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Education

2005	Ph.D., Chemistry, Stanford University, Stanford, CA
1999	A.B., Chemistry, *magna cum laude*, Harvard University, Cambridge, MA

Positions

2021–current	Professor, Department of Chemical and Biological Engineering, University of Colorado Boulder
2022-current	University Associate, National Renewable Energy Labs, Golden, CO
2015–2021	Associate Professor, Department of Chemical and Biological Engineering, University of Colorado Boulder
2014–2015	Associate Professor, Department of Chemical Engineering, University of Virginia
2014–2015	Associate Professor, Department of Chemistry (by courtesy), University of Virginia
2008–2014	Assistant Professor, Department of Chemical Engineering, University of Virginia
2005–2008	NIH NRSA Postdoctoral Fellowship, Columbia University (under Richard A. Friesner)
1999–2005	Graduate Research, Stanford University (under Vijay S. Pande)

Honors and Awards

2020	AICHE CoMSEF Impact Award
2017–current	Psivant Sciences (previous Silicon Therapeutics) Open Science Fellow
2014	NSF CAREER Award
2012	American Chemical Society COMP OpenEye Outstanding Junior Faculty Award
2009	Oak Ridge Associated Universities Ralph E. Powe, Jr. Faculty Enhancement Award
2009	University of Virginia FEST Distinguished Young Investigator Award
2007	Sanibel Symposium IBM-Lowdin Fellowship
2005–2008	NIH Ruth L. Kirschstein NRSA Postdoctoral Fellowship
2004	ACS Chemical Computer Group Graduate Excellence Award
1999–2004	Fannie and John Hertz Graduate Fellowship
1999–2002	Paul Flory Fellowship (Stanford)
1999–2002	William R. and Sara Hart Kimball Stanford Graduate Fellowship
1999	National Science Foundation Graduate Fellowship (declined)
1999	National Defense Science and Engineering Graduate Fellowship (declined)

Refereed Publications (Google Scholar Profile):

1. M. Ramšak, D. A. Ramirez, L. E. Hough, S Vidmar, K. E. Filipič, G. Anderluh, M. R. Shirts, R. Jerala, “Programmable de novo designed coiled coil-mediated phase separation in mammalian cells”, *Nat. Comm.* 14(1), 7973 (2023)
2. A. J. Friedman, H. M. Padgette, L. Kramer, E. T. Liechty, G. W. Donovan, J. M. Fox, M. R. Shirts, “Biophysical rationale for the selective inhibition of PTP1B over TCPTP by nonpolar terpenoids”, *J. Phys. Chem B*, 127, 39, 8305–8316 (2023)
3. E. T. Liechty, A. Hren, L. Kramer, G. Donovan, A. J. Friedman, M. R. Shirts, J. M. Fox “Analysis of neutral mutational drift in an allosteric enzyme,” Prot. Sci., 32(8), e4719, (2023)
4. S. Boothroyd, P. K. Behara, O. C. Madin, D. F. Hahn, H. Jang, V. Gapsys, J. R. Wagner, J. T. Horton, D. L. Dotson, M. W. Thompson, J. Maat, T. Gokey, L.-P. Wang, D. J. Cole, M. K. Gilson, J. D. Chodera, C. I. Bayly, M. R. Shirts*, D. L. Mobley*, “Development and Benchmarking of Open Force Field 2.0.0—the Sage Small Molecule Force Field,” *J. Chem. Theory Comput*, 19 (11), 3251–3275, (2023) (* co-corresponding)
5. O. C. Madin and M. R. Shirts, "Using physical property surrogate models to perform multi-fidelity global optimization of force field parameters", *Digital Disc*, 2, 828–847 (2023)
6. W.-T. Hsu, V. Pimponi, P.T. Merz, G. Bussi, and M. R. Shirts, “Adding alchemical variables to metadynamics to enhance sampling in free energy calculations". *J. Chem. Theory Comput*, 19 (6), 1805–1817 (2023)
7. A. J. Friedman, E. T. Liechty, L. Kramer, A. Sarkar, J. M. Fox, M R. Shirts**,** “Allosteric Inhibition of PTP1B by a Nonpolar Terpenoid,” *J. Phys. Chem. B*, 126 (42) ,8427–8438 (2022)
8. J. Hénin, T. Lelièvre, M. R. Shirts, O. Valsson, L. Delemotte, “Enhanced Sampling Methods for Molecular Dynamics Simulations,” *Living J. Comput. Mol. Sci*. 4 (1), 1583 (2022)
9. S. Sahu, N. A. Schwindt, B. J. Coscia, and M. R. Shirts, “Obtaining and characterizing stable bicontinuous cubic morphologies and their nanochannels in lyotropic liquid crystal membranes,” *J. Phys. Chem. B* 2022, 126 (48) 10098–10110 (2022)
10. T. L. Fobe, C. C. Walker, G. A. Meek, M. R. Shirts, “Folding Coarse-Grained Oligomer Models with PyRosetta,” *J. Chem. Theory Comput.* 18 (10) 6354–6369 (2022)
11. C. C. Walker, T. L. Fobe, M. R. Shirts, “How cooperatively folding are homopolymer molecular knots?” *Macromolecules* 2022, 55, 19, 8419–8437 (2022)
12. S. Boothroyd, L.P. Wang, J. D. Chodera, D. L. Mobley, M. R. Shirts, “The Open Force Field Evaluator: An automated, efficient, and scalable framework for the estimation of physical properties from molecular simulation,” *J. Chem. Theory Comput.* 18 (6), 3566–3576 (2022)
13. S. Boothroyd*, O. C. Madin*, D. L. Mobley, L.-P. Wang, J. D. Chodera, M. R. Shirts, “Improving force field accuracy by training against condensed phase mixture properties,” *J. Chem. Theory Comput.* 18 (6), 3577-3592 (2022) *these authors contributed equally.
14. W.-T. Hsu, D. A. Ramirez, T. Sammakia, Z. Tan, M. R. Shirts, “Identifying signatures of proteolytic stability and monomeric propensity in O-glycosylated insulin using molecular simulation,” *J. Comput. Aid. Drug Des*. 36 (4), 313-328 (2022)
15. O. C. Madin, S. Boothroyd, R. A. Messerly, J. D. Chodera, J. Fass, M. R. Shirts “Bayesian inference-driven model parameterization and model selection for 2CLJQ fluid models,” *J. Chem. Inf. Model*. 62(4), 874–889 (2022)

16. P. T. Merz, W.-T. Hsu, M. W. Thompson, S. Boothroyd, C. C. Walker, and M. R. Shirts, “physical_validation: A Python package to assess the physical validity of molecular simulations” *J. Open Source Soft.* 7(69), 3981 (2022)
17. Y. Qiu, D. Smith, S. Boothroyd, H. Jang, J. Wagner, C. C. Bannan, T. Gokey, V. T. Lim, C. Stern, A. Rizzi, X. Lucas, B. Tjanaka, M. R. Shirts, M. K. Gilson, J. D. Chodera, C. I. Bayly, D. L. Mobley, and L.-P Wang, “Development and Benchmarking of Open Force Field v1.0.0, the Parsley Small Molecule Force Field,” *J. Chem. Theory Comput.*, 17(10), 6262–6280 (2021)
18. S. Zhang, D. F. Hahn, M. R. Shirts, V. A. Voelz, “Expanded ensemble methods can be used to accurately predict protein-ligand relative binding free energies,” *J. Chem. Theory Comput*, 17(10), 6536–6547 (2021)
19. C. C. Walker*, G. A. Meek*, T. L. Fobe, M. R. Shirts, “Using a Coarse-grained Modeling Framework to Identify Oligomeric Motifs with Tunable Secondary Structure,” *J. Chem. Theory Comput.*, 17(10), 6018–6035 (2021) *these authors contributed equally.
20. A. F. Kleman, D. L. Dufek, T. L. Fobe, D. R. McCaslin, B. P. Cary, M. R. Shirts, Michael, S. H. Gellman, "Potential Foldamers Based on an *ortho*-Terphenyl Amino Acid", *Org. Lett.*, 23(12), 4855–4859 (2021)
21. A. S. J. S. Mey, B. K. Allen, H. E. Bruce Macdonald, J. D. Chodera, D. F. Hahn, M. Kuhn, J. Michel, D. L. Mobley, L. N. Naden, S. Prasad, A. Rizzi,, J. Scheen. M. R. Shirts, G. Tresadern, H. Xu,” Best Practices for Alchemical Free Energy Calculations.” *Living J. Comput. Mol. Sci*. 2(1), (2020)
22. N. S. Abraham and M. R. Shirts, “Statistical mechanical approximations to more efficiently determine polymorph free energy differences for small organic molecules,” *J. Chem. Theory Comput.* 16(10), 6503–6512 (2020)
23. B. J. Coscia, C. P. Calderon, and M. R. Shirts, “Statistical Inference of Transport Mechanisms and Long Time Scale Behavior from Time Series of Solute Trajectories in Nanostructured Membranes,” *J. Phys. Chem B*. 124(37), 8110–8123 (2020)
24. B. J. Coscia and Michael R. Shirts, “Capturing Subdiffusive Solute Dynamics and Predicting Selectivity in Nanoscale Pores with Time Series Modeling”, *J. Chem. Theory Comp*. 16(7), 5456–5473 (2020)
25. M. R. Shirts and A. L. Ferguson, “Statistically optimal continuous free energy surfaces from umbrella sampling and multistate reweighting,” *J. Chem. Theory Comp.*16(7), 4107–4125 (2020)
26. A. Rizzi, T. Jensen, D. R Slochower, M. Aldeghi, V. Gapsys, D. Ntekoumes, S. Bosisio, M. Papadourakis, N. M. Henriksen, B. L De Groot, Z. Cournia, A. Dickson, J. Michel, M. K Gilson, M. R. Shirts, D. L Mobley, J. D Chodera, “The SAMPL6 SAMPLing challenge: Assessing the reliability and efficiency of binding free energy calculations”, *J. Comput. Aid. Mol. Des.* 34, 601–633 (2020)
27. G. E. Dwulet, B. J. Coscia, M. R. Shirts, and D. L. Gin, “A Nanostructured Bifunctional Acid-Base Catalyst Resin Formed by Lyotropic Liquid Crystal Monomers”, *Can. J. Chem*. 98(3), 332–336 (2020)
28. V. Balasubramanian, T. Jensen, M. Turilli, P. Kasson, M R. Shirts, and S. Jha, “Adaptive Ensemble Biomolecular Applications at Scale," *SN Comput. Sci.* 1, 104 (2020)
29. N. S. Abraham and M. R. Shirts, “Adding anisotropy to the quasi-harmonic approximation fails to capture accurate organic crystal thermodynamics,” *Cryst. Growth Des.* 19(12), 6911–6924 (2019)

30. E. C. Dybeck, D. P. McMahon, G. M. Day, and M. R. Shirts, “Exploring the Multi-minima Behavior of Small Molecule Crystal Polymorphs at Finite Temperature" *Cryst. Growth Des.* 19(10), 5568–5580 (2019)
31. R. A. Messerly, M. S. Barhaghi, J. J. Potoff, and M. R. Shirts, "Histogram-free reweighting with grand canonical Monte Carlo: Post-simulation optimization of non-bonded potentials for phase equilibria." *J. Chem. & Eng, Data,* 64(9), 3701–3717 (2019)
32. B. J. Coscia and M. R. Shirts, “Chemically Selective Transport in a Cross-Linked H_{II} Phase Lyotropic Liquid Crystal Membrane” *J. Phys. Chem. B*. 123(29), 6314–6330 (2019)
33. M. R. Shirts and N. P. Schieber, “Configurational Mapping Significantly Increases the Efficiency of Solid-Solid Phase Coexistence Calculations via Molecular Dynamics: Determining the FCC-HCP Coexistence Line of Lennard-Jones Particles,” *J. Chem. Phys.* 150(16), 164112 (2019)
34. C. Zanette, C. C. Bannan, C. I. Bayly, J. Fass, M. K. Gilson, M. R. Shirts, J. D. Chodera, D. L. Mobley, “Toward Learned Chemical Perception of Force Field Typing Rules.*” J. Chem. Theory Comput*. 15(1), 402–423 (2019)
35. B. J. Coscia, J. Yelk, M. A. Glaser, D. L. Gin, X. Feng, and M. R. Shirts, “Understanding the Nanoscale Structure of Inverted Hexagonal Phase Lyotropic Liquid Crystal Polymer Membranes” *J. Phys. Chem. B*. 123(1), 289–309 (2019)
36. N. S. Abraham and M. R. Shirts, “An Improved Thermal Gradient Approach for the Quasi-Harmonic Approximation: Making Anisotropic Expansion Feasible,” J. *Chem. Theory Comput*., 14(11) 5904-5919 (2018)
37. D. L. Mobley, C. C. Bannan, A. Rizzi, C. I Bayly, J. D Chodera, V. T Lim, N. M. Lim, K. A Beauchamp, M. R. Shirts, M. K. Gilson, P. K Eastman, “Open Force Field Consortium: Escaping atom types using direct chemical perception with SMIRNOFF v0. 1”, *J. Chem. Theory Comput.*, 14(11) 6076-6092 (2018)
38. D. L. Mobley, M. R. Shirts and D. M. Zuckerman, “Why we need the Living Journal of Computational Molecular Sciences,” *Living J. Comput. Mol. Sci*, 1(1), 2031 (2018)
39. R. A. Messerly, M. R. Shirts, A. F. Kazakov, “Uncertainty quantification confirms unreliable extrapolation toward high pressures for united-atom Mie λ-6 force field*” J. Chem. Phys*. 149(11), 114109 (2018)
40. P. T. Merz and M. R. Shirts, “Testing for Physical Validity in Molecular Simulations”, *PLoS ONE*, 13(9), e0202764 (2018)
41. N. P. Schieber, E. C. Dybeck, and M. R. Shirts, “Using reweighting and free energy surface interpolation to predict solid-solid phase diagrams,” *J. Chem. Phys*. 148 (14), 144104 (2018)
42. R. A. Messerly, S. M. Razavi, M. R. Shirts, “Configuration-Sampling-Based Surrogate Models for Rapid Parameterization of Non-bonded Interactions*” J. Chem. Theory Comput*. 14(6), 3144–3162 (2018)
43. J. E Basconi, G. Carta, M. R. Shirts, “Effects of Protein Properties on Adsorption and Transport in Polymer-grafted Ion Exchangers: A Multiscale Modeling Study” *AIChE J*. 63(10), 4564–4575 (2017)
44. G. D. Ramos Matos, D. Y. Kyu, H. H. Loeffler, J. D. Chodera, M. R. Shirts, and D. L. Mobley, “Approaches for Calculating Solvation Free Energies and Enthalpies Demonstrated with an Update of the FreeSolv Database”, *J. Chem. Eng. Data*, 62(5), 1559–1569 (2017)

