CURRICULUM VITAE

Clare McCabe

Personal Details

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Current Position: Cornelius Vanderbilt Professor of Engineering
Professor of Chemical and Biomolecular Engineering
Professor of Chemistry

Education

1995	- 1999	Ph.D. in Physical Chemistry, University of Sheffield, UK. Thesis title: Statistical Mechanics of Chain Molecules Supervisor: Prof. George Jackson (Chemical Engineering, Imperial College, London)
1992	- 1995	B.Sc. (Hon's) in Chemistry (First Class Honors), University of Sheffield, UK

Professional Experience

Feb.	2017	-	Present		Cornelius Vanderbilt Professor of Engineering, Vanderbilt University
May	2011	-	Present		Professor, Dept. of Chemical & Biomolecular Engineering, Vanderbilt University
May	2011	-	Present		Professor, Dept. of Chemistry, Vanderbilt University
Jan.	2017	-	June	2020	Associate Dean of the Graduate School and founding director of the Office of Postdoctoral Affairs, Vanderbilt University
June	2008	-	May	2011	Associate Professor, Dept. of Chemistry, Vanderbilt University
Sept.	2007	-	Aug.	2011	Associate Professor, Dept. of Chemical & Biomolecular Engineering, Vanderbilt Universityc
Aug.	2004	-	Aug.	2007	Assistant Professor, Dept. of Chemical Engineering, Vanderbilt University
Aug.	2004	-	Aug.	2006	Adjunct Assistant Professor, Department of Chemical Engineering, Colorado School of Mines, Golden, CO
Jan.	2002	-	July	2004	Assistant Professor, Department of Chemical Engineering, Colorado School of Mines, Golden, CO
Oct.	2000	-	Dec.	2001	Research Assistant Professor, Department of Chemical Engineering, University of Tennessee, Knoxville, TN
Jan.	1999	-	Sept.	2000	Postdoctoral Research Associate, Department of Chemical Engineering, University of Tennessee, Knoxville, TN.
Oct.	1997	-	Dec.	1998	Visiting Research Associate at the Institute Superior Tecnico, Lisbon, Portugal

Professional Society Memberships

- Fellow of the American Association for the Advancement of Science, AAAS (2019-)
- Fellow of the American Institute of Chemical Engineers (2019-)
- Fellow of the Royal Society of Chemistry (2007-)
- Senior member of the American Institute of Chemical Engineers (1999-)
- Member, American Chemical Society (2000-)
- Member, Sigma Xi (2000-)
- Member, American Society for Engineering Education (2002-)
- Member, Society of Women Engineers (2003-)
- Member, Biophysical Society (2010-)

Honors and Awards

- 2018 Chancellors Award for Research, Vanderbilt University
- 2014 American Institute of Chemical Engineers (AIChE) Computational Molecular Science and Engineering (CoMSEF) Impact Award
- 2014 Vanderbilt Institute for Nanoscale Science and Engineering Distinguished Service Award
- 2014 Littlejohn Faculty Fellow, Vanderbilt University
- 2011 Vanderbilt University Madison Sarratt Prize for Excellence in Undergraduate Teaching
- 2010 School of Engineering Excellence in Teaching Award
- Jacob Wallenberg Foundation Fellowship from the Royal Swedish Academy of Engineering Sciences (2007 - 2010)
- ACS Women Chemists Committee Lectureship Award, Fall 2002
- UGC Scholarship, University of Sheffield (1995-1998)
- Haworth Medal for Chemistry (first place in graduating class), 1995

Selected Professional Service

National Committees

- Member, National Academy of Sciences, molecular dynamics review panel, 2018, 2019, 2020.
- Member, American Chemical Society Petroleum Research Fund Advisory Board (2017 – 2023)
- Member, Research & New Technology Committee (RANTC) of the American Institute of Chemical Engineers, January 2017 –
- Elected member, Chemical Technology Operating Council (CTOC) of the American Institute of Chemical Engineers, January 2014 – December 2016.
- Elected member, Council for Chemical Research's Governing Board, January 2012 – December 2015.
- Chair of the Nanoscience session at the U.S. Department of Energy Office of Science (Office of Advanced Scientific Computing Research) sponsored workshop *Scientific Impacts And Opportunities For Computing* held January 9 -12, 2008 and co-author of the proceeding workshop report [http://www.sc.doe.gov/ascr/ProgramDocuments/Docs/ScientificImpacts&Oppor.pdf].
- Co-chair of the Self-assembly and Soft Matter Panel, U.S. Department of Energy Office of Science Workshop on Computational Materials Science and Chemistry for Innovation held July 26-28, 2010.
- Secretary, of the non-profit organization Computer Aids for Chemical Engineering Education (CAChE), 2010 - 2012.
- Elected trustee of the non-profit organization Computer Aids for Chemical Engineering Education (CAChE), 2009 –
- Elected member of the Area 1a (Thermodynamics and Transport Properties of the American Institute of Chemical Engineers) Program Committee, November 2006 - November 2009 and November 2009 - November 2011.
- Area 1a (Thermodynamics and Transport Properties of the American Institute of Chemical Engineers) Program Chair for Fall 2011 annual meeting.
- Vice-Chair, of Area 21, the Computational Molecular Science and Engineering Forum (COMSEF) of the American Institute of Chemical Engineers, November 2006 - November 2008.
- Chair of Area 21 (COMSEF) of the American Institute of Chemical Engineers, November 2008 - November 2010.
- Past Chair of Area 21, the Computational Molecular Science and Engineering Forum (COMSEF) of the American Institute of Chemical Engineers, November 2010 - November 2012.
- Area 21 (COMSEF) of the American Institute of Chemical Engineers Programming Chair for the Fall 2007 and 2008 annual meetings.
- Elected to the AIChE-ASME K-7 Joint Committee on Thermophysical Properties (2005 -).
- Secretary, AIChE-ASME K-7 Joint Committee on Thermophysical Properties (2009 -).

