

Samuel (Sam) S. Cho

Wake Forest University · Departments of Physics and Computer Science

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PROFESSIONAL EXPERIENCE

- Associate Professor** *2016 - Present*
Wake Forest University, Winston-Salem, NC
Departments of Physics and Computer Science
- Assistant Professor** *2010 - 2016*
Wake Forest University, Winston-Salem, NC
Departments of Physics and Computer Science
- Post-doctoral Fellow** *2007 - 2010*
University of Maryland, College Park, MD
Advisor: Devarajan Thirumalai
- Doctoral Research Fellow** *2001 - 2007*
University of California, San Diego, La Jolla, CA
Advisor: Peter Wolynes
- Undergraduate Researcher** *1999 - 2001*
University of Maryland, Baltimore, Baltimore, MD
Advisor: Alexander D. MacKerell, Jr.

EDUCATION

- University of California, San Diego** *2001 - 2007*
Ph.D., Physical Chemistry (2007)
M.S., Chemistry (2003)
- University of Maryland, Baltimore County** *1996 - 2001*
B.S., Molecular Biology and Biochemistry (2001)
B.S., Computer Science (2001)

AWARDS AND HONORS

Shively Family Faculty Fellowship (WFU)	2014 - 2017
NIH (NRSA) Post-Doctoral Research Fellowship (UMd)	2007 - 2010
Molecular Biophysics Training Grant (UCSD, NIH)	2003 - 2005
Teaching Assistant Excellence Award (UCSD)	2003
President's Scholar Award (UMBC)	1996 – 2001

PUBLICATION LIST (H-Index: 17; 1,534 Total Citations)

<https://scholar.google.com/citations?user=0g2nL00AAAAJ>

(underlined names are graduate students and italicized names are *undergraduates* mentored by the PI)

1. Izaguirre G, Pietruszko R, **Cho SS**, MacKerell AD. Human aldehyde dehydrogenase catalytic activity and structural interactions with coenzyme analogs. *J. Biomol. Struct. Dyn.* 2001, 19(3):429-447 (Impact Factor: 1.3).
2. Pan YP, Huang N, **Cho SS**, MacKerell AD. Consideration of molecular weight during compound selection in virtual target-based database screening. *J. Chem. Inf. Comp. Sci.* 2003, 43 (1): 267-272 (Impact Factor: 3.6).
3. Wymore T, Hempel J, **Cho SS**, MacKerell AD, Nicholas HB, Deerfield DW. Molecular recognition of aldehydes by aldehyde dehydrogenase and mechanism of nucleophile activation. *Proteins* 2004, 57 (4): 758-771 (Impact Factor: 3.4).
4. Yang SC, **Cho SS**, Levy Y, Cheung MS, Levine H, Wolynes PG, Onuchic JN. Domain swapping is a consequence of minimal frustration. *Proc. Natl. Acad. Sci., USA.* 2004, 101 (38): 13786-13791 (Impact Factor: 9.4).
5. Levy Y, **Cho SS**, Onuchic JN, Wolynes PG. A survey of flexible protein binding mechanisms and their transition states using native topology based energy landscapes. *J. Mol. Biol.* 2005, 346 (4): 1121-1145 (Impact Factor: 4.1).
6. Levy Y, **Cho SS**, Shen T, Onuchic JN, Wolynes PG. Symmetry and frustration in protein energy landscapes: A near degeneracy resolves the Rop dimer-folding mystery. *Proc. Natl. Acad. Sci., USA.* 2005, 102 (7):2373-2378 (Impact Factor: 9.4).
7. **Cho SS**, Levy Y, Onuchic JN, Wolynes PG. Overcoming residual frustration in domain-swapping: The roles of disulfide bonds in dimerization and aggregation. *Phys. Biol.* 2005, 2: S44-55 (Impact Factor 3.1).
8. Ferreira DU, **Cho SS**, Komives EA, Wolynes PG. The energy landscape of modular repeat proteins: Topology determines folding mechanism in the ankyrin family. *J. Mol. Biol.* 2005, 354 (4): 679-692 (Impact Factor: 4.1).