45. E. C. Dybeck, N. S. Abraham, N. P. Schieber, M. R. Shirts, "Capturing Entropic Contributions to Temperature-mediated Polymorphic Transformations Through Molecular Modeling," *Cryst. Growth. Des*. 17(4), 1775–1787 (2017)
46. M. R. Shirts, C. Klein, J. M. Swails, J. Yin, M. K. Gilson, D. L. Mobley, D. A. Case, E. D. Zhong, "Lessons learned from comparing molecular dynamics engines on the SAMPL5 dataset," *J. Comput. Aid. Mol. Des.* 31(1), 146–161 (2017)
47. J. Yin, N. M. Hendriksen, D. R. Slochower, M. R. Shirts, M. W. Chiu, D. L. Mobley, M. K. Gilson, "Overview of the SAMPL5 host–guest challenge: Are we doing better?" *J. Comput. Aid. Mol. Des.* . 31(1), 1–19 (2017)
48. C. C. Bannan, Kalistyn H. Burley, M. Chui, M. R. Shirts, M. K. Gilson, D. L. Mobley, "Blind prediction of cyclohexane-water distribution coefficients from the SAMPL5 challenge," *J. Comput. Aid. Mol. Des.* 30(11), 927–944 (2016)
49. E. C. Dybeck, N. P. Schieber, M. R. Shirts, "Effects of a More Accurate Polarizable Hamiltonian on Polymorph Free Energies Computed Efficiently by Reweighting Point-Charge Potentials," *J. Chem. Theory Comput.* 12, 3491–3505 (2016)
50. L. N. Naden and M. R. Shirts. "Rapid Computation of Thermodynamic Properties Over Multidimensional Nonbonded Parameter Spaces using Adaptive Multistate Reweighting," *J. Chem. Theory Comput.*, 12(4), 1806–1823 (2016)
51. E. C. Dybeck, G. König, B. R. Brooks and M. R. Shirts, "A Comparison of Methods to Reweight from Classical Molecular Simulations to QM/MM Potentials," *J. Chem. Theory Comput*, 12(4), 1466–1480 (2016)
52. M. R. Slovin and M. R. Shirts, "Identifying Differences and Similarities in Static and Dynamic Contact Angles between Nanoscale and Microscale Textured Surfaces Using Molecular Dynamics Simulations," *Langmuir* 31(29), 7980–7990 (2015)
53. L. N. Naden and M. R. Shirts, "A Linear Basis Function Approach to Efficient Alchemical Free Energy Calculations. 2. Inserting and Deleting Charged Molecules," *J. Chem. Theory Comput.* 11(6), 2536–2549 (2015)
54. J. E. Basconi, G. Carta and M. R. Shirts, "Effects of polymer graft properties on protein adsorption and transport in ion exchange chromatography: a multi-scale modeling study," *Langmuir*. 31(14), 4176–4187 (2015)
55. P. V. Klimovich, M. R. Shirts and D. L. Mobley, "Guidelines for the analysis of free energy calculations," *J. Comput. Aid. Mol. Des.* 29(5), 397–411 (2015)
56. J. E. Basconi, G. Carta and M. R. Shirts, "Multi-scale modeling of protein adsorption and transport in macroporous and polymer-grafted ion exchangers," *AIChE J.* 60(11), 3888–3901 (2014)
57. J. I. Monroe and M. R. Shirts, "Converging free energies of binding in cucurbit[7]uril and octa-acid host-guest systems from SAMPL4 using expanded ensemble simulations," *J. Comput. Aid. Mol. Des.* 28(4), 401–415 (2014)
58. E. D. Zhong and M. R. Shirts, "Thermodynamics of coupled protein adsorption and stability using hybrid Monte Carlo simulations," *Langmuir* 30(17), 4952–4961 (2014)
59. L. N. Naden and M. R. Shirts, "A Linear Basis Function Approach to Efficient Alchemical Free Energy Calculations. 1. Removal of Uncharged Atomic Sites," *J. Chem. Theory Comput*., 10(3),1128–1149 (2014)

60. J. I. Monroe, W. G. El-Nahal and M. R. Shirts, “Investigating the mutation resistance of non-nucleoside inhibitors of HIV-RT using multiple microsecond atomistic simulations,” *Proteins* 82(1), 130–144 (2014)
61. C. M. Payne, W. Jiang, M. R. Shirts, M. E. Himmel, M. F. Crowley and G. T. Beckham, “Glycoside hydrolase processivity is directly related to oligosaccharide binding free energy,” *J. Am. Chem. Soc.,* 135(50), 18831–18839 (2013)
62. K. Wang, Y. Yang, J. D. Chodera and M. R. Shirts, “Identifying ligand binding sites and poses using GPU-accelerated Hamiltonian replica exchange molecular dynamics,” *J. Comput. Aid. Mol. Des.* 27 (12), 989–1007 (2013)
63. H. Paliwal and M. R. Shirts, “Using multistate reweighting to rapidly and efficiently explore molecular simulation parameters space for nonbonded interactions,” *J. Chem. Theory Comput*., 9 (11), 4700–4717 (2013)
64. J. E. Basconi and M. R. Shirts, “Effects of temperature coupling algorithms on transport properties and kinetics in molecular dynamics simulations,” *J. Chem. Theory Comput.,* 9 (7), 2887–2899 (2013).
65. H. Paliwal and M. R. Shirts, “Multistate reweighting and configuration mapping together accelerate the efficiency of thermodynamic calculations as a function of molecular geometry by orders of magnitude,” *J. Chem. Phys.,* 138 (15), 154108 (2013)
66. S. Pronk, S. Pali, R. Schulz, P. Larsson, P. Bjelkmar, R. Apostolov, M. R. Shirts, J. C. Smith, P. M. Kasson, D. van der Spoel, B. Hess and E. Lindahl, “GROMACS 4.5: A high-throughput and highly parallel open source molecular simulation toolkit,” *Bioinformatics,* 29 (7), 845–854 (2013).
67. M. R. Shirts, “Simple Quantitative Tests to Validate Sampling from Thermodynamic Ensembles,” *J. Chem. Theory Comput.,* 9 (2), 909–926 (2013)
68. P. Eastman, M. S. Friedrichs, J. D. Chodera, R. J. Radmer, C. M. Bruns, J. P. Ku, K. A. Beauchamp, T. J. Lane, L.-P. Wang, D. Shukla, T. Tye, M. Houston, T. Stich, C. Klein, M. R. Shirts and V. S. Pande, “OpenMM 4.0: A Reusable, Extensible, Hardware Independent Library for High Performance Molecular Simulation,” *J. Chem. Theory Comput.,* 9 (1), 461–469 (2013)
69. J. C. Fuller, R. M. Jackson and M. R. Shirts, “Configurational preferences of arylamide α-helix mimetics via alchemical free energy calculations of relative binding affinities,” *J. Phys. Chem. B,* 111 (35), 10856–10869 (2012)
70. J. C. Fuller, R. M. Jackson, A. Wilson, T. Edwards and M. R. Shirts, “Modeling of Arylamide Helix Mimetics in the p53 Peptide Binding Site of hDM2 Suggests Parallel and Anti-Parallel Conformations are Both Stable,” *PLoS ONE,* 7 (8), e43253 (2012)
71. L. Bu, M. R. Nimlos, M. R. Shirts, J. Stahlberg, M. E. Himmel, M. F. Crowley and G. T. Beckham, “Product binding varies dramatically between processive and nonprocessive cellulase enzymes,” *J. Biol. Chem.,* 287 (29), 24807–24813 (2012)
72. T. T. Pham and M. R. Shirts, “Optimal pairwise and non-pairwise alchemical pathways for free energy calculations of molecular transformation in solution phase,” *J. Chem. Phys.,* 136 (12), 124120 (2012)
73. A. Zhang, S. K. Singh, M. R. Shirts, S. Kumar and E. J. Fernandez, “Distinct aggregation mechanisms of monoclonal antibody under thermal and freeze-thaw stresses revealed by hydrogen exchange,” *Pharm. Res.*, 29 (1), 236–250 (2012)

74. H. Paliwal and M. R. Shirts, "A benchmark test set for alchemical free energy transformations and its use to quantify error in common free energy methods," *J. Chem. Theory Comput.*, 7 (12), 4115–4134 (2011)
75. J. D. Chodera and M. R. Shirts, "Replica exchange and expanded ensemble simulations as Gibbs sampling: Simple improvements for enhanced mixing," *J. Chem. Phys.,* 135 (19), 194110 (2011)
76. T. T. Pham and M. R. Shirts, "Identifying Low Variance Pathways for Free Energy Calculations of Molecular Transformations in Solution Phase," *J. Chem. Phys.*, 135 (3), 034114 (2011)
77. J. D. Chodera, W. C. Swope, F. Noé, J.-H. Prinz, M. R. Shirts and V. S. Pande, "Dynamical reweighting: Improved estimates of dynamical properties from simulations at multiple temperatures," *J. Chem. Phys*., 134 (24), 244107 (2011)
78. L. Bu, G. T. Beckham, M. R. Shirts, M. R. Nimlos, W. S. Adney, M. E. Himmel and M. F. Crowley, "Probing carbohydrate product expulsion from a processive cellulase with multiple absolute binding free energy methods," *J. Biol. Chem.,* 286, 18161–18169 (2011)
79. J. D. Chodera, D. L. Mobley, M. R. Shirts, R. W Dixon, K. Branson and V. S. Pande, "Free energy methods in drug discovery and ligand design: Progress and challenges," *Curr. Opin.. Struc. Biol.*, 21 (2), 150–160 (2011)
80. D. L. Mobley, C. I. Bayly, M. D. Cooper, M. R. Shirts and K. A. Dill, "Small molecule hydration free energies in explicit solvent: An extensive test of fixed-charge atomistic simulations," *J. Chem. Theory Comput.,* 5 (2), 350–358 (2009)
81. M. R. Shirts and J. D. Chodera, "Statistically optimal analysis of multiple equilibrium simulations," *J. Chem. Phys.,* 129 (12), 124105 (2008)
82. M. R. Shirts, D. L. Mobley and J. D. Chodera, "Alchemical free energy calculations: Ready for prime time?" *Ann. Rep. Comput. Chem.,* 3, 41–59 (2007)
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84. M. R. Shirts, D. L. Mobley, J. D. Chodera and V. S. Pande, "Accurate and efficient corrections for missing dispersion interactions in molecular simulations," *J. Phys. Chem. B*, 111 (45), 13052–13063 (2007)
85. K. Zhu, M. R. Shirts, R. A. Friesner and M. P. Jacobson, "Multiscale Optimization of a Truncated Newton Minimization Algorithm and Application to Proteins and Protein-Ligand Complexes," *J. Chem. Theory Comput.,* 3 (2), 640–648 (2007)
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87. E. J. Sorin, Y. M. Rhee, M. R. Shirts and V. S. Pande, "The Solvation Interface is a Determining Factor in Peptide Conformational Preferences," *J. Mol. Biol.,* 356 (1), 248–256 (2006)
88. H. Fujitani, Y. Tanida, M. Ito, G. Jayachandran, C. D. Snow, M. R. Shirts, E. J. Sorin and V. S. Pande, "Direct calculation of the binding free energies of FKBP ligands," *J. Chem. Phys.,* 123 (8), 084108 (2005)
89. M. R. Shirts and V. S. Pande, "Comparison of efficiency and bias of free energies computer by exponential averaging, the Bennett acceptance ratio, and thermodynamic integration," *J. Chem. Phys.,* 122 (14), 144107 (2005)