Editorial

- Editor-in Chief, Fluid Phase Equilibria 2015 - ; Editor, Fluid Phase Equilibria 2012 – 2015
- Member of the editorial board of the international journal Fluid Phase Equilibria, 2006 - 2011.
- Member of the editorial board of the international journal Accounts in Physical Chemistry, 2008 – 2014.
- Guest Editor, Special Issue of *Fluid Phase Equilibria* on ionic liquids (2010).
- Guest Editor, Special Issue of *Fluid Phase Equilibria* for the Proceedings of the 17th Symposium on Thermophysical Properties Conference held June 21st-26th 2009.
- Guest Editor, Special Issue of *Molecular Physics* for the Proceedings of the Foundations of Molecular Modeling and Simulation (FOMMS) conference held July 9th-14th 2006.
- Guest Editor, Special Issue of *Molecular Simulation* for the Proceedings of the Foundations of Molecular Modeling and Simulation (FOMMS) conference held July 9th-14th 2006.

Conference Organization

- Member, Properties and Phase Equilibria for Product and Process Design (PPEPPD) International Organizing Committee, 2017 -.
- Elected Member, Joint ASME-AIChE Committee on Thermophysical Properties that oversees the Triannual Symposia on Thermophysical Properties held in Boulder, CO, 2005 - present.
- Senior advisor, Foundations of Molecular Modeling and Simulation (FOMMS) Conference series held in the US every 3 years (2012-).

Vanderbilt University

- Founding Director, Vanderbilt Office of Postdoctoral Affairs, January 2017 – July 2020.
- Founding Director, Academic Pathways Postdoctoral Fellowship Program, August 2016 – July 2020.
- Member, Vanderbilt Institute for Nanoscale Science and Engineering (VINSE) advisory committee, Fall 2016 – Fall 2018.
- Member, Chancellor's Faculty Advisory Committee on Land Use, Fall 2016.
- Provost's Promotion and Tenure Review Committee, Fall 2015 – Spring 2018.
- Director of the Vanderbilt Institute for Nanoscale Science and Engineering (VINSE) NSF Research Experience for Undergraduates (REU) Site program (and PI of the REU grants), Fall 2009 – present.
- Chair Vanderbilt University Summer Undergraduate Research Program (VUSRP), 2012 - 2017.
- Director of the Graduate Program, Chemical and Biomolecular Engineering, 2007 – 2018.
- Chair, Department of Chemical and Biomolecular Engineering Assistant Professor Search Committee, 2015/2016 (academic years).
- Member, Department of Chemical and Biomolecular Engineering Faculty Search Committees, 2014/2015 and 2016/2017 (academic years).
- Chair, Vanderbilt School of Engineering Committee on Faculty Development and Diversity, 2015 – 2016.
- Member, Graduate Faculty Council, 2009/2010 - 2012/2013 (academic years).
- Director of Graduate Assistance in Areas of National Need (GAANN) program (and PI of GAANN grant) in Advanced Materials, Chemical and Biomolecular Engineering, Fall 2009 – Spring 2013.
- Member, VUSE Dean Search Committee, Fall 2011.
- Member, Department of Chemical and Biomolecular Engineering Chair Search Committee, Fall 2005 - Spring 2007.
- Faculty advisor for the undergraduate chapter of the Society of Women Engineers, Fall 2009 - 2018.

Outreach

- Participated as a mentor to local high school teachers in a summer NSF RET program at Vanderbilt University (2007, 2009 and 2011).
- Participate as a mentor to local high school students in independent study projects 2015, 2017 - 2019.

- Provide interactive demonstrations of our research to visiting middle and high school students and accompanying teachers as part of the Vanderbilt Summer Academy and Governor's School programs. Summers 2005, 2007, 2009, 2011, 2013, 2015, 2016 and 2017.
- Annually mentor several undergraduate students in research projects to expose them to research and encourage them to consider graduate school.

Refereed Journal Publications (*graduate students advised in italics,* **undergraduates advised in bold)**

h-index 48 (Google scholar, https://scholar.google.com/citations?user=ikdrOCMAAAAJ&hl=en)

1. C. McCabe, A. Galindo, A. Gil-Villegas, and G. Jackson, "Predicting the High-Pressure Phase Equilibria of Binary Mixtures of n-Alkanes with the SAFT-VR Approach," *International Journal of thermophysics*, **19**, 1511-1522 (1998).
2. C. McCabe, A. Gil-Villegas, and G. Jackson, "Predicting the High-Pressure Phase Equilibria of Methane + n-Hexane Using the SAFT-VR Approach," *Journal of Physical Chemistry B*, **102**, 4183-4188 (1998).
3. C. McCabe, A. Galindo, A. Gil-Villegas, and G. Jackson, "Predicting the High-Pressure Phase Equilibria of Binary Mixtures of Perfluoro-n-Alkanes + n-Alkanes Using the SAFT-VR Approach," *Journal of Physical Chemistry B*, **102**, 8060-8069 (1998).
4. C. McCabe, A. Gil-Villegas, and G. Jackson, "Gibbs Ensemble Computer Simulation and SAFT-VR Theory of Non-Conformal Square-Well Monomer-Dimer Mixtures," *Chemical Physics Letters*, **303**, 27-36 (1999).
5. C. McCabe, A. Gil-Villegas, G. Jackson, F. Del Rio, "The Thermodynamics of Heteronuclear Molecules Formed from Bonded Square-Well (BSW) Segments Using the SAFT-VR Approach," *Molecular Physics*, **97**, 551-558 (1999).
6. C. McCabe and G. Jackson, 'SAFT-VR Modeling of the Phase Equilibrium of Long-Chain n-Alkanes," *Physical Chemistry Chemical Physics*, **1**, 2057-2064 (1999).
7. E. J. M. Filipe, E. J. S. Gomes de Azevedo, L. F. G. Martins, V. A. M. Soares, J. C. G. Calado, C. McCabe and G. Jackson, "Thermodynamics of Liquid Mixtures of Xenon With Alkanes: Xenon + Ethane and Xenon + Propane," *Journal of Physical Chemistry B*, **104**, 1315-1321 (2000).
8. E. J. M. Filipe, L. F. G. Martins, J. C. G. Calado, C. McCabe and G. Jackson, "Thermodynamics of Liquid Mixtures of Xenon with Alkanes: Xenon + Butane and Xenon + i-Butane," *Journal of Physical Chemistry B*, **104**, 1322-1325 (2000).
9. C. McCabe, S. T. Cui, P. T. Cummings, Peter A. Gordon, and Roland B. Saeger, "Examining the Rheology of 9-Octylheptadeacne to Giga-Pascal Pressures," *Journal of Chemical Physics*, **114**, 1887-1891 (2001).
10. C. McCabe, S. T. Cui, and P. T. Cummings, "Characterizing the Viscosity-Temperature Dependence of Lubricants by Molecular Simulation," *Fluid Phase Equilibria*, **183**, 363-370 (2001).
11. C. McCabe, D. Bedrov, G. D. Smith, and P. T. Cummings, "Discriminating Between Correlated Experimental Viscosity Data Using Molecular Simulation," *Industrial & Engineering Chemistry Research*, **40**, 473-475 (2001).
12. C. McCabe, L. M. B. Dias, E. J. M. Filipe, G. Jackson, "On the Liquid Mixtures of Xenon, Alkanes and Perfluoroalkanes," *Physical Chemistry Chemical Physics*, **3**, 2852-2855 (2001).
13. C. McCabe, A. Galindo, M. N. Garcia-Lisbona and G. Jackson, "Examining the Adsorption (vapor-liquid equilibrium) of Small Hydrocarbons on Low Density Polyethylene with the SAFT-VR Approach," *Industrial & Engineering Chemistry Research*, **40**, 3835-3842 (2001).
14. H.-C. Li, C. McCabe, S. T. Cui, P. T. Cummings, and H. D. Cochran, "Development of a Force Field for Molecular Simulation of the Phase Equilibria of Perfluoro-Methyl-Propyl Ether," *Molecular Physics*, **100**, 265-272 (2002).

