

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

2012-present	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
2017	Meredith Teaching Recognition Award
2016	College Technology Educator of the Year, Technical Alliance of Central New York
2016	ACS OpenEye Outstanding Junior Faculty Award
2015	Nappi Research Competition Award
2015	NSF CAREER award
2015	Faculty Excellence Award, College of Engineering and Computer Science
2014	Syracuse University Nominee to the New York Academy of Sciences' Blavatnik Awards

HONORS AND AWARDS TO UNDERGRADUATE AND GRADUATE MENTEES

2017	First place poster, 3 rd Annual Neuroscience Day, F. J. Irudayanathan (G)
2017	Second place poster, Stevenson Biomaterials Day, Jerry Gomez (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 Syracuse University Graduate School Master of Science Prize, 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 Syracuse University Graduate School Master of Science Prize, Haarika Kamani (G)

PUBLICATIONS

1. 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*, **ASAP**.
2. 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>
3. 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>
4. 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>
5. 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>
6. 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>
7. 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>
8. 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>
9. 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>
10. 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>

11. 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>
12. 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>
13. 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>
14. 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>
15. 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>
16. 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>
17. 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>
18. 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>
19. 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>
20. Non-Born-Oppenheimer molecular dynamics, A. W. Jasper, **S. Nangia**, C.Y. Zhu, and D. G. Truhlar, *Accounts of Chemical Research* **39** 101-108 (2006).
<http://dx.doi.org/10.1021/ar040206v>
21. 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>
22. 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>
23. Introductory lecture: Nonadiabatic effects in chemical dynamics, A. W. Jasper, C.Y. Zhu, **S. Nangia**, and D. G. Truhlar, *Faraday Discussions* **127**, 1-22 (2004).
<http://dx.doi.org/10.1039/b405601a>
24. Coherent switching with decay of mixing: An improved treatment of electronic coherence for non-Born-Oppenheimer trajectories, C.Y. 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>
25. 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.
<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*

RESEARCH AWARDS

Nappi Research Award	\$100,000 (total)
Co-PI	\$45,000
Engineering nanocarriers for brain tumor treatment	6/1/2016 - 5/31/2017
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	\$500,000
PI	
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	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) 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).
- (Poster, Invited) Enabling transport across the blood brain barrier, Shikha Nangia, *251th ACS National Meeting, San Diego CA* (March 13–17, 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).
- (Poster) Unraveling the molecular architecture of blood brain barrier tight junctions, Flaviyan Jerome Irudayanathan and Shikha Nangia, *GRC Membrane Protein Folding*, Boston, MA (June 21-26, 2015).
- (Poster) Role of membrane composition and s-palmitoylation along the secretion pathway of transmembrane proteins insights from multiscale molecular dynamics of claudin-5, Flaviyan Jerome Irudayanathan and Shikha Nangia, *GRC Membrane Protein Folding*, Boston, MA (June 21-26, 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).

- (Poster) Investigation of mechanism of interaction of antimicrobial peptides with bacterial membrane, Alexia Pena, Huilin Ma, 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).
- (Poster) Investigating telodendrimer based cancer drug delivery micelles, Wenjuan Jiang, Juntao Luo, and Shikha Nangia, *GRC Drug Carriers in Medicine & Biology, Waterville valley, NH* (August 17-22, 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.
- (Poster) Investigation of Intracellular Vesicular Transport using multiscale molecular dynamics approach, Julie Hess 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).
- (Poster) Reaction mechanisms and dissolution rates of quartz in acidic, basic, and neutral media, at *234th ACS National Meeting, Boston MA* (August 19–23, 2007).
- (Poster) Army Ants Algorithm for Surface Hopping Calculations on Chemical Systems with Coupled Electronic States,” at *Computational Chemical Dynamics from Gas-Phase to Condensed-Phase Systems*, University of Minnesota, Minneapolis (October 7-9, 2004).
- (Poster) Army Ants Algorithm for Efficient Trajectory Surface Hopping, at *Non-adiabatic Effects in Chemical Dynamics*, Faraday Discussions 127, Oxford, UK (5–7 April 2004).