90. M. R. Shirts and V. S. Pande, "Solvation free energies of amino acid side chain analogs for common molecular mechanics water models," *J. Chem. Phys.*, 122 (13), 134508 (2005)
91. M. R. Shirts, E. Bair, G. Hooker and V. S. Pande, "Equilibrium free energies from nonequilibrium measurements using maximum likelihood methods," *Phys. Rev. Lett.,* 91 (14), 140601 (2003)
92. M. R. Shirts, J. W. Pitera, W. C. Swope and V. S. Pande, "Extremely Precise Free Energy Calculations of Amino Acid Side Chain Analogs: Comparison of Common Molecular Mechanics Force Fields for Proteins," *J. Chem. Phys.,* 119 (11), 5740–5761 (2003)
93. V. S. Pande, I. Baker, J. Chapman, S. P. Elmer, S. Khaliq, S. M. Larson, Y. M. Rhee, M. R. Shirts, C. Snow, E. Sorin and B. Zagrovic, "Atomistic protein folding simulations on the submillisecond time scale using worldwide distributed computing," *Biopolymers,* 68 (1), 91–109 (2003)
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98. M. Shirts and V. S. Pande, "Screen Savers of the World Unite!" *Science,* 290 (5498), 1903–1094 (2000)

Book Chapters

99. M. R. Shirts and D. L. Mobley, "An Introduction to Best Practices in Free Energy Calculations," in Eds. L. Monticelli and E. Salonen, *Biomolecular Simulations: Methods and Protocols*, New York: Humana Press (2013)
100. M. R. Shirts, "Best Practices in Free Energy Calculations for Drug Design," in Ed. R. Baron, *Computer Aided Drug Design*, New York: Humana Press (2012)
101. M. R. Shirts, D. L. Mobley and S. P. Brown, "Free Energy Calculations in Structure-Based Drug Design," in *Drug Design: Structure- and Ligand-Based Approaches*, Eds. K. M. Merz, D. Ridge and C. H. Reynolds, New York: Cambridge University Press (2010)

Preprints and Papers in Review or in Press

102. M. R. Shirts, "Reweighting from the mixture distribution as a better way to describe the Multistate Bennett Acceptance Ratio," arXiv:1704.00891 (2017)
103. N. S. Abraham, M. T. Hock, M. R. Shirts, "Probing the force field sensitivity of entropy and enthalpy differences in organic polymorphs using classical potentials" arXiv, https://arxiv.org/abs/2010.10225 (2020)
104. H. Paliwal and M. R. Shirts, "A water model with improved thermodynamic properties over a large pressure and temperature range optimized using multistate reweighting and configuration space mapping," in revision at *J. Chem. Theory Comput.*, preprint at ChemRxiv at https://doi.org/10.26434/chemrxiv-2023-383m4 (2023)

105. D. A. Ramirez, L. E. Hough, M. R. Shirts, "Coiled-coil domains are sufficient to drive liquid-liquid phase separation of proteins in molecular models", bioRxiv 2023.05.31.543124 (2023)
106. K. Takaba, I. Pulido, P K. Behar. C. E. Cadendar, A. J. Friedman, M. M. Henry, H. M. Opeskin, C. R. Iacovella, A. M. Nagle, A. M. Payne, M. R. Shirts, D. L. Mobley, J. D. Chodera, Y. Wang. "Machine-learned molecular mechanics force field for the simulation of protein-ligand systems and beyond", preprint at arXiv:2307.07085 submitted to *Chem.. Sci* .(2023)
107. S. Lee, M. R. Shirts and A. P. Straub, "Predicting organic solute rejection in reverse osmosis and nanofiltration with machine learning and molecular fingerprints," submitted to *Envron. Sci. Technol.*. (2023)
108. W.-T. Hsu and M. R. Shirts, "Ensemble of expanded ensembles: A generalized ensemble approach with enhanced flexibility and parallelizability" preprint at arXiv:2308.06938 (2023)
109. C. M. Davel*, T. Bernat*, J. R. Wagner, and M. R. Shirts, "Parameterization of general organic polymers within the Open Force Field framework", preprint at ChemRxiv (10.26434/chemrxiv-2023-f2zxd-v2), in press at *J. Chem. Info. Model*. (2023) ((* co-first authors)

Software Development Projects

1. GROMACS (https://www.gromacs.org), 2008–current. GROMACS is the most popular classical molecular simulation code in the world (>8,000 Google Scholar paper citations since 2009). I am one of the core developers and a co-writer for the integrator core and free energy calculation code. License: LGPL open source.
2. *pymbar* (https://github.com/choderalab/pymbar), 2008–current. *pymbar* is an analysis code for computing thermodynamic quantities for simulations from multiple thermodynamic states. I am one of two co-creators and co-developers. *pymbar* has been downloaded by approximately 800 unique users. License: GPL open source.
3. *physical_validation* (https://github.com/shirtsgroup/physical_validation), 2012–current. Previously known as *checkensemble, physical_validation* is an analysis tool that validates the statistical fit of simulations to NPT, NVT, and NVμ ensembles. I and former postdoc Pascal Merz are the main developers. License: MIT open source.
4. Open Force Field toolkit (https://github.com/openforcefield). 2018-current. A set of tools for parameterizing and applying general organic force fields. I am one of the lead PI's of the overall Open Force Field Initiative. License: MIT open source.
5. CG_OpenMM (https://github.com/shirtsgroup/cg_openmm). 2020-current. A framework for characterization and optimization of coarse-grained oligomers to optimize them for phase behavior between secondary structure elements.
6. CG_pyRosetta (https://github.com/shirtsgroup/cg_pyrosetta). 2020-current. An add-on module to Rosetta/pyRosetta for identifying and optimizing coarse-grained oligomers for low energy structures with folding behavior.

Community Websites

1. i-CoMSE (https://www.icomse.org), co-PI, 2022–current. Website for community educational resources in computational molecular sciences, part of the efforts of the Institute for Computational Molecular Science Education.

2. Alchemistry.org (https://www.alchemistry.org), co-maintainer, 2009–current. Community website with tutorials and information about statistical mechanical calculations for computing free energies.
3. Open Force Field Initiative (https://www.openforcefield.org), 2019–current. Community resource for the Open Force Field Initiative, distributes code and information about organic molecule force field development.

Invited Talks

1. Chemical Physics / Physical Chemistry Seminar, University of Colorado Boulder, January 2024
2. Statistical Thermodynamics and Molecular Simulation Seminar Series (Virtual), December 2023
3. Boston Free Energy Conference, Plenary and Opening Speaker, Cambridge, MA, May 2023
4. FOMMS 2022, Plenary speaker in "Molecular Simulation Fundamentals" Delavan, WI, July 2022
5. Scuola Internazionale Superiore di Studi Avanzati, Biophysics Program Seminar, Trieste, Italy (virtual), May 2022
6. Iowa State Chemistry Department, Departmental Seminar, Ames, IA, April 2022
7. 2nd Workshop on Computational Chemistry as Strategical Tool for The Development of Functional Materials Fluminense University, Rio de Janeiro, Brazil (Virtual), November 2021
8. University of Denver, Chemistry & Biochemistry Departmental Seminar, Denver, CO, October 2021
9. Lawrence Livermore National Labs, Computational Chemistry and Material Science Summer Program (Virtual), August 2021
10. AbbVie CADD Council Seminar Series (Virtual), August 2021
11. MERCURY Conference for Undergraduate Computational Chemistry, Plenary Speaker (Virtual), July 2021
12. Workshop on Free Energy Methods in Drug Design, (Virtual), June 2021
13. Folding@Home Science talk (Virtual), June 2021
14. ACS Spring National meeting, in "Recent Development of Molecular Mechanics Force Fields for Proteins, Nucleic Acids" session (Virtual), April 2021
15. ACS Spring National meeting, in "Molecular Crystal Polymorphism: How, When and Why Molecules Pack in the Solid State" session (Virtual), April 2021
16. AICHE National Meeting, "Making Molecular Simulation as Useful as Possible in Chemical Engineering," COMSEF Plenary Session, San Francisco, CA (Virtual), November 2020
17. Vienna Algorithms, Biomolecules and Computer Seminar, University of Vienna, Vienna, Austria, (Virtual) October 2020
18. Notre Dame Chemical and Biomolecular Engineering, Departmental Seminar, graduate student nominated speaker, South Bend, IN (Virtual), October 2020
19. ATOMS (Applied Thermodynamics and Molecular Simulation) seminar, Federal University of Rio de Janeiro (Virtual), September 2020
20. MERCURY Conference for Undergraduate Computational Chemistry, Plenary Speaker, Furman University, Greenville, SC, July 2020 (Cancelled due to COVID-19)
21. 2020 Workshop on Free Energy Methods in Drug Design, Boston, MA, May 2020 (Cancelled due to COVID-19)
22. ACS Spring National Meeting, "Molecular Crystal Polymorphism: How, When & Why Molecules Pack in the Solid State", Philadelphia, PA, March 2020 (Cancelled due to COVID-19)

23. ACS Spring National Meeting, “Recent Developments of Molecular Mechanics Force Fields for Proteins, Nucleic Acids, Small Molecules & Materials” session, Philadelphia, PA, April 2020 (Cancelled due to COVID-19)
24. Center for Computational Biology Seminar, University of Kansas, Lawrence, KS, February 2020
25. Biological Physics Seminar, Arizona State University, Tempe, AZ, February 2020
26. MolSSI Workshop on Molecular Dynamics Software Interoperability, New York, NY, November 2019
27. Cyberloop for Computational Bionanomaterials Design Workshop, "Molecular simulations infrastructure: GROMACS, OpenFF, and SCALE-MS", Boulder, CO, October 2019
28. Rational Solid Form Design Summit, Cambridge, MA, October 2019
29. Materials Genome Initiative Seminar, NIST, Gaithersburg MD, August 2019
30. CECAM workshop, “Open source software for enhanced-sampling simulations,” Lugano, Switzerland, July 2019
31. "Free energy calculations: Entering the fourth decade of adventures in Chemistry and Biophysics", Santa Fe, NM, June 2019
32. Computing@PNNL seminar, Pacific Northwest National Labs, Richland, WA, June 2019
33. ACS Spring National Meeting, “Sustainable Software for Computational Molecular Science” session, Orlando, FL, April 2019
34. ACS Spring National Meeting, “ACS Award for Computers in Chemical & Pharmaceutical Research in Honor of Arnie Hagler” session, Orlando, FL, April 2019
35. Physics Colloquium, Department of Physics, Brigham Young University, Provo, UT, November 2018
36. Departmental Seminar, Department of Chemical and Biological Engineering, University at Buffalo, SUNY, Buffalo, NY, November 2018
37. AICHE, November 2018, COMSEF Hands on with Molecular Simulation Workshop, Pittsburgh, PA 2018
38. Research Seminar, Pfizer Materials Science and Drug Product Design, Groton, CT, October 2018
39. Research Seminar, Bristol-Myers Squibb, New Brunswick, NJ, August 2018
40. FOMMS 2018, "Workshop on Simulation Reproducibility," Delavan, WI, July 2018
41. 20th Symposium on Thermophysical Properties, “Predicting Solid State Phase Diagrams Using Multistate Reweighting and Coordinate Mapping” Boulder, CO, June 2018
42. Departmental Seminar, Department of Chemistry, Temple University, Philadelphia, PA, March 2018
43. Departmental Seminar, Department of Chemistry, University of Arkansas, Fayetteville, AR, March 2018
44. Departmental Seminar, Department of Chemistry, New Mexico Institute of Mining and Technology, Socorro, NM, February 2018
45. AIChE National Meeting, “How to Recognize Garbage," COMSEF Hands on with Molecular Simulation Workshop, Minneapolis, MN, October 2017
46. Center for Computational Mathematics Colloquium, University of Colorado Denver, Denver, CO, March 2017
47. SIAM CSE2017, “Warp-bridge sampling to improve efficiency of calculations on physical chemistry,” Atlanta, CA, February 2017
48. University of Washington, Department of Chemical Engineering Seminar, Seattle, WA, January, 2017