15. S. Bair, C. McCabe, and P. T. Cummings, "Comparison of Non-Equilibrium Molecular Dynamics with Experimental Measurements in the Nonlinear Shear-Thinning Regime", *Physical Review Letters,* **88**, 058302 (2002).
16. C. McCabe, C. W. Manke and P. T. Cummings, "Predicting the Newtonian Viscosity of Complex Fluids from High Strain Rate Molecular Simulations", *Journal of Chemical Physics,* **116**, 3339 – 3343 (2002).
17. C. McCabe, Y. V. Kalyuzhnyi and P. T. Cummings, "Thermodynamic Properties of Freely-Jointed Hard-Sphere Multi-Yukawa Chain Fluids: Theory and Simulation," *Fluid Phase Equilibria*, **194**, 185-196 (2002).
18. S. Furukawa, C. McCabe, P. T. Cummings, T. Nitta, "Non-Equilibrium Molecular Dynamics Simulation Studies On the Behavior of Hydrocarbon-Isomers In Silicalite," *Fluid Phase Equilibria*, **194**, 309–317 (2002).
19. Y. V. Kalyuzhnyi, C. McCabe, P. T. Cummings and G. Stell, "Structural and Thermodynamic Properties of a Multicomponent Freely-Jointed Hard-Sphere Multi-Yukawa chain fluid," *Molecular Physics*, **100**, 2499-2517 (2002).
20. R. P. Bonifácio, E. J. M. Filipe, C. McCabe, M. F. Costa Gomes, A. A. H. Pádua, "Predicting the Solubility of Xenon in n-Hexane and n-Perfluorohexane: A Simulation and Theoretical Study," *Molecular Physics*, **100**, 2547-2553 (2002).
21. E. J. M. Filipe, L. M. B. Dias, J. C. G. Calado, C. McCabe and G. Jackson, "Is Xenon an Enobled Alkane?" *Physical Chemistry Chemical Physics,* **4**, 1618-1621 (2002).
22. S. Bair, C. McCabe, and P. T. Cummings, "Calculation of Viscous EHL Traction for Squalane Using Molecular Simulation and Rheometry", *Tribology Letters*, **13**, 251-254 (2002).
23. J. L. Rivera, C. McCabe, and P. T. Cummings, "Layering Behavior and Axial Phase Equilibria of Pure Water and Water + Carbon Dioxide Inside Single Walled Carbon Nanotubes", *Nano Letters*, **2**, 1427-1431 (2002).
24. L. M. B. Dias, R P. Bonifácio, E. J. M. Filipe, J. C. G. Calado, C. McCabe and G. Jackson, "Liquid-Vapor Equilibrium of {xBF_3 + (1-x) n-butane} at 195.49K," *Fluid Phase Equilibria,* **205**, 163-170 (2003).
25. J. L. Rivera, C. McCabe, and P. T. Cummings, "Molecular Simulations of Liquid-Liquid Interfacial Properties: Water / *N*-Alkane and Water + Methanol / *N*-Alkane Systems, *Physical Review E,* **67**, article number 011603 (2003).
26. S. T. Cui, C. McCabe, P. T. Cummings, and H. D. Cochran, "Molecular Dynamics Study of the Nano-Rheology of n-Dodecane Confined Between Planar Surfaces," *Journal of Chemical Physics*, **118**, 8941-8944 (2003).
27. J. C. Pàmies, C. McCabe, P. T. Cummings, and L. F. Vega, "Coexistence Densities of Methane and Propane by Quench Molecular Dynamics and Gibbs Ensemble Monte Carlo Simulations," *Molecular Simulation*, **29**, 463-470 (2003).
28. J. L. Rivera, C. McCabe, and P. T. Cummings, "Oscillatory Behavior of Double-Walled Nanotubes Under Extension: A Simple Nanoscale Damped Spring," *Nano Letters,* **3**, 1001-1005 (2003).
29. H.-C. Li, C. McCabe, S. T. Cui, P. T. Cummings, and H. D. Cochran, "On the Development of a General Force Field for the Molecular Simulation of Perfluoroethers," *Molecular Physics,* **101**, 2157–2169 (2003).
30. C. McCabe, A. Galindo and P. T. Cummings, "Anomalies in the Solubility of Alkanes in Near-Critical Water," *Journal of Physical Chemistry B*, **107**, 12307-12314 (2003).
31. C. McCabe, O. Borodin, D. Bedrov, G. D. Smith, and P. T. Cummings, "Transport Properties of Perfluoroalkanes Using Molecular Dynamics Simulation: Comparison of United- and Explicit-Atom Models," *Industrial & Engineering Chemistry Research,* **42**, 6956-6961 (2003).