NEWS AND MEDIA

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

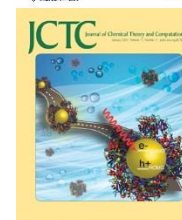
2015

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).

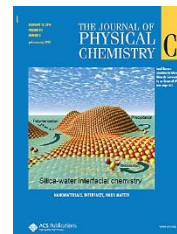


2012

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

2016-present	Nandhini Rajagopal, Ph.D. student <i>Molecular architecture of tight junctions</i>
2016-present	Ginger Star Peterman Ph.D. student <i>Outer membrane of gram-negative membrane</i>
2015-present	Huilin Ma, Ph.D. student <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>
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

2016	Tara Picudella (Chemical Engineering)
2016	Masud Dikita Llewellyn (Chemical Engineering)
2016-present	Jerry Gomez (Chemical Engineering)
2016	Natalie Edelstein (Bioengineering)(Dean's Leadership Award)
2015-present	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

2016	Yatin Zirath (student), Christian Brothers Academy, DeWitt
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

2015-2017	CEN 601- BMCE Seminar, <i>Coordinator</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>
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

2017	Nominated to participate in the upcoming career development event at ASEE Summer School for Chemical Engineering Faculty, <i>Raleigh</i> , NC State University (July 29-Aug. 3)
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

PEER REVIEWED JOURNAL PUBLICATIONS

Citation metrics reported from Web of Science, Scopus, and Google Scholar

	Total Citations	h-index
Web of Science	791	13
Scopus	798	13
Google Scholar	845	13

ACADEMIC SERVICE

2017	Organizer, Molecular engineering of soft matter: Spanning small molecules to macromolecules, Telluride Science Research Center, Telluride, CO (June 20-June 24)
2017	Organizer, 3 rd Annual Neuroscience Day, Syracuse University, Syracuse (April 7, 2017)
2016	Chair, Development of Intermolecular Potential Models, AIChE Annual Meeting, San Francisco (November 13-18)

- 2016 Chair, Biomimetic and Biohybrid Materials and Devices, 2015 AIChE Annual Meeting, San Francisco (November 13-18)
- 2016 Research Panel, 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. *Emphasis on stem cells and regenerative medicine research*
- 2015 Co-chair, Biomimetic and Biohybrid Materials and Devices, 2015 AIChE Annual Meeting, Salt Lake City, UT
- 2015 Research Panel, New Faculty Orientation Program, Syracuse University
- 2015-present Member, Department of Psychology Faculty Search Committee. *Emphasis on Cognition, Brain, & Behavior science*
- 2014 Biomedical and Chemical Engineering Department Seminar Series Coordinator
- 2014 Presenter, workshop sponsored by Women in Science and Engineering (WiSE)
- 2014-present Member, Department of Physics Faculty Search Committee. *Emphasis on Experimental soft matter physics*
- 2014-present Member, Graduate Admissions Committee
- 2013-present BMCE faculty representative for College of engineering and computer science website
- 2012-present committee
- 2014 Member, Soft Interfaces IGERT @ SU Graduate Recruitment Committee
- 2014 Website coordinator, Department of Biomedical and Chemical Engineering
- 2014 Co-chair, Biomimetic and Biohybrid Materials and Devices I and II, 2014 AIChE Annual Meeting, Atlanta, GA
- 2012-2013 Presenter, workshop sponsored by Women in Science and Engineering (WiSE)
- 2012-2013 Member of the Conference Program Committee, 39th Annual Northeast Bioengineering Conference, Syracuse
- 2013-present Portfolio Reviewer, Women in Science and Engineering–Future Professoriate Program (WiSE–FPP)
- 2013-2014 Soft Interfaces IGERT @ SU Graduate Admissions Committee
- 2012-2013 Member, Department of Biomedical and Chemical Engineering Faculty Search Committee, *Emphasis on energy and emerging energy technology*
- 2013-2014 Member, Department of Biology and Chemistry Faculty Search Committee. *Emphasis on experimental biochemistry*
- 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