9. **Cho SS**, Levy Y, Wolynes PG. P versus Q: Structural reaction coordinates capture protein folding on smooth landscapes. *Proc. Natl. Acad. Sci., USA*. 2006, 103 (3): 586-591 (Impact Factor: 9.4).
10. Ferreira DU, Cervantes CF, Truhlar SME, **Cho SS**, Wolynes PG, Komives EA. Stabilizing I κ B α by 'consensus' design. *J. Mol. Biol.* 2007, 365 (4): 1201-1216 (Impact Factor: 4.1).
11. **Cho SS**, Weinkam P, Wolynes PG. Origins of barriers and barrierless folding of BBL. *Proc. Natl. Acad. Sci., USA*. 2008, 105 (1):118-123 (Impact Factor: 9.4).
12. Pincus DL, **Cho SS**, Hyeon C, Thirumalai D. Minimal models for protein and RNA: From folding to function., Chapter 6 in *Progress in Molecular Biology and Translational Science* edited by P. Michael Conn (2008) Academic Press, Vol. 84 (Impact Factor: 3.9).
13. Lenz P, **Cho SS**, Wolynes PG. Analysis of single molecule folding studies with replica correlation functions. *Chem. Phys. Lett.* 2009, 471 (4-6):310-314 (Impact Factor: 2.3).
14. **Cho SS**, Levy Y, Wolynes PG. Quantitative criteria for native energetic heterogeneity influences in the prediction of protein folding kinetics. *Proc. Natl. Acad. Sci., USA*. 2009, 106 (2):434-439 (Impact Factor: 9.4).
15. **Cho SS**, Pincus DL, Thirumalai D. Assembly mechanisms of RNA pseudoknots are determined by the stabilities of the constituent secondary structures. *Proc. Natl. Acad. Sci., USA*. 2009, 106 (41):17349-17357 (Impact Factor: 9.4).
16. Patro R, Ip CY, Bista S, **Cho SS**, Thirumalai D, Varshney A. MDMap : A system for data-driven layout and exploration of molecular dynamics simulations. *IEEE Symposium on Biological Data Visualization*, 2011, 111-118.
17. **Cho SS**, Reddy G, Straub JE, Thirumalai D. Molecular mechanism for the entropic stabilization of proteins by TMAO. *J. Phys. Chem. B* 2011, 115, 13401-13407 (Impact Factor: 3.7).
18. Biyun S, **Cho SS**, Thirumalai D. Folding of human telomerase RNA pseudoknot using ion-jump and temperature quench simulations. *J. Amer. Chem. Soc.* 2011, 133, 20634-20643 (Impact Factor: 9.9). Selected for "Spotlight on Recent JACS Publications": <http://pubs.acs.org/doi/pdf/10.1021/ja211674d>
19. Guthold M, **Cho SS**. Fibrinogen unfolding mechanisms are not too much of a stretch. *Structure*, 2011, 19, 1536-1538 (Impact Factor: 6.3).
20. Koculi E, **Cho SS**, Thirumalai D, Woodson SA. Folding of P5abc RNA is determined by direct coupling of secondary and tertiary structures. *Nucl. Acid Res.* 2012, 40, 1-10 (Impact Factor: 8.3).
21. Lipscomb TJ, Zou A, **Cho SS**. Parallel Verlet neighbor list algorithm for GPU-optimized MD simulations. *Proceedings of the ACM Conference on Bioinformatics, Computational Biology and Biomedicine*, 2012, 321-328 (21% acceptance rate).