32. C. McCabe and S. B. Kiselev, "A Crossover SAFT-VR Equation of State for Pure Fluids: Preliminary Results for Light Hydrocarbons," *Fluid Phase Equilibria*, **219**, 3-9 (2004).
33. C. McCabe and S. B. Kiselev, "Application of Crossover Theory to the SAFT-VR Equation of State: SAFT-VRX for Pure Fluids," *Industrial & Engineering Chemistry Research*, **43**, 2839-2851 (2004).
34. L. M. B. Dias, E. J. M. Filipe, J. C. G. Calado, and C. McCabe, "Thermodynamics of Liquid (Xenon + Methane) Mixtures," *Journal of Physical Chemistry B*, **108**, 7377-7381 (2004).
35. M.-J. Lee, C. McCabe, P. T. Cummings, "Square-Well Chain Molecules: A Semi-Empirical Equation of State and Monte Carlo Simulation Data," *Fluid Phase Equilibria,* **221**, 63-72 (2004).
36. S. Bair and C. McCabe, "A Study of Mechanical Shear Bands in Liquids at High-Pressure," *Tribology International*, **37**(10) 783-789 (2004).
37. Y. V. Kalyuzhnyi, C. McCabe, **E. Whitebay** and P. T. Cummings, "Equation of State and Liquid-Vapor Equilibria of One- and Two-Yukawa Hard-Sphere Chain Fluids: Theory and Simulation", *Journal of Chemical Physics*, **121**(16), 812-8137 (2004).
38. C. McCabe, S. C. Glotzer, J. Kieffer, M. Neurock and P. Cummings, "Multiscale Simulation of the Synthesis, Assembly and Properties of Nanostructured Organic/Inorganic Hybrid Materials," Journal of Theoretical and Computational Nanoscience, **1**(4), 265-279 (2004).
39. J. L. Rivera, C. McCabe and P. T. Cummings, "The oscillatory damped behavior of incommensurate double-walled carbon nanotubes," *Nanotechology,* **16,** 186-198 (2005).
40. G. Pan, J. F. Ely, C. McCabe and D. Isbister, "Operator splitting algorithm for iso-kinetic SLLOD molecular dynamics," *Journal of Chemical Physics,* **122**, 9, 4114 (2005).
41. L. Sun, *H. G. Zhao*, S. B. Kiselev and C. McCabe, "Application of SAFT-VRX to Binary Phase Behaviour: Alkanes," *Fluid Phase Equilibria*, **228-229**, 275-282 (2005).
42. **P. Morgado**, C. McCabe and E. J. M. Filipe, "Modeling the phase behavior and excess properties of alkane + perfluoroalkane binary mixtures with the SAFT-VR approach," *Fluid Phase Equilibria*, **228-229**, 389-393 (2005).
43. L. Sun, *H. G. Zhao*, S. B. Kiselev and C. McCabe, "Predicting Mixture Phase Equilibria and Critical Behavior using the SAFT-VRX Approach," *Journal of Physical Chemistry B,* **109**, 9047-9058 (2005).
44. A. Striolo, C. McCabe and P. T. Cummings, "Thermodynamic and Transport Properties of Polyhedral Oligomeric Silsesquioxanes in Poly(Dimethyl Siloxane)," *Journal of Physical Chemistry B,* **109** 14300 - 14307 (2005).
45. A. Striolo, C. McCabe and P. T. Cummings, "Effective Interactions between Polyhedral Oligomeric Silsesquioxanes Dissolved in normal Hexadecane from Molecular Simulation," *Macromolecules*, **38**, 8950-8959 (2005).
46. *Y. Peng*, *H. G. Zhao* and C. McCabe, "On the Thermodynamics of Diblock Chain Fluids from Simulation and the Heteronuclear Statistical Associating Fluid Theory for Potentials of Variable Range," *Molecular Physics,* **104**(4), 571-586 (2006).
47. *T. C. Ionescu*, F. Qi, C. McCabe, A. Striolo, J. Kieffer and P. T. Cummings, "Evaluation of Force Fields for Molecular Simulation of Polyhedral Oligomeric Silsesquioxanes," *Journal of Physical Chemistry B,* **110**, 2502 - 2510 (2006).
48. *H. G. Zhao* and C. McCabe, "Phase Behavior of Dipolar Fluids from a Modified Statistical Associating Fluid Theory for Potentials of Variable Range," *Journal of Chemical Physics,* **125**, 104504 (2006).
49. A. Striolo, C. McCabe and P. T. Cummings, "Organic-Inorganic Telechelic Molecules: Solution Properties from Simulations" *Journal of Chemical Physics*, **125**, 104504 (2006).
50. *H. G. Zhao*, **P. Morgado**, C. McCabe and A. Gil-Villegas, "Predicting the Phase Behavior of Nitrogen + n-Alkanes for Enhanced Oil Recovery from the SAFT-VR Approach: Examining the

Effect of the Quadrupole Moment," *Journal of Physical Chemistry B*, **110** (47) 24083-24092 (2006).