49. Dassault Systèmes BIOVIA, ASTS Seminar (virtual), October 2016
50. Basque Center for Applied Mathematics, Scientific Seminar, Bilbao, Spain, August 2016
51. Barcelona Supercomputing Center, Life Sciences Seminar, Barcelona, Spain, July 2016
52. University of California Irvine, Department of Chemistry Computational Chemistry Seminar, July 2016
53. 2016 Workshop on Free Energy Methods in Drug Design: Targeting Cancer, Boston, MA, May 2016
54. Syracuse University, Department of Biomedical and Chemical Engineering Seminar, Syracuse, NY, March 2016
55. Physical Chemistry Seminar, Colorado State University, Fort Collins, CO, November 2015
56. Banff International Research Station, "Free Energies: A Mathematical Perspective" workshop, Oaxaca, Mexico, July 2015
57. Snowmass Summer Biophysics Workshop, Snowmass, CO, July 2015
58. NIST Computational Soft Materials Group seminar, Gaithersburg, MD, May 2015
59. ACS National Meeting, "Modeling Complex Biomolecules" session, Denver, CO, March 2015
60. University of Colorado Boulder, Department of Chemical Engineering Departmental Seminar, Boulder, CO, January 2015
61. University of Illinois at Urbana-Champaign, Department of Materials Science and Engineering Colloquium, Champaign, IL, December 2014
62. Virginia Commonwealth University, Institute for Structural Biology & Drug Discovery, Richmond, VA, November 2014
63. Georgia Tech University, Department of Chemical Engineering Seminar, Atlanta, GA, August 2014
64. Telluride Summer Research Center, "Molecular Recognition," Telluride, CO, August 2014
65. 6th US-Poland Workshop on the Thermodynamics of Complex Fluids and Interfaces, Warsaw, Poland, June 2014
66. 2014 Workshop on Free Energy Methods in Drug Design, Boston, MA, May 2014
67. Max F. Perutz Laboratories, Biophysical Sciences Seminar, Vienna, Austria, June 2014
68. University of Pennsylvania, Penn Institute for Computational Science Seminar, Philadelphia, PA, April 2014
69. "Uncertainty Quantification in Materials Modeling" Workshop, Institute of Mathematics and its Applications, University of Minnesota, Minneapolis, MN, December 2013
70. Vanderbilt University, Departmental Seminar, Department of Chemical and Biomolecular Engineering, Nashville, TN, November 2013
71. George Mason University, Computational Materials Science Center Colloquium, Fairfax, VA, November 2013
72. University of Wisconsin-Madison, Departmental Seminar, Department of Chemical and Biological Engineering, Madison, WI, October 2013
73. University of Wisconsin-Madison, Theoretical Chemistry Institute Seminar, Madison, WI, October 2013
74. National Institute of Standards and Technology Workshop on Atomistic Simulations for Industrial Needs, Gaithersburg, MD, August 2013
75. Snowmass Summer Biophysics Workshop, "Free Energy Calculations: Three Decades of Adventure in Chemistry and Biophysics," Snowmass, CO, July 2013

76. National Institute of Standards and Technology, Chemical Sciences Division Seminar, Gaithersburg, MD, February 2013
77. University of California, Riverside, Department of Chemistry, Physical Chemistry Seminar, Riverside, CA, January 2013
78. University of Pittsburgh, Departmental Seminar, Department of Chemical Engineering, Pittsburgh, PA, September 2012
79. University of Virginia, Department Colloquium, Department of Statistics, Charlottesville, VA, August 2012
80. FOMMS 2012, Plenary Session, "Workshop on Benchmarking and Validation," Mt. Hood, OR, July 2012
81. ETH-Zürich, Physical Chemistry Colloquium, Zürich, Switzerland, June 2012
82. CECAM Workshop, "Free Energy Calculations: From Theory to Applications," Paris, France, June 2012
83. ACS 2012 Middle Atlantic Region Meeting, "Frontiers in the Application of Computational Chemistry to Biological Systems," Baltimore, MD, May 2012
84. Second Workshop on Free Energy Methods in Drug Design: Going the Last Mile, Boston, MA, May 2012
85. University of Virginia, Big Data Summit, "Algorithms and Analytics" Session, May 2012
86. University of Delaware, Departmental Lecture, Department of Physics, Newark, DE, March 2012
87. 52nd Sanibel Symposium, St. Simon's Island, GA, February 2012
88. University of Tennessee, Genome Science and Technology Program, Knoxville, TN, February 2012
89. Oak Ridge National Laboratories, Center for Molecular Biophysics, Oak Ridge, TN, February 2012.
90. University of Maryland, Chem-Phys/Phys-Chem Seminar Series, College Park, MD, November 2011
91. Telluride Summer Research Center, "Free Energy Simulation: From academic research to industrial application," Telluride, CO, July 2011
92. Brigham Young University, Departmental Seminar, Department of Chemical Engineering, Provo, UT, March 2011
93. University of Virginia, NIH Biotechnology Training Program, Faculty Lecture Series, Charlottesville, VA, September 2010
94. Shanghai International Conference on Biophysics and Molecular Biology Society, Shanghai-Jiashan, China, August 2010
95. Hong Kong University of Science and Technology, Departmental Seminar, Department of Chemistry, Hong Kong, August 2010
96. Telluride Summer Research Center: Algorithmic Developments in Advanced Sampling, Telluride, CO, June 2010
97. National Renewable Energy Laboratory, Biomolecular Sciences Group Seminar, Golden, CO, October 2009
98. Drexel University, Chemistry Department Seminar, Philadelphia, PA, November 2008
99. University of Virginia, Chemistry Department Seminar, Charlottesville, VA, October 2008
100. GROMACS User Group Workshop, Göttigen, Germany, September 2008
101. ACS National Meeting, "Free Energy Methods in Academia and Industry," Philadelphia, PA, August 2008
102. 47th Sanibel Symposium, St. Simons Island, GA, February 2007

103. National Institute of Standards and Technology, "Validating modeling and experimental methods to enable drug discovery," Gaithersburg, MD, April 2006
104. CUP VII, OpenEye Scientific Software, Santa Fe, NM, March 2006
105. Gordon Conference, Computer-assisted Drug Design, "Mini-talk," Tilton, NH, August 2005
106. Brigham Young University, Physical Chemistry Seminar, Provo, UT, December 2004
107. Gordon Conference in Computational Chemistry, July 2002 (invited to talk based on poster)
108. Stanford University, Biomedical Computation at Stanford (BCATS), Stanford, CA, October 2000

Contributed Conference Presentations

1. AIChE National Meeting, "Improved Theories of Cooperative Folding of Oligomers and Demonstrations in Coarse-Grained Models" in "Thermodynamics of Biomolecular Folding and Assembly", Orlando, FL, November 2023
2. AIChE National Meeting, "The Open Force Field "Rosemary" Release and New Approaches to Chemically Transferable Force Fields" in in "Development of Intermolecular Potentials", Orlando, FL, November 2023
3. ACS Annual Meeting, "Improved theories of cooperative folding of oligomers and demonstrations in coarse-grained models," in "Molecular Mechanics", San Francisco, CA, August 2023
4. ACS Annual Meeting, "Open force field initiative: open software, open data" in "Free and Source Software: Harnessing the Power of Data", San Francisco, CA, August 2023
5. AIChE National Meeting, "Statistical Inference of Transport Mechanisms from Time Series of Solute Trajectories in Polymer Membranes" in "Microscale Transport Processes", Phoenix, AZ, November 2022
6. AIChE National Meeting, "The Open Force Field v2.0 and Extensions to Biopolymers" in "Development of Intermolecular Potentials", Phoenix, AZ, November 2022
7. AIChE National Meeting, "How Much Do Disorder and Entropy in Molecular Crystals?" in "Advancements in Particle Engineering and Material Sciences in Pharmaceutical Process Development" session, Virtual, November 2021
8. AIChE National Meeting, "The Open Force Field Initiative: Current Efforts Towards Transferable Force Fields for Biological and Organic Molecules," Development of Intermolecular Potential Models session, Virtual, November 2020
9. AIChE National Meeting, "Disorder and Entropy in Molecular Crystals", in Computational Solid State Pharmaceutics session, Virtual, November 2020
10. AIChE National Meeting, "Modeling of Chemically-Specific Separations in Lyotropic Liquid Crystal Self-Assembled Nanoporous Membranes" in Membrane Modeling and Simulation I session, Virtual, November 2020
11. AIChE National Meeting, "Let's Not Use Histograms: Bayesian Inference of Potentials of Mean Force with Umbrella Sampling and Multistate Reweighting" in Recent Advances in Multiscale Methodologies, Virtual, November 2020
12. ACS Spring National Meeting, "Bayesian inference of continuous potentials of mean force from umbrella sampling and multistate reweighting," "Molecular Mechanics" session, Philadelphia, PA, March 2020 (Cancelled due to COVID-19)
13. ACS Spring National Meeting, "No more histograms: Variational and Bayesian approaches to estimating potentials of mean force", "Molecular Mechanics" session, Orlando, FL, April 2019

14. AIChE National Meeting, “No More Histograms: Variational and Bayesian Approaches to Estimating Potentials of Mean Force”, Pittsburgh, PA, October 2018
15. AIChE National Meeting, “The Living Journal of Computational Molecular Science: Improving Community Use of Molecular Simulation Methods through a New Publishing Model”, Pittsburgh, PA, November 2018
16. AIChE National Meeting, “Automated Tests for Physical Validity in Molecular Dynamics and Monte Carlo Simulations”, Minneapolis, MN, November 2017
17. AIChE National Meeting, "Capturing the Role of Temperature and the Sensitivity to Energy Function Complexity in Crystal Polymorph Stability Using Molecular Modeling," Minneapolis, MN, October 2017
18. ACS National Meeting, “Understanding the molecular details of protein adsorption in polymer-grafted ion exchangers,” BIOT: Downstream Processes session, San Francisco, CA, April 2017
19. ACS National Meeting, “Capturing the role of temperature in crystal polymorph stability using molecular modeling,” COMP: Material Science session, San Francisco, CA, April 2017
20. ACS National Meeting, “Understanding and applying multistate reweighting in a broad molecular simulation context,” COMP: Molecular Mechanics session, San Francisco, CA, April 2017
21. AIChE National Meeting, “Recent Advances in Molecular Simulation Methods, “Molecular Simulation of Protein Adsorption and Molecular Recognition Processes” and “Thermophysical Properties of Biological Systems” sessions, Salt Lake City, UT, November 2015
22. ACS National Meeting, “Molecular Mechanics” session, Denver, CO, March 2015.
23. AIChE National Meeting, “COMSEF Plenary Session” and “Software Engineering in and for the Molecular Sciences” sessions, Atlanta, GA, November 2014
24. ACS National Meeting, “Drug Design,” “Molecular Mechanics” and “Computational Studies of Water” sessions, Dallas, TX, March 2014
25. AIChE National Meeting, “Recent Advanced in Molecular Simulation Methods,” San Francisco, CA, November 2013
26. Folding@Home Developers Meeting, Stanford, CA, August 2013
27. AIChE National Meeting, “COMSEF Plenary Session,” Pittsburgh, PA, October 2012
28. ACS National Meeting, “Molecular Mechanics” sessions, Philadelphia, PA, August 2012
29. AIChE National Meeting, “Recent Advances in Molecular Simulation Methods” and “Beyond Standard Hardware: GPUs, Cloud Computing, and Crowdsourcing” session, Minneapolis, MN, October 2011
30. ACS National Meeting, “Drug Discovery” session, Denver, CO, September 2011
31. SAMPL3: Free Energy Calculation Method Blind Challenge, Stanford, CA, August 2011
32. ACS National Meeting, “Computers in Chemistry: Molecular Mechanics” sessions, Anaheim, CA, March 2011
33. AIChE National Meeting, “Molecular Modeling and Simulation of Complex Molecules” session, Salt Lake City, UT, November 2010
34. ACS National Meeting, “Computers in Chemistry: Molecular Mechanics” session, San Francisco, CA, March 2010
35. AIChE National Meeting, “Thermophysical Properties of Biological Systems” and “Recent Advances in Molecular Simulation Methods” sessions, Nashville, TN, November 2009