22. Proctor AJ, Lipscomb TJ, Zou A, Anderson, JA, **Cho SS**. Performance analyses of a parallel Verlet neighbor list algorithm for GPU-optimized MD simulations. *Proceedings of the ASE/IEEE International Conference on Biomedical Computing*, 2012, 14-19. (7.5% acceptance rate, Best Paper Award)
23. Proctor AJ, Lipscomb TJ, Zou A, Anderson, JA, **Cho SS**. GPU-optimized coarse-grained MD simulations of protein and RNA folding and assembly. *ASE Science Journal*, 2012, 1, 1-11. (3.9% acceptance rate)
24. Li R, Ge H, **Cho SS**. Sequence-dependent base stacking interactions guide tRNA folding energy landscapes. *J. Phys. Chem. B*, 2013, 117, 12943-12952 (Impact Factor: 2.3).
25. Proctor AJ, Stevens CA, **Cho SS**. GPU-optimized hybrid neighbor/cell list algorithm for coarse-grained MD simulations of protein and RNA folding and assembly. *Proceedings of the ACM Conference on Bioinformatics, Computational Biology and Biomedicine*, 2013, 633-640 (29% acceptance rate).
26. Li R, Chen R, Chen P, Wen Y, Ke P-C, **Cho SS**. Computational and experimental characterizations of silver nanoparticle-apolipoprotein biocorona, *J. Phys. Chem. B*, 2013, 117, 13451-13456 (Impact Factor: 3.6).
27. **Cho SS**, Pauca VP, Johnson D, James Y. Computational Thinking for the Rest of Us: A Liberal Arts Approach to Engaging Middle and High School Teachers with Computer Science Students. *Proceedings of Society for Information Technology & Teacher Education International Conference*, 2014 (30% acceptance rate).
28. Leuchter JD, Green AT, Gilyard J, Rambarat CG, **Cho SS**. Coarse-grained and atomistic MD simulations of RNA and DNA folding. *Israel J. Chem. Special Issue: 2013 Nobel Prize in Chemistry: Computational Chemistry of Biomolecules*, 2014, 54: 1152-1164 (Impact Factor: 2.7).
29. Burg J, Pauca VP, Turkett W, Fulp E, **Cho SS**, Santago P, Cañas D, Gage HD. Engaging Non-Traditional Students in Computer Science through Socially-Inspired Learning and Sustained Mentoring. *Proceedings of the 46th ACM Technical Symposium on Computer Science Education*, 2015, 639-644 (36% acceptance rate).
30. Li R, Macnamara, LM, Leuchter JD, Alexander RW, **Cho SS**. MD Simulations of tRNA and Aminoacyl-tRNA Synthetases: Dynamics, Folding, Binding, and Allostery. *International Journal of Molecular Sciences, Special Issue: Functions of Transfer RNA*, 2015, 16:15872-15902 (Impact Factor: 2.3).
31. Li R, Stevens CA, **Cho SS**. Molecular dynamics simulations of protein-nanoparticle biocorona formation. *Modeling, Methodologies and Tools for Molecular and Nano-scale Communications*, Eds. Junichi Suzuki, Tadashi Nakano, Michael J. Moore, 2017, 241-256, Springer Publishing.

32. Li W, Lucioni T, Li R, Bonin K, **Cho SS**, Guthold M. Stretching single fibrin fibers hampers their lysis, *Acta Biomaterialia*, 2017, 60:264-274.

CURRENT SUPPORT

NVIDIA CUDA Research Center (PI: \$10,000 est. equipment)	2012 – 2017
NVIDIA CUDA Teaching Center (PI: \$10,000 est. equipment)	2011 – 2017

PAST SUPPORT

National Science Foundation, CBET (Co-PI: \$300,000, PI: Pu-Chun Ke, Clemson University, Dept. Physics and Astronomy)	2012 – 2015
Center for Molecular Communication and Signaling (WFU) (PI: \$20,000)	2012 – 2014
Google CS4HS (PI: \$15,000, Co-PI: Paúl Pauca, WFU Dept. Computer Science)	2012 – 2013
Science Research Fund (WFU) (PI: \$10,000)	2011 – 2012
NIH NRSA Postdoctoral Fellowship (UMd)	2007 – 2010