51. G. Pan and C. McCabe, "Prediction of Viscosity for Molecular Fluids at Experimentally Accessible Shear Rates Using the Transient Time Correlation Function Formalism: Application to n-Decane," *Journal of Chemical Physics,* **125** (19), 4527 (2006).
52. L. Sun, *H. G. Zhao* and C. McCabe, "Predicting the Phase Equilibria of Petroleum Fluids with the SAFT-VR Approach," *AIChE Journal*, **53**(3), 720-731 (2007).
53. A. Martinez, **M. Castro**, C. McCabe and A. Gil-Villegas, "Predicting adsorption isotherms using a 2D SAFT-VR approach," *Journal of Chemical Physics*, **126**(7), 4707 (2007).
54. **P. Morgado**, *H. G. Zhao*, C. McCabe, F. J. Blas, L. P. N. Rebelo, E. J. M. Filipe, "Liquid Phase Behavior of Perfluoroalkylalkane Surfactants," *Journal* of *Physical Chemistry B*, **111**(11), 2856-2863 (2007).
55. *Y. Peng* and C. McCabe, "Molecular Simulation and Theoretical Modeling of Polyhedral Oligomeric Silsesquioxanes," *Molecular Physics*, **105**(2-3), 261-272 (2007).
56. *L. M. B. Dias*, E. J. M. Filipe, C. McCabe, T. Cordeiro, and J. Calado, "Liquid Mixtures of Xenon with Fluorinated Species: Xenon + Sulfur Hexafluoride, *Journal of Physical Chemistry B*, **111**, 5284-5289 (2007).
57. H.-C. Li, C.-Y. Lee, C. McCabe, A. Striolo, and M. N Neurock, "Ab Initio Analysis of the Structural Properties of Alkyl-Substituted Polyhedral Oligomeric Silsesquioxanes," *Journal of Physical Chemistry A*, **111**, 3577-3584 (2007).
58. *H. G. Zhao*, M. C. dos Ramos, and C. McCabe, "Development of an Equation of State for Electrolyte Solutions by Combining the Statistical Associating Fluid Theory and the Mean Spherical Approximation for the Non Primitive Model," *Journal of Chemical Physics*, **126**(24), 4503 (2007).
59. *H. G. Zhao, Y. Ding* and C. McCabe, "Phase behavior of dipolar associating fluids from the SAFT-VR+D equation of state," *Journal of Chemical Physics*, **127**(8), 4514 (2007).
60. E. R. Chan, A. Striolo, C. McCabe, S. C. Glotzer and P. T. Cummings, "Coarse-Grained Force Field for Simulating Polymer-Tethered Silsesquioxane Self-Assembly in Solution," *Journal of Chemical Physics*, **127**, 114102 (2007).
61. A. Striolo, C. McCabe, P. T. Cummings, E. R. Chan and S. C. Glotzer, "Aggregation of POSS Monomers in Liquid Hexane: A Molecular-Simulation Study," *Journal of Physical Chemistry B*, **111**, 12248 (2007).
62. **P. Morgado**, R. Tomás, H. G. Zhao, M. C. dos Ramos, F. J. Blas, C. McCabe and E. J. M. Filipe, "Solution Behaviour of Perfluoroalkanes and Perfluoroalkylalkane Surfactants in n-octane," *Journal of Physical Chemistry C*, **111** (43), 15962 -15968, (2007).
63. L. Zhong, J. F. Matthews, M. F. Crowley, *T. Rignall*, C. Talon, J. M. Cleary, R. C. Walker, G. Chukkapalli, C. McCabe, M. R. Nimlos, C. L. Brooks, M. E. Himmel, and J. W. Brady, "Interactions of the Complete Cellobiohydrolase I from Trichoderma reesei with Microcrystalline Cellulose Ib," *Cellulose*, **15** (2) 261-273 (2008).
64. X. Zhao, *T. R. Rignall*, C. McCabe, W. S. Adney, M. E. Himmel, "Molecular simulation evidence for processive motion of Trichoderma reesei Cel7A during cellulose depolymerization," *Chemical Physics Letters*, **460** 284–288 (2008).
65. M. C. dos Ramos, **K. D. Goff**, H. G. Zhao and C. McCabe, "Modeling the Phase Behaviour of H_2S + n-Alkane Binary Mixtures Using the SAFT-VR+D Approach," *Journal of Physical Chemistry B*, **112** (31) 9417-9427 (2008).
66. *A. M. Cione*, O. A. Mazyar, *B. D. Booth*, C. McCabe, and G. K. Jennings, "Deposition and Wettability of [bmim] [triflate] on Self-Assembled Monolayers," *Journal of Physical Chemistry C*, **113**, 2384-2392 (2009).

67. *Y. Peng*, **K. D. Goff**, M. C. dos Ramos and C. McCabe, "Developing a Group-Contribution-Based SAFT-VR Equation of State," *Fluid Phase Equilibria*, **277** 131–144 (2009).
68. O. A. Mazyar, G. K. Jennings, and C. McCabe, "Frictional Dynamics of Alkylsilane Monolayers on SiO_2: Effect of 1-n-butyl-3-methylimidazolium Nitrate as a Lubricant," *Langmuir*, **25** (9), 5103–5110 (2009).
69. O. A. Mazyar, G. Pan and C. McCabe, "Transient time correlation function calculation of the viscosity of a molecular fluid at low shear rates: a comparison of stress tensors," *Molecular Physics*, **107** (14) 1423-1429 (2009).
70. *P. S. Redmill*, **S. C. Capps**, P. T. Cummings, and C. McCabe, "A Molecular Dynamics Study of the Gibbs Free Energy of Solvation of Fullerene Particles in Octanol and Water," *Carbon,* **47** 2865 – 2874 (2009).
71. *B. D. Booth, S. G. Vilt*, C. McCabe, and G. K. Jennings, "Tribology of Monolayer Films: Comparison between n-Alkanethiols on Gold and n-Alkyl Trichlorosilanes on Silicon," *Langmuir,* **25** (17), 9995–10001 (2009).
72. *S. G. Vilt*, **Z. Leng**, *B. D. Booth*, C. McCabe, and G. K. Jennings, "Surface and Frictional Properties of Two-Component Alkylsilane Monolayers and Hydroxyl-Terminated Monolayers on Silicon," Journal of Physical Chemistry C, **113** (33), 14972–14977 (2009).
73. M. C. dos Ramos and C. McCabe, "Modeling the Phase Behavior, Excess Enthalpies and Henry's Constants of the H_2O + H_2S Binary Mixture Using the SAFT-VR+D Approach," *Fluid Phase Equilibria*, **290** 137-147 (2010).
74. *Y. Peng*, **K. D. Goff**, M. C. dos Ramos and C. McCabe, "Predicting the Phase Behavior of Polymer Systems with the GC-SAFT-VR Approach," *Industrial & Engineering Chemistry Research*, **49** (3), 1378-1394 (2010).
75. *K. R. Hadley* and C. McCabe, "On the Investigation of Coarse-Grained Models for Water: Balancing Computational Efficiency and the Retention of Structural Properties," *Journal of Physical Chemistry* B, **114** (13), 4590–4599 (2010).
76. *K. R. Hadley* and C. McCabe, "A Coarse-Grained Model for Amorphous and Crystalline Fatty Acids," *Journal of Chemical Physics*, **132**, 134505 (2010). *Selected for inclusion in the Virtual Journal of Biological Physics Research.*
77. *P. S. Redmill* and C. McCabe, "Molecular Dynamics Study of the Behavior of Selected Nanoscale Building Blocks in a Gel-Phase Lipid Bilayer," *Journal of Physical Chemistry B,* **14** (28), 9165–9172 (2010).
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Other Refereed Publications and Conference Proceedings