36. ACS National Meeting, “Computers in Chemistry: Molecular Mechanics” sessions, Washington, DC, August 2009
37. ACS National Meeting, “Computers in Chemistry: Molecular Mechanics” session, Salt Lake City, UT, March 2009
38. AIChE National Meeting, “Molecular Modeling of Biophysical Processes” and “Recent Advances in Molecular Simulation Methods” sessions, Philadelphia, PA, November 2008
39. AIChE National Meeting, “Molecular Modeling of Biophysical Processes” and “Recent Advances in Molecular Simulation Methods” sessions, Salt Lake City, UT, November 2007
40. ACS National Meeting, “Computers and Chemistry: Drug Discovery” and “Computers and Chemistry: Current Techniques in Molecular Simulation of Biological Processes” sessions, Boston, MA, August 2007
41. ACS National Meeting, “Computers and Chemistry: Free Energy Computations in Drug Discovery” session, San Francisco, CA, September 2006
42. ACS National Meeting, “Computers and Chemistry: Structure-Based Drug Design” session, Washington, DC, September 2005
43. ACS National Meeting, “Computers and Chemistry: General Contributions” session, Philadelphia, PA, August 2004
44. ACS National Meeting, “Computers and Chemistry: General Contributions” and “Computers and Chemistry: Rational Drug Design” sessions, Anaheim, CA, March 2004
45. CECAM Workshop on “Component Architecture, Open Standards, and Parallel Algorithms,” Lyon, France, October 2003

Conference Presentations by Students and Postdocs (presenter underlined)

1. Wei-Tse Hsu, Valerio Piomponi, Pascal Merz, Giovanni Bussi and Michael R Shirts, “Advancing Alchemical Free Energy Methods: Enhanced Flexibility, Parallelizability and Configurational Sampling” (poster), AIChE National Meeting, Orlando, FL, November 2023
2. Wei-Tse Hsu, Valerio Piomponi, Pascal Merz, Giovanni Bussi, Michael Shirts, “Expanding alchemical free energy calculations: From enhanced configurational sampling to ensemble simulation methods,” ACS Annual Meeting, San Francisco, August 2023
3. Anika J. Friedman, Michael R. Shirts, Jerome M. Fox, “Allosteric inhibition via nonpolar terpenoid inhibitors” Biophysical Society Annual Meeting, San Diego, February 2023
4. Dominique A. Ramirez, Loren E. Hough, Michael R. Shirts, “Coiled-coil domains can drive liquid-liquid phase separation,” Biophysical Society Annual Meeting, San Diego, February 2023
5. Nathanael E. Schwindt, Subin Sahu, Douglas L. Gin, Richard D. Noble (poster), “Understanding the Normal Bicontinuous Cubic Phase in Gemini Lyotropic Liquid Crystals in Order to Design Selective Separations”, AIChE National Meeting, Phoenix, AZ, November 2022
6. Wei-Tse Hsu, Pascal R. Merz, Giovanni Bussi and Michael R. Shirts, “Accelerated Free Energy Calculations by Joint Biasing in Configurational and Alchemical Space in Metadynamics” in “Recent Advances in Molecular Simulation Methods,” AIChE National Meeting, Phoenix, AZ, 2022
7. Christopher C. Walker, Sarah Mellett, Theodore L. Fobe, and Michael L. Shirts, “How Does Foldamer Side Chain Entropy Affect Folding Cooperativity?” in “Thermodynamics of Biomolecular Folding and Assembly”, AIChE National Meeting, Phoenix, AZ, November 2022

8. Anika J. Friedman, Jerome M. Fox, and Michael R. Shirts, "Determining the mechanism of allosteric inhibition of PTP1B by amorphadiene using molecular dynamics simulations", ACS National Meeting, Chicago, IL, August 2022
9. Theodore L. Fobe, Christopher C. Walker and Michael R. Shirts, "Folding coarse-grained foldamer models with PyRosetta", ACS National Meeting, Chicago, IL, August 2022
10. Wei-Tse Hsu, Pascal R. Merz, Giovanni Bussi and Michael R. Shirts, "Accelerated Free Energy Calculations by Joint Biasing in Configurational and Alchemical Space in Metadynamics," ACS National Meeting, Chicago, IL, August 2022
11. Theodore L. Fobe, Christopher C. Walker and Michael R. Shirts (poster), "Folding coarse-grained foldamer models with PyRosetta", RosettaCon, Leavenworth, WA, August 2022
12. Owen C. Madin, John D. Chodera, Michael. K. Gilson, David L. Mobley, and Michael R. Shirts (poster), "Improving Lennard-Jones parameters by training against condensed phase mixture data," ACS National Meeting, Boston, MA, March 2022
13. Owen C. Madin, John D. Chodera, Michael. K. Gilson, David L. Mobley, and Michael R. Shirts, "Surrogate-enabled Bayesian parameterization of nonbonded force field parameters," in "Molecular Mechanics," ACS National Meeting, Boston, MA, March 2022
14. Anika J. Friedman, Jerome M. Fox, and Michael R. Shirts (poster), "Determining the mechanism of allosteric inhibition of PTP1B by amorphadiene using molecular dynamics simulations", ACS National Meeting, Boston, MA, March 2022
15. Wei-Tse Hsu, Dominique A. Ramirez, Zhongping Tan, Tarek Sammakia and Michael R. Shirts, "Investigating the Influence of O-Linked Glycosylation on the Proteolytic Stability and Dimerization Propensity of Insulin using Molecular Dynamics," in "Molecular Mechanics", ACS National Meeting, Boston, MA, March 2022
16. Wei-Tse Hsu, Pascal R. Merz, Giovanni Bussi and Michael R. Shirts (poster), "Using alchemical variables within the metadynamics framework to improve sampling in free energy calculations," ACS National Meeting, Boston, MA, March 2022
17. Wei-Tse Hsu, Dominique A. Ramirez, Zhongping Tan, Tarek Sammakia and Michael R. Shirts, "Gaining Mechanistic Insights into the Influence of O-Linked Glycosylation on Insulin Properties with Molecular Dynamics" (poster), AIChE National Meeting, Boston, MA, November 2021
18. Christopher C. Walker, Garret L. Meek, Theodore L. Fobe, and Michael L. Shirts, "Using a Coarse-Grained Modeling Framework to Identify Oligomeric Motifs with Tunable Secondary Structure" in "Thermodynamics of Biomolecular Folding and Assembly", AIChE National Meeting, Boston, MA, November 2021
19. Owen C. Madin, John D. Chodera, Michael. K. Gilson, David L. Mobley, and Michael R. Shirts, "Development and Benchmarking of Small Molecule Force Fields in the Open Force Field Initiative" AIChE National Meeting, Boston, MA, November 2021
20. Wei-Tse Hsu, Pascal R. Merz, Giovanni Bussi and Michael R. Shirts, "Improved Configurational Sampling by the introduction of Alchemical Variable in Metadynamics" in "Recent Advances in Molecular Simulation Methods," AIChE National Meeting, Boston, MA, November 2021
21. Theodore L. Fobe, Christopher C. Walker and Michael R. Shirts, "Exploring Non-Biological Foldamer Secondary Structure Using Tuneable Coarse-Grained Models" in "Recent Advances in Multiscale Methodologies", AIChE National Meeting, Boston, MA, November 2021
22. Owen C. Madin, Simon Boothroyd, Richard A. Messerly and Michael R, Shirts, "Bayesian Model Selection: Applying Parsimony to Build Better Molecular Models", in "Data-Driven Design and Modeling", AIChE National Meeting, Boston, MA, November 2021

23. Subin Sahu, Benjamin J. Coscia, Nathanael Schwindt, Michael R. Shirts, “Obtaining stable bicontinuous cubic structures in lyotropic liquid crystals” ACS Annual Meeting, August 2021.
24. Wei-Tse Hu, Pascal Merz, Giovanni Bussi, and Michael R. Shirts, Adding alchemical variables to metadynamics to enhance sampling in free energy calculations, ACS Spring Meeting (virtual), April 2021
25. Owen C. Madin, Simon Boothroyd, Richard Messerley, and Michael R. Shirts, Bayesian Model Selection: Occam’s Razor Applied to Molecules, ACS Spring Meeting (virtual), April 2021
26. Theodore L. Fobe and Michael R. Shirts, “CG Pyrosetta: A Coarse-Grained Configurational Search Tool for General Heteropolymers,” AIChE National Virtual Meeting, November 2020
27. Owen C. Madin, Richard A. Messerly, Simon Boothroyd and Michael R. Shirts (poster), “Bayesian Model Selection for Non-Covalent Interactions,” AIChE National Virtual Meeting, November 2020
28. Wei-Tse Hsu, Pascal T. Merz, Giovanni Bussi, and Michael R. Shirts (poster), “Introduction of Alchemical Variables in Metadynamics to Enhance Configurational Sampling,” AIChE National Virtual Meeting, November 2020
29. Nathan S. Abraham and Michael R. Shirts, “Bridging the Gap between Static Lattice Energy and Full Free Energy Differences of Organic Crystal Polymorphs When Predicting Crystal Energy Landscape,” AIChE National Virtual Meeting, November 2020
30. Simon Boothroyd, Owen Madin and Michael R. Shirts (poster), “Open Force Field Initiative: New Strategies for Parameterizing Non-Bonded Interactions,” AIChE National Virtual Meeting, November 2020
31. Theodore L. Fobe, Garrett A. Meek, and Michael R. Shirts (poster), “CG PyRosetta: Coarse-grained conformational search tool for general heteropolymers,” COMP and Sci-Mix session, ACS Spring National Meeting (Cancelled due to COVID-19)
32. Garrett A. Meek, Theodore L. Fobe and Michael R. Shirts, “Leveraging coarse-grained models to design heteropolymers with novel secondary structure”, “Molecular Modeling” session, ACS Spring National Meeting (Cancelled due to COVID-19)
33. Theodore L. Fobe, Garrett A. Meek, and Michael R. Shirts (Poster), “CG PyRosetta: A Coarse-Grained Configuration Search Tool for General Foldamer Secondary Structure”, Winter RosettaCon, New York, NY February 2020
34. Nathan S. Abraham and Michael R. Shirts (poster), "Building Computational Tools to Help Guide Experimentalists in the Discovery of New Solid Phases of Organic Materials," AIChE National Meeting, Orlando, FL, November 2019
35. Benjamin J. Coscia and Michael R. Shirts, "Chemically Dependent Transport of Small Polar Solutes in a Cross-Linked HII Phase Lyotropic Liquid Crystal Membrane," AIChE National Meeting, Membrane Modeling and Simulation session, Orlando, FL, November 2019
36. Nathan S. Abraham and Michael R. Shirts, "Probing the Sensitivity of Point Charge Potentials in an Attempt to Improve Their Ability to Rank the Stability of Pharmaceutical Polymorphs," AIChE National Meeting, Computational Solid State Pharmaceutics session, Orlando, FL, November 2019
37. Benjamin J. Coscia and Michael R. Shirts (poster), "Transport Mechanisms of Polar Solutes in a Cross-Linked HII Phase Lyotropic Liquid Crystal Membrane," AIChE National Meeting, Orlando, FL, November 2019
38. Owen C. Madin, Richard A Messerly and Michael R. Shirts (poster), "A Bayesian Approach to Model Selection and Parameterization for Non-Bonded Interactions," AIChE National Meeting, Computational Molecular Science and Engineering Forum Poster session, Orlando, FL, November 2019

39. Pascal T. Merz, Mark Abraham, and Michael R. Shirts (poster), "New integrator framework for GROMACS", ACS Fall 2019 National Meeting, COMP Session, San Diego, CA 2019
40. Owen C. Madin and Michael R. Shirts (poster), "Force field complexity assessed via Bayesian inference and reversible jump Monte Carlo sampling", ACS Fall 2019 National Meeting, COMP and Sci-Mix Sessions, San Diego, CA 2019
41. Pascal T. Merz and Michael R. Shirts, "Physical validity in molecular simulations," ACS Fall 2019 National Meeting, Molecular Mechanics session, San Diego, CA, August 2019
42. Benjamin J. Coscia and Michael R. Shirts (poster), "Transport Mechanisms of Polar Solutes in a Cross-Linked HII Phase Lyotropic Liquid Crystal Membrane," AIChE National Meeting, Computational Molecular Science and Engineering Forum Poster Session, Orlando, FL, November 2019
43. Benjamin J. Coscia and Michael R. Shirts (presenter), "Chemically Dependent Transport of Small Polar Solutes in a Cross-Linked HII Phase Lyotropic Liquid Crystal Membrane," AIChE National Meeting, Membrane Modeling and Simulation, Orlando, FL, November 2019
44. Benjamin J. Coscia, and Michael R. Shirts (oral), " Understanding Transport of Small Solutes in the Pores of a Nanostructured Lyotropic Liquid Crystal Membrane," AIChE National Meeting, Pittsburgh, PA, October 2018
45. Nathan S. Abraham, Eric C. Dybeck, Natalie P. Schieber and Michael R. Shirts (oral), "Understanding the Effect of Changing Complexities of Potential Energy Functions on the Entropic Contribution to Free Energy Differences of Organic Polymorphs," AIChE National Meeting, Pittsburgh, PA, October 2018
46. Benjamin J. Coscia and Michael R. Shirts (poster), "The Influence of Pore Structure on Transport in Lyotropic Liquid Crystal Membranes," AIChE National Meeting, Pittsburgh, PA, October 2018
47. Nathan S. Abraham, Eric C. Dybeck, and Michael R. Shirts (poster) "Challenging Statistical Mechanics Approximations in Organic Crystal Thermodynamics," AIChE National Meeting, Pittsburgh, PA, October 2018
48. Benjamin J. Coscia and Michael R. Shirts (poster), "Understanding the Effect of Nanoscopic Pore Structure on Transport in Lyotropic Liquid Crystal Membranes," FOMMS, Delavan, WI, July 2018
49. Nathan S. Abraham and Michael. R. Shirts (oral), “Improved Thermal Gradient Quasiharmonic Approximations for Thermodynamic Properties of Organic Crystals with the Inclusion of Anisotropy,” Gordon Research Seminar on Crystal Engineering, Newry, ME, June 2018
50. Nathan S. Abraham and Michael. R. Shirts (poster), “Improved Thermal Gradient Quasiharmonic Approximations for Thermodynamic Properties of Organic Crystals with the Inclusion of Anisotropy,” Gordon Research Conference on Crystal Engineering, Newry, ME, June 2018
51. Benjamin J. Coscia, Xunda Feng, Joe Yelk, Matthew Glaser, Douglas L. Gin, and Michael R. Shirts (oral), "Understanding the Effect of Nanoscopic Pore Structure on Transport in Lyotropic Liquid Crystal Membranes," AIChE National Meeting, Minneapolis, MN, November 2017
52. Eric C. Dybeck and Michael R. Shirts (oral)AIChE National Meeting, “Exploring the Multi-Minima Behavior of Organic Crystal Polymorphs at Finite-Temperature," Minneapolis, MN, October 2017
53. Natalie P. Schieber and Michael R. Shirts (oral) "Prediction of Solid State Phase Diagrams Using Multistate Reweighting and Jacobian Mapping." AIChE National Meeting, Minneapolis, MN, October 2017