INVITED CONFERENCES/WORKSHOPS

1. Mesilla Chemistry Workshop: Multi-Scale Modeling of Biological Molecules (2009), Mesilla, NM. Ordered and/or parallel RNA folding mechanisms.
2. American Physical Society National Meeting (2009), Pittsburgh, PA. Stabilities of constituent hairpins determine whether RNA folds via ordered and/or parallel mechanisms.
3. NVIDIA GPU Technology Conference (2012), San Jose, CA. GPU-based molecular dynamics simulations of protein and RNA assembly. (competitive)
4. American Chemical Society National Meeting (2012), Philadelphia, PA. MD simulations of telomerase RNA pseudoknot and ribosome assembly.

5. ACM Conference on Bioinformatics, Computational Biology and Biomedicine (2012), Orlando, FL. Parallel neighbor lists for GPU-optimized MD simulations. (competitive; 21% acceptance rate)
6. ASE International Conference on BioMedical Computing (2012), Washington, DC. Performance analyses of a parallel Verlet neighbor list algorithm for MD simulations. (competitive; 7.5% acceptance rate)
7. American Physical Society National Meeting (2013), Baltimore, MD. Parallel Neighbor List Algorithm for GPU-Optimized MD Simulations.
8. ACM Conference on Bioinformatics, Computational Biology and Biomedicine (2013), Washington, DC. GPU-optimized hybrid neighbor/cell list algorithm for coarse-grained MD simulations of protein and RNA folding and assembly. (competitive; 29% acceptance rate)
9. Society for Information Technology & Teacher Education International Conference (2014), Jacksonville, FL. Computational Thinking for the Rest of Us: A Liberal Arts Approach to Engaging Middle and High School Teachers with Computer Science Students.
10. Kavli Institute for Theoretical Physics China: Macromolecular dynamics: structure, function and diseases (2014), Beijing, China. Coarse-Grained GPU Optimized MD Simulations of Biomolecular Folding and Assembly.
11. NVIDIA GPU Technology Conference (2015), San Jose, CA. GPU-Optimized Algorithms for Coarse-Grained MD Simulations of Protein-Nanoparticle Biocorona Formation. (competitive)

INVITED SEMINARS

1. Wake Forest University, Structural and Computational Biophysics Discussion Group (2010), Winston Salem, NC, RNA Folding and Ribosome Assembly.
2. University of Virginia, Department of Chemistry (2012), Charlottesville, VA. GPU-based molecular dynamics simulations of protein and RNA assembly.
3. University of North Carolina, Greensboro, Department of Computer Science (2012), Greensboro, NC. GPU-optimized molecular dynamics simulations of ribosome assembly.
4. University of Maryland School of Pharmacy, Department of Pharmaceutical Sciences (2013), Baltimore, MD. tRNA Folding Energy Landscapes and GPU-Optimized MD Simulations.
5. Winston-Salem State University, Department of Chemistry (2013), Winston-Salem, NC. Coarse-Grained MD Simulations of Protein and RNA Folding and Assembly.

6. Wake Forest University, Structural and Computational Biophysics Discussion Group (2013), Winston Salem, NC. Coarse-Grained GPU Optimized MD Simulations of Biomolecular Folding and Assembly.
7. Nanjing University, Department of Physics (2014), Nanjing, China. Coarse-Grained GPU Optimized MD Simulations of Biomolecular Folding and Assembly.
8. Wake Forest University, Structural and Computational Biophysics Discussion Group (2015), Winston Salem, NC. Computational and Experimental Characterization of rDNA and rRNA G-Quadruplexes and Their Interactions with Small Molecules.