1. C. McCabe, P. T. Cummings, S. T. Cui, P. A. Gordon, and R. B. Saeger, "Determining the Pressure-Viscosity Coefficient by Molecular Simulation," *Proceedings of the First International Conference on the Foundations of Molecular Modeling and Simulation (FOMMS 2000)*, American Institute of Chemical Engineers Symposium Series No. 325, **97,** 199-202 (2000).
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15. G. Varga, J. Sallai, A. Ledeczi, C. R. Iacovella, C. McCabe, and P. T. Cummings, "Enabling Cross-Domain Collaboration in Molecular Dynamics Workflows," Proceedings of the Fourth International Conference on Advanced Collaborative Networks, Systems and Applications, Seville, Spain (2014).
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Book Chapters

1. P. T. Cummings and C. McCabe, "Molecular Rheology," *2002 Yearbook of Science and Technology*, McGraw-Hill, New York (2001).
2. P. T. Cummings and C. McCabe, "Tribology at the Nanoscale," *Encyclopedia of Nanoscience and Nanotechnology*, Marcel Dekker (2004).
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Reports

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2. C. McCabe and I. Aronson "Self-assembly and soft matter," in Report of the Department of Energy Workshop on Computational Materials Science and Chemistry for Innovation July 26–27, 2010, Office of Science, Department of Energy. Available online at http://www.ornl.gov/sci/cmsinn/CMSC_Workshop_Report.pdf

Invited Presentations

1. C. McCabe, "Phase Behavior of Chain Molecules using the SAFT-VR Approach," XII School on Complex Fluids, San Luis, Potosi, Mexico, September 1st 1999.
2. C. McCabe, "Molecular Modeling of Phase Equilibria and Transport Properties," Dept. Chemical Engineering, University of Tennessee, Knoxville, September 19th 2000.
3. C. McCabe, "Molecular Modeling of Phase Equilibria and Transport Properties," Dept. Chemical Engineering and Petroleum Refining, Colorado School of Mines, Golden, Colorado, November 3rd 2000.
4. C. McCabe, "Molecular Modeling and Simulation of Fluorinated Systems," Dept. Chemical Engineering, Colorado School of Mines, Golden, Colorado, February 23rd 2001.
5. C. McCabe, "Phase Behavior and Transport Properties of Hydrocarbon Systems," Dept. Chemical Engineering, University of Florida, Gainesville, Florida, March 1st 2001.
6. C. McCabe, "Examining the Rheology of Fluorinated Molecules by Molecular Simulation," Dept. of Materials and Applied Chemistry, Nihon University, Tokyo, Japan, May 16th 2001.
7. C. McCabe, "Examining the Rheology of Fluorinated Molecules by Molecular Simulation," Dept. Chemical Science and Engineering, Osaka University, Osaka, Japan, May 18th 2001.
8. C. McCabe, "Phase Behavior and Transport Properties of Perfluorocarbon Systems," Dept. Chemical Engineering, Instituto Superior Técnico, Lisboa, Portugal, May 31st 2001.
9. C. McCabe, "Molecular Modelling of Phase Equilibria and Transport Properties," Research School of Chemistry, Australian National University, Canberra, Australia, September 21st 2001.

10. C. McCabe, "Molecular Modelling of Phase Equilibria and Transport Properties," Dept. Applied Physics, Royal Melbourne Institute of Technology, Melbourne, Australia, September 27th 2001.
11. C. McCabe, "Characterizing the High Pressure Behaviour of Lubricant Basestocks," ExxonMobil Research and Engineering, Corporate Strategic Research, Annandale, NJ, March 19th 2002.
12. P. T. Cummings, S. T. Cui, C. McCabe, and H. D. Cochran, "Molecular Simulation of the Structure and Rheology of Nano-Confined Fluids", ACS National meeting, Orlando, FL, April 10th 2002.
13. C. McCabe, "Molecular Modeling of Phase Equilibria and Transport Properties," Physical and Chemical Properties Division, National Institute of Standards and Technology, Boulder, CO, May 26th 2002.
14. C. McCabe, "Molecular Modeling of Phase Equilibria and Transport Properties," Department of Chemical Engineering, Wayne State University, Detroit, MI, November 15th 2002.
15. C. McCabe, "Molecular Modeling of Complex Fluids: Phase Equilibria and Rheology," Department of Chemical Engineering, Vanderbilt University, Nashville, TN, March 17th 2003.
16. C. McCabe, "Molecular Simulation of Rheological Processes", ACS National meeting, New Orleans, LA, 27th March 2003.
17. C. McCabe, "Molecular Simulation of Rheological Processes: Application to Lubricant Basestocks", NCS 2003 - NREL Workshop on Computational Science in Materials Science, Chemistry and Biology, April 3rd 2003.
18. C. McCabe, "Accurate Modeling of Phase Equilibria Including the Critical Region Using a Molecular-Based Equation of State," Molecular Thermodynamics and Molecular Simulation (MTMS) 03, Akiu, Sendai, Japan May 28th 2003.
19. C. McCabe, "Molecular Simulation of Rheological Properties," MTMS Post Congress Symposium, Tokyo, Japan, May 31st 2003.
20. C. McCabe, "Molecular Modeling of Complex Fluids and Materials," Department of Chemical Engineering, Vanderbilt University, Nashville, TN, March 15th 2004.
21. C. McCabe, "Molecular Modeling of Fluids Near to and Far from the Critical Region," CERC3 Workshop on Neoteric Solvents as Reaction Media: Reality and Future, St. Malo, France, April 17th 2004.
22. C. McCabe, "Molecular Modeling of the Hydrated T. Reesei Linker Peptide", 2nd NREL Computational Sciences Workshop - Computational Biology: Focus on Hydrogen, Biomass, and Nanoscience, September 10th 2004.
23. C. McCabe, "Molecular Modeling of Complex Fluids," Department of Chemical Engineering, Tennessee Tech University, Cookeville, TN, October 14th 2004.
24. C. McCabe, "Multiscale Simulation of the Nano-Scale Assembly of Hybrid Materials," Annual meeting of AIChE, Austin, TX, November 9th 2004.
25. C. McCabe, "Molecular Modeling of Complex Fluids and Nanostructured Materials," 1st US - China Workshop on Chemical Engineering, Beijing, China, August 9 -12 2005.
26. C. McCabe, "Multiscale simulation of the assembly and properties of nanostructured organic/inorganic hybrid materials," 230th ACS National Meeting, Washington, DC, August 28th 2005.
27. C. McCabe, "Computational Nanotechnology: From Atomistic Simulation to Thermodynamic Models," Tutorial on Computational Methods in Nanotechnology," AIChE Annual Meeting, Cincinnati, Ohio, October 30th 2005.
28. C. McCabe, "Molecular Modeling of Complex Fluids and Materials," Department of Chemical Engineering, University of Memphis, Memphis, Tennessee, April 5th 2006.
29. C. McCabe, "Multiscale simulation of the assembly and properties of nanostructured organic/inorganic hybrid materials," Molecular Thermodynamics and Molecular Simulation 06, Chiba, Japan, May 24th 2006.