54. Benjamin J. Coscia, Xunda Feng, Joe Yelk, Matthew Glaser, Doug Gin, and Michael R. Shirts (poster), "Understanding the Nanoscopic Structure of Lyotropic Liquid Crystal Membranes Using Molecular Dynamics Simulations," AIChE National Meeting, Minneapolis, MN, October 2017
55. Nathan S. Abraham and Michael R. Shirts (poster), "Improved Thermal Gradient Quasiharmonic Approximations for Thermodynamic Properties of Organic Crystals with the Inclusion of Anisotropy", AIChE National Meeting, Minneapolis, MN, October 2017
56. Natalie P. Schieber, Nathan S. Abraham, Eric C. Dybeck, and Michael R. Shirts (poster) "Differences in Relative Free Energy Versus Temperature Curves for Small Organic Molecules between Quantum Mechanical and Classical Potentials," AIChE National Meeting, Minneapolis, MN, October 2017
57. Nathan S. Abraham, Eric C. Dybeck and Michael R. Shirts (oral), "Can Lattice Dynamics with Anisotropic and Isotropic Thermal Expansion Accurately Estimate Thermodynamic Properties of Crystals Pharmaceutics Compared to Molecular Dynamics?" AIChE National Meeting, Minneapolis, MN, October 2017
58. Nathan S. Abraham and Michael R. Shirts (poster), "Evaluation of anisotropic, isotropic, and no thermal expansion in the (quasi-)harmonic approximation to accurately calculate thermodynamic properties of organic crystals," ACS National Meeting, Washington, DC, August 2017
59. Nathan S. Abraham and Michael R. Shirts (oral), "Improved isotropic and anisotropic thermal gradient approaches for the quasiharmonic approximation to predict thermodynamic properties of organic crystals," ACS National Meeting, Washington, DC, August 2017
60. Benjamin J. Coscia and Michael R. Shirts (poster), "Understanding the microscopic structure of lyotropic liquid crystal membranes using molecular dynamics simulations", Presenter: (Poster) ACS National Meeting, Washington, DC, August 2017
61. Pascal T. Merz and Michael R. Shirts (oral) "Testing for physical validity in molecular dynamics", ACS National Meeting, Washington, DC, August 2017
62. Natalie P. Schieber, Eric C. Dybeck, and Michael R. Shirts (oral), Predicting relative polymorph stability using multistate reweighting methods and Jacobian mapping, ACS National Meeting, San Francisco, CA, April 2017
63. Eric C. Dybeck, Nathan S. Abraham, Natalie P. Schieber, and Michael. R. Shirts (oral), "Polymorphic Transformations at Ambient Conditions Elucidated with Molecular Dynamics," AIChE National Meeting, San Francisco, CA, November 2016
64. Drew Biedermann, Geoffrey M. Geise, and Michael R. Shirts (poster), "Molecular Dynamics Modeling of Water and NaCl Transport in Sulfonated Poly(arylene ether sulfone) Desalination Membranes", AIChE Student National Meeting, San Francisco, CA, November 2016
65. Eric C. Dybeck, Natalie P. Schieber, and Michael. R. Shirts (poster), "Effects of polarization and entropy on crystal polymorph free energies," ACS National Meeting, Philadelphia, PA, August 2016
66. Levi N. Naden and Michael R. Shirts (poster), "Rapid Computation of Thermodynamic Properties over a Large Multidimensional Space of Nonbonded Parameters," 2016 Meeting on Free Energy Calculations in Drug Design: Targeting Cancer, Boston, MA, May 2016
67. Eric C. Dybeck, Brittany Z. Bruns, Natalie P. Schieber, and Michael. R. Shirts (oral), "Exploring Polymorph Free Energy Landscapes with Hamiltonian Reweighted Molecular Dynamics," AIChE National Meeting, Salt Lake City, UT, November 2015

68. Levi N. Naden and Michael R. Shirts (poster), “Rapid Computation of Thermodynamic Properties over a Large Multidimensional Space of Nonbonded Parameters,” AIChE National Meeting, Salt Lake City, UT, November 2015
69. Drew Biedermann, Geoffrey M. Geise, and Michael R. Shirts (poster), “Effect of Sulfonate Functional Groups on Transport and Sorption Behavior of NaCl in Disulfonated Poly(Arylene Ether Sulfone) Membranes”, AIChE Student National Meeting, Salt Lake City, UT, November 2015
70. Levi N. Naden and Michael R. Shirts (oral), “Rapid computation of thermodynamic properties over a large multidimensional space of nonbonded parameters,” ACS National Meeting, Boston, MA, August 2015
71. Eric C. Dybeck, Brittany Z. Bruns, Natalie P. Schieber, Gerhard Koenig and Michael. R. Shirts (oral), “Exploring polymorph free energy landscapes with Hamiltonian reweighted molecular dynamics,” ACS National Meeting, Boston, MA, August 2015
72. Eric C. Dybeck, Natalie P. Schieber, Brittany Z. Bruns, and Michael R. Shirts (poster), Reweighting to Expensive Hamiltonians to Explore Polymorph Free Energy Landscapes With High Accuracy. FOMMS 2015, Mt. Hood, OR, July 2015
73. Levi N. Naden and Michael R. Shirts (oral), “Extending a Linear Basis Function Approach to Alchemically Solvating Charged Particles and Changing Atomic Identity,” AIChE National Meeting, Atlanta, GA, November 2014
74. Brittany Zimmerman and Michael R. Shirts (poster), “Improved Approaches for Optimizing Force Fields Using Multistate Reweighting and Diverse Data Sources,” AIChE National Meeting, Atlanta, GA, November 2014
75. Joseph. E. Basconi, Giorgio Carta, and Michael R. Shirts (poster), “Multi-scale modeling of protein adsorption and transport in macroporous and polymer-grafted ion exchangers,” PREP: International Symposium on Preparative and Process Chromatography, July 2014
76. Levi N. Naden and Michael R. Shirts (oral), “A linear basis function approach to efficient alchemical free energy calculations,” Washington DC Molecular Theory and Computation Symposium, Rockville, MD, June 2014
77. Joseph. E. Basconi, Giorgio Carta, and Michael R. Shirts (oral), “Multi-scale modeling of protein adsorption and transport in macroporous and polymer-grafted ion exchangers,” Washington DC Molecular Theory and Computation Symposium, Rockville, MD, June 2014
78. Levi N. Naden and Michael R. Shirts (oral), “A linear basis function approach to efficient alchemical free energy calculations,” ACS National Meeting, Dallas, TX, March 2014
79. Joseph. E. Basconi, Giorgio Carta, and Michael R. Shirts (oral), “Elucidating the Details of Protein Transport in Polymer-Grafted Ion Exchangers Through Multi-Scale Modeling,” AICHE National Meeting, San Francisco, CA, November 2013
80. Levi N. Naden and Michael R. Shirts (oral), “A Linear Basis Function Approach to Efficient Molecular Transformation Free Energy Calculations,” AICHE National Meeting, San Francisco, CA, November 2013
81. Ellen D. Zhong and Michael R. Shirts (oral), “Modeling Protein Conformational Stability On Chromatography Media With a Gō-Like Model,” AICHE National Meeting, San Francisco, CA, November 2013

82. Himanshu Paliwal and Michael R. Shirts (oral), "Accelerating Screening of Simulation Parameter Spaces By Orders of Magnitude Using Reweighting and Configuration Space Mapping Algorithms," AICHE National Meeting, San Francisco, CA, November 2013
83. Kai Wang, Yanzhi Yang, John D. Chodera, and Michael R. Shirts (oral), "Identifying Ligand Binding Sites and Poses Using Hamiltonian Replica Exchange Molecular Dynamics: Model Systems and a Validation Study Using the Astex Diverse Set," AICHE National Meeting, San Francisco, CA, November 2013
84. Jacob I. Monroe and Michael R. Shirts (poster), "Converged Free Energies of Binding in Cucurbit[7]Uril and Octa-Acid Host Systems from Expanded Ensemble Simulations", AICHE National Student Meeting, San Francisco, CA, November 2013
85. Joseph E Basconi, "Molecular Modeling of Protein Transport in Polymer-Grafted Ion Exchangers," University of Virginia Engineering Research Symposium, Charlottesville, VA, April 2013
86. Kai Wang, John D. Chodera and Michael R. Shirts (oral), "Identifying Drug Binding Locations and Poses Using Hamiltonian Replica Exchange Molecular Dynamics," AIChE National Meeting, Pittsburgh, PA, October 2012
87. Himanshu Paliwal and Michael R. Shirts (oral), "Using Multistate Reweighting to Rapidly Explore Molecular Parameter Space," AIChE National Meeting, Pittsburgh, PA, October 2012
88. Joseph E. Basconi, Giorgo Carta and Michael R. Shirts (oral), "Molecular Modeling of Protein Transport in Polymer-Grafted Ion Exchangers," AIChE National Meeting, Pittsburgh, PA, October 2012
89. Ellen D. Zhong and Michael R. Shirts (poster, 1st prize in student competition, computing and process control section), "Modeling Protein Conformational Stability on Chromatography Media with a Gō-Like Model," AIChE Student National Meeting, Pittsburgh, PA, October 2012
90. Arjan C. Kool, Himanshu Paliwal, John D. Chodera, and Michael R. Shirts (poster), "Efficient Thermodynamic Property Computation Using Molecular Simulation Over Thousands and Millions of Thermodynamic States," AIChE Student National Meeting, Pittsburgh, PA, October 2012
91. Jacob I. Monroe, Walid G. El-Nahal and Michael R. Shirts (poster), "Microsecond-Scale Simulations to Determine NNRTI Function Upon Drug Resistant Mutations in HIV-RT," AIChE Student National Meeting, Pittsburgh, PA, October 2012
92. Levi N. Naden, Tri T. Pham and Michael R. Shirts (poster), "Linear Basis Function Approaches to Efficient Free Energy Calculations," AIChE National Meeting, Pittsburgh, PA, October 2012
93. Joseph E. Basconi and Michael R. Shirts (oral), "Modeling protein transport in charged chromatographic gels using coarse-grained molecular dynamics simulation," ACS National Meeting, Philadelphia, PA, August 2012
94. Kai Wang and Michael R. Shirts (oral), "Identifying drug binding locations and poses using Hamiltonian replica exchange molecular dynamics," ACS National Meeting, Philadelphia, PA, August 2012
95. Levi N. Naden, Tri T. Pham and Michael R. Shirts (poster), "Linear basis function approaches to efficient free energy calculations," ACS National Meeting, Philadelphia, PA, August 2012
96. Kai Wang, John D. Chodera, and Michael R. Shirts (poster), "Applications of GPU-accelerated replica exchange molecular dynamic simulations of proteins," ACS National Meeting, Philadelphia, PA, August 2012