POSTER PRESENTATIONS

1. American Chemical Society Meeting (2000), Washington, DC. MD simulations of NAD(+) coenzyme analogs in the active site of ALDH reveal the impact of chemical substitutions on enzymatic activity.
2. Gordon Research Conference: Protein Folding Dynamics (2004), Ventura, CA. The principle of minimal frustration in domain-swapping.
3. Biophysical Society Meeting (2004), Baltimore, MD. Application of the principle of minimal frustration to structure prediction of domain-swapping proteins.
4. Protein Society Meeting (2006), San Diego, CA. Minding your p's and q's: Structural reaction coordinates capture protein folding on smooth landscapes.
5. Protein Society Meeting (2008), San Diego, CA. Two state or not two state: Origins of barriers and barrierless folding of BBL.
6. Biophysical Society Meeting (2010), San Francisco, CA. Assembly mechanisms of RNA pseudoknots are determined by the stabilities of the constituent secondary structures.
7. Biophysical Society Meeting (2014), San Francisco, CA. Computational and experimental characterizations of silver nanoparticle-apolipoprotein biocorona.

MANUSCRIPT PEER REVIEWER (Total: 44)

Proceedings of the National Academy of Sciences (1), PLoS One (1), PLoS Computational Biology (6), Biophysical Journal (1), Nucleic Acids Research (3), Journal of Physical Chemistry B (4), Proteins: Structure, Function, and Bioinformatics (5), Journal of Physical Chemistry Letters (1), Journal of Molecular Biology (1), Physical Chemistry Chemical Physics (1), ChemPhysChem (1), ACS Chemical Neuroscience (1), ACS Catalysis (1), IEEE Transactions on NanoBioscience (1), Environmental Science Nano (2), Springer Publishing (3), Journal of

Chemical Information and Modeling (5), BMC Research Notes (1), BMC Biophysics (1), Israel Journal of Chemistry (2), Nanotechnology Reviews (1), Journal of Molecular Graphics and Modeling (1)

GRANT PROPOSAL REVIEWER

National Institutes of Health (MSFB Study Section), National Science Foundation, Department of Energy, Oak Ridge Associated Universities

CONFERENCE PROGRAM COMMITTEE MEMBER

1. 8th International Conference on Bio-inspired Information and Communications Technologies (2014), Boston, MA.

CLASSES TAUGHT (Total: 548 Undergraduate / 39 Graduate Students)

1. Fall 2010: PHY 320/620: Physics of Biological Macromolecules (9U/5G)
2. Spring 2011: CSC 221: Data Structures and Algorithms I (13U)
3. Fall 2011: CSC 221: Data Structures and Algorithms I (12 U)
4. Fall 2011: CSC 391/691: GPU Programming (4U/8G)
5. Spring 2012: PHY 113: General Physics (81U)
6. Fall 2012: CSC 391/691: GPU Programming (5U/2G)
7. Fall 2012: PHY 320/620: Physics of Biological Macromolecules (6U/9G)
8. Spring 2013: CSC 221: Data Structures and Algorithms I (10U)
9. Spring 2013: PHY 113: General Physics (15U)
10. Fall 2013: CSC 221: Data Structures and Algorithms I (35U)
11. Fall 2013: PHY 113: General Physics (25U)
12. Spring 2014: CSC 221: Data Structures and Algorithms I (19U)
13. Spring 2014: PHY 113: General Physics (47U)
14. Fall 2014: PHY 320/620: Physics of Biological Macromolecules (11U/4G)
15. Fall 2015: PHY 113: General Physics (56U)
16. Fall 2015: CSC 391/691: GPU Programming (12U/4G)

17. Spring 2016: PHY 114: General Physics II (53U)
18. Spring 2016: CSC 221: Data Structures and Algorithms I (25U)
19. Fall 2016: PHY 320/620: Physics of Biological Macromolecules (10U/1G)
20. Fall 2016: CSC 391/691: Machine Learning (9U)
21. Fall 2016: CSC 391/691: Many Core Algorithms (1U/1G)
22. Spring 2017: CSC 111: Introduction to Computer Science (30U)
23. Fall 2017: PHY 113: General Physics (43U)
24. Fall 2017: CSC 391/691: GPU Programming (10U/5G)
25. Fall 2017: CSC 391: High Performance Computing (6U)