30. C. McCabe, "Molecular Modeling of the Hydrated T. reesei Linker Peptide," Center for Nanophase Materials Sciences User Meeting, Oak Ridge National Laboratory, Oak Ridge, Tennessee, June 15th 2006.
31. C. McCabe, "Molecular Modeling of Complex Fluids and Materials," Department of Chemical Engineering, University of Auburn, Auburn, Alabama, October 4th 2006.
32. C. McCabe, "Molecular Modeling of Complex Fluids and Materials," Department of Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, Indiana, October 25th 2006.
33. C. McCabe, "Molecular Modeling of Complex Fluids Using a SAFT Based Approach," Department of Chemical Engineering, National University of Singapore, Singapore, August 23rd 2007.
34. C. McCabe, "Molecular Modeling of Complex Fluids and Materials," Department of Chemistry, Chiba University, Chiba-shi, Japan, September 12th 2007.
35. C. McCabe, "Molecular Modeling of Complex Fluids," Society of Chemical Engineers of Japan 39th Autumn Meeting, University of Hokkaido, Sapporo, Japan, September 13th 2007.
36. C. McCabe, "Molecular Modeling of Nanostructured Systems," Department of Chemical and Materials Engineering, University of Cincinnati, Cincinnati, Ohio, October 4th 2007.
37. C. McCabe, "Molecular Modeling of Complex Fluids and Materials," Department of Chemistry, Vanderbilt University, Nashville, TN, December 10th 2007.
38. C. McCabe, "Using Molecular Modeling to Understand Enzymatic Cellulose Hydrolysis," Scientific Impacts and Opportunities in Computing workshop, Maui, HI, January 10th 2008.
39. C. McCabe, "Molecular Modeling of Complex Fluids with a SAFT-Based Approach," Department of Chemistry, University of Kansas, Lawrence, KS, February 19th 2008.
40. C. McCabe, "Molecular Modeling of Complex Fluids," ACS Spring National Meeting, New Orleans, LA, April 6th 2008.
41. C. McCabe, "Using Molecular Modeling to Understand Enzymatic Cellulose Hydrolysis," AIChE Spring National Meeting, New Orleans, LA, April 8th 2008.
42. C. McCabe, "Molecular and Coarse-Grained Modeling of Complex Systems," MICHELIN Technology Center, Clermont-Ferrand, France, May 23rd 2008.
43. C. McCabe, "Molecular modeling of fluids: From molecular simulation and molecular theory to engineering systems," 5th Chemical Engineering Conference for Collaborative Research in Eastern Mediterranean Countries (EMCC-5)," Cetraro, Italy, May 26th 2008.
44. C. McCabe, "Using Molecular Modeling to Understand Enzymatic Cellulose Hydrolysis," Department of Process and Energy, Delft University of Technology, The Netherlands, June 4th 2008.
45. C. McCabe, "Molecular Modeling of Complex Fluids and Materials," Department of Chemical and Biomolecular Engineering, Rice University, Houston TX, October 2nd 2008.
46. C. McCabe, "Molecular Modeling of Nanostructured Systems," Center for Simulational Physics 22nd Annual Workshop, Recent Developments in Computer Simulation Studies in Condensed Matter Physics, University of Georgia, Athens, GA, February 23rd 2009.
47. C. McCabe, "Molecular Modeling of Complex Fluids," Department of Chemical and Materials Engineering, University of Kentucky, Lexington, KY, April 15th 2009.
48. X. Zhao, C. Taylor, C. McCabe, W. S. Adney and M. E. Himmel, "Role of Cel7A Linker in Enzymatic Hydrolysis of Cellulose Chains: A Simulation Study," U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, 2009 Nanoscale Science Research Centers Contractors Meeting, Annapolis, MD, June 4th 2009.
49. C. McCabe, "A Molecular Based Approach to Modeling Complex Fluids," Foundations of Molecular Modeling and Simulation (FOMMS 2009), Blaine, WA, July 12 - 16th 2009.