97. Himanshu Paliwal and Michael R. Shirts (oral), "Validation of free energy calculation methods: Thermodynamic sampling of large parameter spaces using multistate reweighting methods," ACS National Meeting, Philadelphia, PA, August 2012
98. Tri T. Pham and Michael R. Shirts (oral), "Reducing the Statistical Error of Free Energy Calculations Through Functional Optimization of Pair Potential Pathways," AIChE National Meeting, Minneapolis, MN, October 2011
99. Himanshu Paliwal and Michael R. Shirts (oral), "A Benchmark Test Set for Free Energy Methods and Its Use to Test Free Energy Estimators and Dependence on Molecular Simulation Parameters," AIChE National Meeting, Minneapolis, MN, October 2011
100. Tri T. Pham and Michael R. Shirts (oral), "Identifying low variance pathways of intermediates for free energy calculations," ACS National Meeting, Denver, CO, August 2011
101. Walid G. El-Nahal and Michael R. Shirts (poster), "A Molecular Dynamics Simulation Study of HIV-RT Inhibitor Susceptibility to Mutation," (3rd place in student competition, computing and process control section), AICHE National Meeting, Salt Lake City, UT, November 2010

Sponsored Research

2023
Agency: University of Colorado Boulder Innovative Seed Grant Program
Project Title: "Understanding the biological role of coiled-coil proteins in liquid-liquid phase separation"
PI: Michael R. Shirts
Amount: $50,000
Dates: 7/1/2023-6/30/2024

2022
Agency: NSF
Project Title: NSF-BSF: Ion transport and selectivity in salt-rejecting membranes operating at elevated salinities and pressures
PIs: Anthony Straub (CU Boulder), Co-PI Michael R. Shirts
Dates: 8/1/2022-7/31/2025
Amount: $450,000 (CU total, Shirts component approximately $169,000)

Agency: NIH/NIGMS
Project Title: Supplement: Open data-driven infrastructure for building biomolecular force fields for predictive biophysics and drug design
PIs: Michael R. Shirts
Dates: 6/1/2022-5/31/2023
Amount: $10,760 (Undergraduate research)

Agency: NIH/NIGMS
Project Title: Markov State Model approaches for folding, binding and design"
PI: Vince Voelz (Temple University),
Amount: $152,495 (Shirts component)

Dates: 7/1/2022-6/30/2027

Agency: NSF XSEDE Supercomputing Program
Project Title: Understanding organic crystal polymorph stability, transport in charged polymeric membranes, and peptide binding ensembles using molecular dynamics
PIs: Michael Shirts
Amount: 2.72 million CPU compute units and 4K GPU compute units. Estimated value of these awarded resources by XSEDE is $36,145
Dates: 10/1/202-9/30/2022

2021
Agency: NSF
Project Title: Collaborative Research: CyberTraining: Implementation: Medium:
Establishing Sustainable Ecosystem for Computational Molecular Science Training and Education
PIs: Eric Jankowski (Boise State), Neeraj Rai (Mississippi State), Sapna Sarupria (U. Minnesota), Michael R. Shirts, Jindal Shah (Oklahoma State)
Dates: 10/1/2021-9/31/2025
Amount: $104,845 (Shirts portion)

Agency: NIH/NIGMS
Project Title: Supplement: Open data-driven infrastructure for building biomolecular force fields for predictive biophysics and drug design
PIs: Michael R. Shirts
Dates: 10/1/2021-9/31/2022
Amount: $327,462 (Open Software development supplement)

Agency: NSF XSEDE Supercomputing Program
Project Title: Understanding organic crystal polymorph stability, transport in charged polymeric membranes, and peptide binding ensembles using molecular dynamics
PIs: Michael Shirts
Amount: 5.67 million CPU compute units and 15.2K GPU compute units. Estimated value of these awarded resources by XSEDE is $ 36,145.60.
Dates: 7/1/2021-6/30/2022

2020
Agency: NIH/NIGMS
Project Title: Supplement: Open data-driven infrastructure for building biomolecular force fields for predictive biophysics and drug design
PIs: Michael R. Shirts
Dates: 3/1/2020-2/28/2021
Amount: $96,003 (Equipment supplement)

Agency: NIH/NIGMS

Project Title: Supplement: Open data-driven infrastructure for building biomolecular force fields for predictive biophysics and drug design
PIs: Michael R. Shirts
Dates: 3/1/2020-2/28/2021
Amount: $157,074 (Open Software development supplement, Shirts portion)

Agency: NIH/NIBIB
Project Title: Glycoengineering of therapeutic peptides for improved treatment of human diseases, R01
PIs: Tarek Sammakia (CU Boulder)
Dates: 5/1/2020-4/30/2022
Amount: $80,000 (Shirts portion)

2019
Agency: DTRA
Project Title: High-MVTR, Stretchable, Biomimetic Porous Polymer Membranes for Chemical/Biological Defense (CBD)
PI: Josh Uzarski (Army Research Labs), Co-I's Doug Gin, Rich Noble, Michael Shirts
Dates: 3/1/2020-8/31/2022
Amount: $642,140 ($190,344 Shirts group amount).

Agency: NIH/NIGMS
Project Title: Open data-driven infrastructure for building biomolecular force fields for predictive biophysics and drug design, R01GM132386
PIs: Michael Shirts and John Chodera (MSKCC), Co-I's Michael Gilson (UC-San Diego). David Mobley (UC Irvine), and Lee-Ping Wang (UC Davis)
Dates: 3/1/2020-2/28/2024
Amount: $2,489,686 ($1,330,000 CU Boulder amount).

Agency: NSF XSEDE Supercomputing Program
Project Title: Understanding organic crystal polymorph stability, transport in charged polymeric membranes, and peptide binding ensembles using molecular dynamics
PIs: Michael Shirts
Amount: 3.92 million CPU compute units and 98.6K GPU compute units. Estimated value of these awarded resources by XSEDE is $122,620.
Dates: 10/1/2019-9/30/2020

2018
Agency: DOE Basic Energy Sciences
Project Title: What are the principles controlling biomimetic polymer secondary structure?
PIs: Michael Shirts (Joel Kaar co-I)
Amount: $782,171
Dates: 6/1/2018-5/31/2021

Agency: NSF OCI
Project Title: Collaborative Research: NCSI Framework: Software: SCALE-MS - Scalable Adaptive Large Ensembles of Molecular Simulations, NSF OCI-1835720
PIs: Michael Shirts, Peter Kasson (U. Virginia), Matteo Turilli (Rutgers), Kristen Fichthorn (Penn State),
Amount: $286,504 (CU portion)
Dates: 1/1/2019-12/31/2021

Agency: ACS Petroleum Research Fund
Project Title: Engineering molecular selectivity in self--assembled nanostructured membranes
PRF#59814-ND7
PIs: Michael Shirts
Amount: $110,000
Dates: 1/1/19-8/31/21

Agency: NSF XSEDE Supercomputing Program
Agency: DOE Basic Energy Sciences
Project Title: Understanding organic crystal polymorph stability, transport in charged polymeric membranes, and peptide binding ensembles using molecular dynamics
PIs: Michael Shirts
Amount: 3.38 million CPU compute units and 56K GPU compute units. Estimated value of these awarded resources by XSEDE is $96,511
Dates: 7/1/2018-6/30/2019

2017
Agency: NSF
Project Title: “D3SC: EAGER: Collaborative Research: A probabilistic framework for automated force field parameterization from experimental datasets”, NSF CHE-1738975
PIs: Michael Shirts and John Chodera
Amount: $118,918 (Shirts portion)
Dates: 8/1/2017 to 7/31/2019

Agency: NSF XSEDE Supercomputing Program
Project Title: “Understanding organic crystal polymorph stability, transport in charged polymeric membranes, and peptide binding ensembles using molecular dynamics simulations", NSF TG-MCB130021
PI: Michael R. Shirts
Amount: 2.95 million CPU hours, 95K GPU hours. Estimated value of these awarded resources by XSEDE is $130,321
Dates: 7/1/2017 to 6/30/2018

2016
Agency: National Institutes of Health, NIGMS
Project Title: “Hardening and Development of the GROMACS Molecular Simulation Engine,”
R01GM115790

PIs: Peter Kasson and Michael R. Shirts
Amount: $1,074,131 (Shirts portion $555,000)
Dates: 5/1/2016-4/30/2020

Agency: University of Colorado Boulder Innovative Seed Grant Program
Project Title: “Understanding the Molecular Details of Protein Binding Plasticity Through Atomistic Computer Simulation”
PI: Michael R. Shirts
Amount: $49,806
Dates: 7/1/2016-12/31/2017

Agency: NSF XSEDE Supercomputing Program
Project Title: “Understanding polymorph stability in organic crystals and transport in charged polymeric membranes using molecular dynamics simulation", NSF TG-MCB130021
PI: Michael R. Shirts
Amount: 3.53 million SU (compute units). Estimated value of these awarded resources by XSEDE is $240,424.00
Dates: 7/1/2016 to 6/30/2017

2014
Agency: Jeffress Trust Awards Program in Interdisciplinary Research
Project Title: “Understanding and Predicting Pharmaceutical Binding to Blood Plasma Proteins”
PI: Michael R. Shirts
Amount: $100,000
Dates: 6/30/2014 to 12/31/2015

Agency: NSF Division of Engineering, CBET program
Project Title: “CAREER: Understanding the thermodynamics of crystalline materials using advanced molecular simulation sampling methods,” NSF-CBET 1351635
PI: Michael R. Shirts
Amount: $449,976
Dates: 5/1/2014 to 4/30/2019

2012
Agency: NSF XSEDE Supercomputing Program
Project Title: “Modeling biological macromolecules in chromatography and drug design,” NSF TG-MCB130021
PI: Michael R. Shirts
Amount: Allocation of 250K supercomputer hours on NICS Keeneland GPU cluster, 2.8 million hours on Kraken supercomputer
Dates: 1/1/2013 to 7/30/2014

Agency: NSF Division of Chemistry, Theory, Models and Computational Methods Program

Project Title: “Highly multidimensional thermodynamic property prediction for chemical design using atomistic simulations,” NSF CHE-1152786
PI: Michael R. Shirts
Amount: $413,961
Dates: 5/15/2012 to 4/30/2015

2011
Agency: NSF Division of Chemical, Bioengineering, Environmental, and Transport Systems
Project Title: “Integrated Program for Conformational Effects in Protein Chromatography,” NSF CBET-1134256
PI: Erik J. Fernandez, Co-PIs: Michael R. Shirts, John P. O’Connell
Amount: $300,000
Dates: 9/1/2011 to 8/31/2014

Agency: NSF Teragrid Supercomputing Program
Project Title: “GPU-accelerated calculation of ligand binding affinities to biological macromolecules,” TG-MCB100015
PI: John D. Chodera (UC-Berkeley), Co-PIs: Michael R. Shirts, David L. Mobley (University of New Orleans)
Amount: Allocation of 1.27 million hours on NCSA Lincoln GPU cluster (shared between PIs)
Dates: 4/1/2011 to 9/30/2012

Agency: NRBSC Anton Specialized Supercomputer Program
Project Title: “The effects of nonnucleoside inhibitors on the structure and dynamics of HIV wild type reverse transcriptase and drug resistant mutants,” PSCA10097P
PI: Michael R. Shirts
Amount: 50,000 hours on the Anton supercomputer, National Resource for Biomedical Supercomputing
Dates: 11/1/2011 to 5/31/2012

2010
Agency: NSF Division of Chemical, Bioengineering, Environmental, and Transport Systems
Project Title: “Nanoscopic Understanding of Protein Transport and Structure Dynamics in Charged Gels for Protein Chromatography,” NSF CBET-1032727
PI: Giorgo Carta, Co-PI: Michael R. Shirts
Amount: $303,000
Dates: Dates: 8/15/2010 to 7/31/2013 (extended to 7/31/2014)

Agency: NSF NRCA Supercomputer Program
Project Title: “Comparison of molecular dynamics and 2D-IR spectroscopy for HIV-RT ligand binding”
PI: Michael R. Shirts
Amount: Allocation of 200,000 supercomputer hours on NCSA Kraken Cray cluster

2009

Agency: NSF NRCA Supercomputer Program
Project Title: "GPU-accelerated calculation of ligand binding affinities to biological macromolecules"
PI: John Chodera, co-PIs: Michael Shirts, David Mobley
Amount: Allocation of 250,000 hours on NCSA Lincoln GPU cluster (shared between PIs)

Agency: University of Virginia FEST Distinguished Young Investigator Award
Project Title: "Fighting drug resistance through *in silico* counter-evolution"
PI: Michael Shirts
Amount: $50,000

Agency: Oak Ridge Associated Universities Ralph E. Powe, Jr. Faculty Enhancement Award
Project Title: "Constructing and validating a robust benchmark set for solution phase molecular design using free energy calculations"
PI: Michael R. Shirts
Amount: $10,000 ($5,000 in match by U.Va.)