OUTREACH AND SERVICE

Wake Forest University Dept. Physics Graduate Committee Member	<i>2010 – 2017</i>
Wake Forest University Dept. Computer Science Graduate Committee Member	<i>2010 – 2017</i>
Wake Forest University Lower Division Advisor	<i>2012 – 2015</i>
Organizer of Computational Thinking Workshop for Teachers	<i>2012 – 2014</i>
Wake Forest University Fulbright Fellowship Committee Member	<i>2012 – 2017</i>
Wake Forest University STEM@Wake Committee Member	<i>2012 – 2017</i>
Grace Hopper Women in Computing Scholarship Committee Member	<i>2015 – 2016</i>
Wake Forest University Health Professions Committee Member	<i>2016 – 2017</i>
Biophysical Society Committee for Inclusion and Diversity	<i>2017 – 2020</i>

STUDENTS MENTORED

1. *Tyson Lipscomb (WFU, Computer Science, M.S.), 2011 – 2012
2. *Rongzhong Li (WFU, Physics, Ph.D.), 2011 – Present
3. *Anqi Zou (WFU, Computer Science, B.S., Mathematical Business, B.S.), 2011 – 2012
4. *Andrew Proctor (WFU, Computer Science, M.S.), 2012 – 2013
5. *Heming Ge (Cornell University, Physics, B.S.), 2012 (summer)
6. *Jessica Leuchter (WFU, Chemistry, B.S.), 2013 – 2014
7. *Cody Stevens (WFU, Computer Science, B.S., M.S.), 2013 – 2015
8. *Adam Green (WFU, Biology, B.S.), 2013 – 2014
9. *Julian Gilyard (WFU, Computer Science, B.S., Mathematical Economics, B.S.), 2013 – 2016
10. *Cecilia Rambarat (WFU, Chemistry, B.S.), 2013 – 2015
11. William Nicholson (WFU, Biophysics, B.S.), 2014 – 2015
12. Lauren Nelson (WFU, Physics, M.S.), 2014 – Present
13. Manal Ahmidouch (WFU, Biophysics, B.S.), 2014 – Present
14. Sajant Anand (WFU, Physics, B.S., Computer Science, B.S.), 2015 – Present
15. Daniel Vickers (WFU, Biophysics, B.S.), 2015 – Present
16. Melisa Carranza (WFU, Computer Science, M.S.), 2016 – 2017
17. Smiti Kaul (WFU, Computer Science, B.S., Mathematics, B.A.), 2016 – Present
18. Kedi Zheng (WFU, Computer Science, B.S.), 2017 – Present
19. Meijian Guan (WFU, Computer Science, M.S.), 2017 – Present
20. Haoze Du (WFU, Computer Science, M.S.), 2017 – Present
21. Caroline Kuczynski (WFU, Physics, B.S.), 2017 – Present

* Author in at least one peer-reviewed publication

THESES SUPERVISED

Rongzhong Li (Ph.D., Physics), *Molecular Dynamics Simulations of Bio-molecular Dynamics, Folding, and Assembly*, 2015.

Tyson Lipscomb (M.S., Computer Science), *GPU-Optimized Molecular Dynamics Simulations*, 2012.

Andrew Proctor (M.S., Computer Science), *GPU-Optimized Hybrid Neighbor/Cell List Algorithm for Coarse-grained Molecular Dynamics Simulations*, 2013.

Cody Stevens (M.S., Computer Science), *GPU-Optimized Graph Theory Analysis of Allosteric Protein Signaling Networks*, 2014.

Jessica Leuchter (B.S., Chemistry), *Molecular Dynamics Simulations of a Refined Modeled MetRS:tRNA^{Met} Complex*, 2014.

William Nicholson (B.S., Physics), *Quantifying the Stability of Acridines to Putative Ribosomal DNA G-quadruplexes*, 2015.

Julian Gilyard (B.A., Computer Science), *Multi-Threaded Machine Learning Algorithms for Low-Volatility Stock Options*, 2016.

