft matter: Spanning small molecules to macromolecules, Telluride Science Research Center, Telluride, CO (June 20-June 24)
- 2017 *Chair*, Modeling of Lipid Membranes and Membrane Proteins, 2017 AIChE Annual Meeting, Minneapolis (October 29-November 3)
- 2017 *Organizer*, 3<sup>rd</sup> Annual Neuroscience Day, Syracuse University, Syracuse (April 7, 2017)
- 2016-2018 *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)
- 2015 *Member*, Department of Biomedical and Chemical Engineering Faculty Search Committee
- 2015 *Co-chair*, Biomimetic and Biohybrid Materials and Devices, 2015 AIChE Annual Meeting, Salt Lake City, UT
- 2015 *Panelist*, New Faculty Orientation Program, Syracuse University
- 2015 *Member*, Department of Psychology Faculty Search Committee
- 2015-2017 *Coordinator*, Biomedical and Chemical Engineering Department Seminar Series
- 2014 *Presenter*, workshop sponsored by Women in Science and Engineering (WiSE)
- 2014 *Member*, Department of Physics Faculty Search Committee. *Emphasis on Experimental soft matter physics*
- 2014-present *Member*, Graduate Admissions Committee, Department of Biomedical and Chemical Engineering
- 2013-present *Member*, BMCE faculty representative for College of engineering and computer science website committee
- 2012 *Member*, Soft Interfaces IGERT @ SU Graduate Recruitment Committee
- 2012-present *Website coordinator*, Department of Biomedical and Chemical Engineering
- 2014 *Co-chair*, Biomimetic and Biohybrid Materials and Devices I and II, 2014 AIChE Annual Meeting, Atlanta, GA
- 2014 *Presenter*, workshop sponsored by Women in Science and Engineering (WiSE)
- 2013 *Member*, 39th Annual Northeast Bioengineering Conference Program Committee
- 2013 *Reviewer*, Women in Science and Engineering–Future Professoriate Program (WiSE–FPP)
- 2013 *Member*, Soft Interfaces IGERT @ SU Graduate Admissions Committee
- 2013 *Member*, Department of Biomedical and Chemical Engineering Faculty Search Committee,

- 2012-2013 *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

#### **BROADER IMPACT AND OUTREACH**

- 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