Teaching Experience

Colorado (2016–Present):

Spr. 2021–22	Instructor, CHEN 5838: Special Topics: Numerical Methods in Python
Spr. 2021–22	Instructor, CHEN 5838: Special Topics: Introduction to Machine Learning
Spr. 2019	Instructor, CHEN 4838/5838: Special Topics: Advanced Statistical Methods
Fall 2016–21	Instructor, CHEN 1211, General Chemistry for Engineers
Spring 2016	Instructor, CHEN 5750, Numerical Methods in Chemical Engineering

Virginia (2008–2015):

Fall 2014	Instructor, ChE 6665, Techniques for Chemical Engineering Analysis and Design
Spr. 2009–15	Instructor, ChE 2216, Modeling and Simulation in Chemical Engineering
Fall 2009–13	Instructor, ChE 6615, Advanced Thermodynamics

Ph.D. Students Mentored

University of Colorado (2015-Present)

1. Natalie Schieber, Chemical Engineering Ph.D. awarded 2018
2. Bryce Manubay, Chemical Engineering M.S. awarded 2018
3. Travis Jensen, Chemical Engineering M.S. awarded 2018
4. Nathan Abraham, Chemical Engineering Ph.D. awarded 2020
5. Ben Coscia, Chemical Engineering Ph.D. awarded 2020
6. Owen Madin, Chemical Engineering Ph.D. awarded 2022
7. Wei-Tse Hsu, Chemical Engineering Ph.D. candidate, Ph.D. awarded 2023
8. Theodore (Lenny) Fobe, Chemical Engineering Ph.D. candidate, Ph.D. awarded 2023
9. Anika Friedman, Biological Engineering Ph.D. candidate, 2020-current
10. Nathanael Schwindt, Chemical Engineering Ph.D. candidate, 2020-current

11. Dominique Ramirez, Biochemistry Ph.D. candidate, 2021-current
12. Yu-Tang Lin, Chemical Engineering M. S. awarded, 2022
13. Timotej Bernat, Chemical Engineering Ph.D. candidate, 2022-current
14. Barbara Morales, Chemistry Ph.D. candidate, 2023-current
15. Julianne Hoeflich, Chemical Engineering Ph.D. candidate, 2023-current
16. Annette Thompson, Chemical Engineering Ph.D. candidate (joint with Jerome Fox), 2023-current

University of Virginia (2008-2016)

17. Himanshu Paliwal, Chemical Engineering Ph.D. awarded April 2014
18. Joseph Basconi, Chemical Engineering Ph.D. awarded May 2015
19. Kai Wang, Chemical Engineering M.S. awarded, 2016
20. Levi Naden, Chemical Engineering, Ph.D. awarded August 2016
21. Brittany Bruns, Chemical Engineering, Ph.D. Candidate 2012–2015 (transferred to UC Berkeley law school)
22. Eric Dybeck, Chemical Engineering Ph.D. awarded December 2016
23. Tyler Prillaman, Chemical Engineering M.S. awarded May 2016

Undergraduate Students Mentored

University of Colorado Boulder (2016-current)

1. Norma Langdon (B.S. 2018), 2016-2018
2. Marcus Hock (B.S. 2019), 2017-2019
3. Tanner Bobak (B.S. 2020), 2017-2018
4. Megan Becker (B.S. 2020), 2017
5. Jenna Trost (B.S. 2021), 2018-2020
6. Lucas St. Germain (B.S. 2021), 2018
7. Thomas Schoderbek (B.S. 2021), 2019
8. Erast Davidjuk (B.S. 2021), 2019-2021
9. Conner Vogel (B. S. 2022), 2019-2021
10. Peter Dvorak (B.S. 2023), 2020-2021
11. Antonia Lim (B.S. 2023), 2020-2023
12. Connor Davel (B.S. 2023), 2020-2023
13. Hannah Padgette (B.S. 2023), 2020-2023
14. Sarah Mellett (B.S. 2023), 2021-2023
15. Ethan Coleman (B.S. 2025), 2022-2023
16. Anastasia Shrimpton (B.S. 2024), 2023-current
17. Patrick Frankel (B.S. 2025), 2023-current

University of Virginia (2008-2016)

18. Walid El-Nahal, Chemical Engineering (B.S. 2011), 2009–2011
19. Michael Zhu, Chemical Engineering (B.S. 2011), 2009–2011
20. Karan Mehra, Chemical Engineering (B.S. 2012), 2010–2011
21. Christopher Lee, Chemistry and Computer Science (B.S. 2011), 2010–2011

22. Christoph Klein, Chemical Engineering (B.S. 2012), 2010–2012
23. Arjan Kool, Chemical Engineering (B.S. 2013), 2011–2014
24. Ellen Zhong, Chemical Engineering (B.S. 2014), 2011–2014
25. Yanzhi Yang, Chemical Engineering (B.S. 2014), 2012–2014
26. Jacob Monroe, Chemical Engineering (B.S. 2014), 2012–2014
27. Kelly Glitzos, Chemical Engineering (B.S. 2015), 2012 (REU summer student).
28. Hari Devanathan, Computer Science (B.S. 2015), 2012–2013.
29. Mitch Slovin, Chemical Engineering (B.S. 2015), 2013–2015
30. Jacob Rosenthal, Chemical Engineering (B.S. 2015), 2014–2015.
31. Alex Yang, Chemical Engineering (B.S. 2016), 2013–2016
32. Andrew Biedermann, Chemical Engineering (B.S. 2017), 2014–2017
33. Saehee Jung, Chemical Engineering (B.S. 2018), 2014–2015

Postdoctoral Researchers Mentored

University of Colorado Boulder (2016-current)
1. Pascal Merz, Ph.D. 2017 (ETH Zurich), 2017-2021
2. Garrett Meek, Ph.D. 2016 (Michigan State), 2018-2019
3. Simon Boothroyd, Ph.D. 2018 (University of Lancaster), 2019-2020
4. Matt Thompson, Ph.D. 2019 (Vanderbilt University), 2020-2022
5. Christopher Walker, Ph.D. 2020 (North Carolina State University) 2020-2022
6. Subin Sahu, Ph.D. 2018 (University of Oregon) 2020-2022

University of Virginia (2008-2015)
7. Tri Pham, Ph.D. 2009, Monash University, (Australia), 2009–2011

Visitors Mentored

University of Virginia (2008-2015)
1. Jonathan Fuller, University of Leeds, (U.K.), Ph.D. 2010, summer visitor, 2009

University of Colorado Boulder (2016)
2. Can Pervane, University of Southampton (U.K), semester visitor 2017
3. Sayalee Patankar, (Research Science Institute high school student, Summer 2020)
4. Isabell Strawn (REU Student, University of Idaho, Summer 2020)
5. Theo Julien (Boulder High School student, Fall 2021-2022)
6. Marcos Serrou do Amaral (Sabbatical visitor, Professor, Universidade Federal de Mato Grosso do Sul, Spring 2024)

Conference Organization

1. Chair and organizer, “Molecular Simulation” sessions, 22nd Symposium on Thermophysical Properties, Boulder, CO, 2024

2. Chair and organizer, “Molecular Simulation” sessions, 21st Symposium on Thermophysical Properties, Boulder, CO, 2021
3. Chair and organizer, “Making Molecular Simulation a Mainstream Chemical Engineering Tool: Reproducibility, Robustness, and Usability”, Orlando, FL, November 2019.
4. Chair and organizer, “Making Molecular Simulation a Mainstream Chemical Engineering Tool: Reproducibility, Robustness, and Usability”, Pittsburgh, PA, November 2018.
5. Organizer, “Developing community best practices for molecular simulation software”, NIST Gaithersburg, MD, August 2017
6. Chair and organizer, “Making Molecular Simulation a Mainstream Chemical Engineering Tool: Reproducibility, Robustness, and Usability”, San Francisco, CA, November 2016.
7. Co-organizer, “2016 Workshop on Free Energy Methods in Drug Design: Going the Last Mile,” Boston, MA, May 2016.
8. Chair and Organizer, “3rd Workshop on Free Energy Methods in Drug Design,” Boston, MA, May 2014.
9. Chair and Organizer, 2013 GROMACS USA Workshop, University of Virginia, Charlottesville, VA, September 2013 (in charge of conference organization and logistics, including writing NSF proposal for support).
10. Co-chair, “Development of Intermolecular Force Fields,” AIChE National Meeting, Pittsburgh, PA, October 2012.
11. Co-organizer, “2nd Workshop on Free Energy Methods in Drug Design: Going the Last Mile,” Boston, MA, May 2012.
12. Chair, “Model Development for Complex Biological Systems,” and Co-chair, “Development of Intermolecular Force Fields,” AIChE National Meeting, Minneapolis, MN, October 2011.
13. Co-chair, “Recent Advances in Molecular Simulation Methods,” AIChE National Meeting, Salt Lake City, UT, November 2010.
14. Co-organizer, “2010 Workshop on Free Energy Methods in Drug Design: Going the Last Mile,” Boston, MA, May 2010.
15. Chair, “Recent Advances in Molecular Simulation Methods,” AIChE National Meeting, Nashville, TN, November 2009.

National Service

- Co-PI, Institute for Computational Molecular Science Education, 2021-current
- Founder and Managing Editor, *Living Journal of Computational Molecular Science*, 2018-current
- Organizing committee member, Symposium on Thermophysical Properties, 2018-current
- Scientific Advisory Board, Midwest Integrated Center for Computational Materials, 2019-current
- Institute for Computational Molecular Science Education, Co-PI, 2021-current
- AIChE COMSEF Liaison Director (2014-2017)
- Participant, DARPA Ideation Technology Exchange Workshop, January 2014. A DARPA-run workshop to brainstorm technologies to invest in over the next 10–20 years.

University Service:

University of Colorado Boulder (2016-current)

- Founder, PULSE (Public Policy for Undergraduates Learning Science and Engineering), public policy program for science and engineering undergraduates at CU (2017-2020)
- Campus Liaison for Fannie and John Hertz Foundation, 2018-current
- Faculty Member, Material Science Program, 2020-current
- Faculty Member, IQ Biology program, 2016–current

University of Virginia (2008-2015)
- Member, U.Va. Computational Science Advisory Council, 2008–2014.
- Campus Liaison for Fannie and John Hertz Foundation Student Summer Program, 2010.
- Reviewer, Harrison Undergraduate Research Awards, 2011, 2013–15

College Service:
University of Colorado Boulder (2016-current)
- Member, College-wide Engineering Proposal Review Committee

University of Virginia (2008-2015)
- Discussion Group Leader, Undergraduate Common Reading Experience, 2008–2013
- Journal Club Coordinator, NIH Biotechnology Training Program, 2009–2011
- Organizer, "Pharmaceutical Industry: In the Trenches" seminar series, brought five lecturers to speak on aspects of pharmaceutical development to a group of Biomedical Engineering, Chemical Engineering, and Chemistry undergrads, 2011

Departmental Service
University of Colorado Boulder (2016-current)
- Member, Graduate Studies Committee (2016–2017, 2020-2023)
- Member, Leadership Committee (2016–2017)
- Member, Undergraduate Studies Committee (2017-2020, 2023-current)

University of Virginia (2008-2016)
- Department Website and Social Media Coordinator, 2009–2015
- Department Newsletter Editor, 2011–2015
- Department Seminar Coordinator, 2009–2012, 2014
- Class of 2013 Advisor (30 students), 2010–2013
- Class of 2017 Advisor (30 students), 2014-2015
- Departmental Contact for Center for Diversity, 2012–2015
- Faculty Search Committee, 2013–2015
- Departmental Chair Search Committee, 2014–2015
- Departmental Faculty Representative, Society of Women Engineers, 2010–2014

Consulting
- Osmo.ai, 2023-current
- Relay Therapeutics, 2022-current

- Consultant and Open Science Fellow, Silicon Therapeutics, 2017-2021, Roivant Sciences, 2021-2022, Psivant Sciences, 2022-current
- Schrödinger, Inc.: Assisted in the design of protein structure prediction software, 2006
- D.E. Shaw Research and Development: Assisted in the design of computer hardware specialized for biomolecular simulations, 2003

Society Memberships
American Chemical Society
American Institute of Chemical Engineers
American Society for Engineering Education

Peer Reviewer for Journals
Biochemistry
Biophysical Journal
Bioorganic & Medicinal Chemistry
Digital Discovery
European Journal of Biophysics
Industrial & Engineering Chemistry Research
Fluid Phase Equilibria
Journal of the American Chemical Society
Journal of Biological Chemistry
Journal of Chemical Physics
Journal of Chemical Theory and Computation
Journal of Computational Chemistry
Journal of Computational and Applied Mathematics
Journal of Computer-Aided Molecular Design
Journal of Computational Physics
Journal of Medicinal Chemistry
Journal of Physical Chemistry B
Journal of the Royal Society Interface
Physical Chemistry Chemical Physics
Proteins: Structure, Function, and Bioinformatics
Proceedings of the National Academy of Sciences USA
PLoS Computational Biology
PLoS ONE
Science Advances