Melisa Carranza (M.S., Computer Science), *Dynamic Parallelism in GPU-Optimized Barnes Hut Trees for Molecular Dynamics Simulations*, 2017.

SELECTED STUDENT PRESENTATIONS

Rongzhong Li, *Ion Concentration Dependent MD Simulations of tRNA Folding Mechanisms*, Gordon Research Conference: Protein Folding Dynamics, Ventura, CA, 2011 (poster).

Tyson Lipsomb, *GPU-Based Molecular Dynamic Simulations Optimized with CUDPP and CURAND Libraries*, NVIDIA GPU Technology Conference, San Jose, CA, 2012 (competitively selected poster; ~60% acceptance rate).

Anqi Zou, *Single vs. Double Precision MD Simulations: Correlation is Length-Scale Dependent*, NVIDIA GPU Technology Conference, San Jose, CA, 2012 (competitively selected poster; ~60% acceptance rate).

Rongzhong Li, *Molecular Conformational Signaling Networks Determine Ion Concentration Dependent tRNA Folding Mechanisms*, Center for Molecular Communication and Signaling Fall Retreat, Winston-Salem, NC, 2012 (invited talk).

Rongzhong Li, *Ion Concentration Dependent MD Simulations of tRNA Folding Mechanisms*, American Physical Society Meeting, Baltimore, MD, 2013 (invited talk).

Andrew Proctor, *Performance Analyses of a Parallel Verlet Neighbor List Algorithm for GPU-Optimized MD Simulations*, NVIDIA GPU Technology Conference, San Jose, CA, 2013 (competitively selected poster; ~60% acceptance rate).

Jessica Leuchter, *Molecular Dynamics Simulations of a Refined Modeled MetRS:tRNA^{Met} Complex*, 552nd WE-Heraeus Seminar at the Karlsruhe Institute of Technologie (Germany), 2014 (invited poster).

Adam Green, *Validation and Physical Characterization of Ribosomal G-Quadruplexes with MD Simulations*, Biophysical Society Meeting, San Francisco, CA, 2015 (poster).

Cody Stevens, *GPU Optimized Allosteric Communication Network Analyses of Molecular Dynamics Simulations*, NVIDIA GPU Technology Conference, San Jose, CA, 2014 (competitively selected poster; ~60% acceptance rate).

Rongzhong Li, *A True Random Number Generator Algorithm from Digital Camera Image Noise for Varying Light Conditions*, North Carolina Academy of Science Annual Meeting, 2015 (invited talk).

Cecilia Rambarat, *Atomistic and Coarse-Grained MD Simulations of the Intrinsically Disordered Bacillus Subtilis Ribonuclease P Protein*, Biophysical Society Meeting, Baltimore, MD, 2015 (poster).

William Nicholson, *Quantifying the Stability of Acridines to Putative Ribosomal G-Quadruplexes*, Biophysical Society Meeting, Baltimore, MD, 2015 (poster).

Rongzhong Li, *A True Random Number Generator Algorithm from Digital Camera Image Noise for Varying Light Conditions*, IEEE Southeast Conference, Fort Lauderdale, FL, 2015 (invited talk).

Manal Ahmidouch, *Computational and Experimental Characterization of Ribosomal DNA and RNA G-quadruplexes*, Biophysical Society Meeting, New Orleans, LA, 2017 (poster).

Lauren Nelson, *MD Simulations and Experimental Characterization of Neuroglobin and Mutants*, Second Molecular Biophysics Symposium at Virginia Tech, Blacksburg, VA, 2017 (invited talk).

SELECTED MEDIA COVERAGE

- J. Amer. Chem. Soc. Spotlight highlighting manuscript in collaboration with coworkers from University of Maryland and Zhejiang University (China): <http://pubs.acs.org/doi/pdf/10.1021/ja211674d>
- Wired.co.uk profiles research group: <http://www.wired.co.uk/news/archive/2012-02/17/videogame-gpus-for-cancer-simulations>
- Wake Forest University News profiles research of undergraduate group member, Anqi Zou: <http://news.wfu.edu/2012/02/16/can-a-video-game-cure-cancer/>

- Wake Forest University's Student Newspaper, Old Gold and Black, profiles undergraduate research group member, Anqi Zou:
<http://oldgoldandblack.com/?p=17732>
- Fox 8 News profiles our research group and Computer Science MS group member, Tyson Lipscomb, is interviewed:
<http://myfox8.com/2012/02/16/videogames-take-a-role-in-treating-cancer-at-wake-forest/>
- Wake Forest University News ranks news of our research group #4 of top 10 science research stories of the 2011-2012 academic year:
<http://news.wfu.edu/2012/06/21/spotlight-on-science/>
- Mashable (and Huffington Post) selects Wake Forest University as one of the "Top 10 Colleges for Tech" and specifically highlights our Computational Thinking Workshop:
<http://mashable.com/2012/08/24/best-tech-colleges/#UFFhF1sHvmq5>
- Wake Forest University News profiles Computational Thinking Workshop and Computer Science MS group member, Andrew Proctor, is interviewed:
<http://news.wfu.edu/2012/09/04/computers-in-the-middle/>
- Fox 8 News profiles Computational Thinking Workshop and Computer Science MS group member, Andrew Proctor, is interviewed:
<http://myfox8.com/2012/09/21/buckley-report-computers-in-middle-school/>
- NVIDIA's CUDA Week in Review Newsletter spotlights thesis of Computer Science MS group member, Tyson Lipscomb:
<http://www.nvidia.com/content/newsletters/web/CUDA-Week-in-Review-sept-28-12-web.html>
- Wake Forest University's Student Newspaper, Old Gold and Black, profiles Physics Colloquium speaker, Prof. Alexander D. Mackerell (invited my Sam Cho):
<http://oldgoldandblack.com/?p=27434>
- NVIDIA's CUDA Week in Review Newsletter spotlights thesis of Computer Science MS group member, Andrew Proctor:
<http://www.nvidia.com/content/newsletters/web/CUDA-Week-in-Review-july-03-13-web.html>
- Wake Forest University News profiles research of undergraduate group member, Jessica Leuchter: <http://news.wfu.edu/2014/02/28/the-birds-and-the-bees-of-proteins/>
- Wake Forest News profiles Manal Ahmidouch and Melisa Carranza in an article about gender diversity in STEM: <http://news.wfu.edu/2017/01/24/gender-diversity-in-stem-lets-change-the-world-together/>

- Wake Forest News profiles Manal Ahmidouch in an article about receiving her travel award to the internationally attended Biophysical Society Meeting:
<http://news.wfu.edu/2017/02/07/undergrads-cancer-research-success-earns-international-attention/>
- Spectrum News features Manal Ahmidouch in a segment on gender diversity in STEM:
<http://www.twcnews.com/nc/triad/news/2017/03/21/gender-equality-in-stem-careers-a-long-way-off--statistics-reveal.html>

THESIS COMMITTEE MEMBER

David Harrison (Ph.D., Physics; 2017), Evan Welchman (Ph.D., Physics; 2017), Ye Zheng (Ph.D., Chemistry; 2016), Amanda Smelner (Ph.D., Physics; 2016), Andrea Belanger (Ph.D., Physics, 2015), Jie Liu (Ph.D., Physics, 2015), Yuyang Zhu (Ph.D., Chemistry, 2015), Steven Johnson (M.S., Computer Science, 2015), Abdulmalik Obaid (Senior Thesis, Physics, 2015), Kelli Simms (Senior Thesis, Physics, 2015), Xinran Zhang (Senior Thesis, Physics, 2015), Papri Banerjee (Ph.D., Chemistry), Lee Ann Graham (Ph.D., Chemistry, 2012), Ivan Azarov (Ph.D., Physics, 2011) Don Nguyendac (Senior Thesis, Physics, 2011), Brandon Turner (Senior Thesis, Physics, 2011)

Last Updated: December 22, 2017