50. C. McCabe, "A Molecular Based Approach to Modeling Complex Fluids," Molecular Thermodynamics and Molecular Simulation 2009, Kanasawa University, Kanasawa, October 5th 2009. [Keynote].
51. C. McCabe, "A Molecular Based Approach to Modeling Complex Fluids," 5th US-Sino Joint Conference of Chemical Engineering, Beijing, China, October 15th 2009.
52. X. Zhao, T. Rignall, C. McCabe, W. S. Adney, and M. E. Himmel, "Molecular Simulation Evidence for Processive Motion of Trichoderma reesei Cel7A during Cellulose Depolymerization," MRS Fall Meeting, Boston, Massachusetts, November 30th 2009.
53. C. McCabe, "Molecular modeling of fluids: From molecular simulation and molecular theory to engineering systems," Mardi Gras Conference 2010: Computational Materials and Methods, Cook Conference Center, Louisiana State University, Baton Rouge, LA, February 12th 2010.
54. C. McCabe, "Developing Coarse-Grained Models for the Molecular Simulation of the Self Assembly of Skin Lipids," 12th International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD), Suzhou, Jiangsu, China, May 18th 2010. [Plenary]
55. C. McCabe, "Molecular Modeling of Complex Fluids Using a SAFT Based Approach," Midwest Thermodynamics and Statistical Mechanics meeting, University of Notre Dame, South Bend, IN, June 3rd 2010.
56. C. McCabe, "Developing Coarse-Grained Models for the Molecular Simulation of the Self Assembly of Skin Lipids," Pennsylvania State University, State College, June 22nd 2010.
57. C. McCabe, "Developing Coarse-Grained Models for the Molecular Simulation of the Self Assembly of Skin Lipids," SciDAC 2010 Conference, Chattanooga, TN, July 13th 2010.
58. C. McCabe, "On the Development of SAFT Based Approaches for Modeling Charged and Polar Fluids," 20 Years of the SAFT Equation: Recent Advances and Challenges, Barcelona, Spain, September 21st 2010.
59. C. McCabe, "Developing Coarse-Grained Models for the Molecular Simulation of the Self Assembly of Skin Lipids," SUNY at Buffalo, Buffalo, NY, October 27th 2010.
60. C. McCabe, "Developing Coarse-Grained Models for the Molecular Simulation of the Self Assembly of Skin Lipids," Coarse-Grained Methods and Self-Assembly, CECAM-USI, Lugano, Switzerland, July 27th 2011.
61. C. McCabe, "Understanding the Self-Assembly of Skin Lipids," New Mexico State University, Las Cruces, NM, September 9th 2011.
62. C. McCabe, "Elucidating protein-carbohydrate interactions in cellulase enzymes with molecular simulation," National Institute for Computational Sciences Workshop on Modeling Advanced Materials, Systems Biology and Alternative Energy: Building Capabilities and Collaborations for Cyber-Enabled Discovery, University of Tennessee, Knoxville, TN, October 11th 2011.
63. C. McCabe, "Evolving the SAFT-VR Equation of State into a General Modeling Platform for Complex Fluids," Session in honor of Jan Sengers, AIChE Annual Meeting, Minneapolis MN, October 18th 2011.
64. C. McCabe, "Molecular modeling of fluids: From molecular simulation and molecular theory to engineering systems," The 9th International Conference on Separation Science and Technology, JeJu, Korea, October 22nd -29th 2011. [Plenary]
65. C. McCabe, "On the Development of SAFT Based Approaches for Modeling Charged and Polar Fluids," 6th Sino-US Joint Chemical Engineering Conference, Beijing, China, November 7th – 10th 2011.
66. C. McCabe, "Novel Lubrication Schemes for Silicon-Based Microelectromechanical Devices," University of Melbourne, Melbourne, Australia, November 25th 2011.
67. C. McCabe, "Accurate Modeling of the Thermodynamics of Electrolytes using the SAFT-VR+DE," Royal Society of Chemistry Workshop on Electrolytes, Imperial College, London, January 6th 2012.

68. G. T. Beckham, L. Bu, C. J. Dibble, S. Kim, C. M. Payne, M. G. Resch, D. W. Sammond, C. B. Taylor, M. E. Himmel, C. McCabe, M. F. Crowley, "Understanding fungal glycosyl hydrolases and oxidative enzymes with simulation and experiment," 62nd Annual Meeting of the Society for Industrial Microbiology and Biotechnology, Washington, DC, August 15th 2012.
69. C. McCabe, "Developing Coarse-Grained Models for the Molecular Simulation of the Self Assembly of Skin Lipids," Department of Chemical Engineering, University of Michigan, Ann Arbor, Michigan, May 1st 2013.
70. C. McCabe, "Lubrication Schemes for Silicon-Based Microelectromechanical Devices," Advances in Non-equilibrium Simulation, Imperial College, June 26th 2013.
71. C. McCabe, "Studying the Self Assembly of Skin Lipids," VII Brazilian Meeting on Simulational Physics, Joao Pessoa, Brazil, August 6th 2013.
72. C. McCabe, "Understanding the Self-Assembly of Skin Lipids," Aachen Conference on Computational Engineering Science, RWTH Aachen University, September 11th 2013.
73. C. R. Iacovella, C. McCabe, and P. T. Cummings, "Improved Computational Models via Synthesis Mimetic Simulation: Applications to Nano-Confined Systems," I3Ms Seminar Series, Aachen Institute for Advanced Study in Computational Engineering Science, RWTH Aachen, Germany, January 13th 2014.
74. P. T. Cummings, C. R. Iacovella, C. McCabe, A. Ledeczi and G. Karsai, "Automating Computational Materials Discovery through Model-Integrated Computing," International Conference on Computational Science (ICCS) 2014, Cairns, Queensland, Australia, June 10th 2014.
75. G. Das, L. A. Mitchell, M.D. LeVan, C. McCabe and P. T. Cummings; "Towards a predictive theory of adsorption through a combination of SAFT-VR and classical density functional theory" 10th International Conference on Separation Science and Technology (ICSST14), Nara, Japan, October 30th 2014. [Keynote lecture]
76. C. McCabe, "Extending SAFT by Utilizing Liquid State Fluid Theories: Polar Fluids, Electrolyte Solutions, and Adsorption Phenomena," AIChE Annual Meeting, Atlanta GA, November 17th 2014.
77. C. McCabe, "Understanding the Self-Assembly of Skin Lipids," AIChE Annual Meeting, Atlanta GA, November 19th 2014.
78. C. R. Iacovella, G. Varga, J. Sallai, A. Ledeczi, C. McCabe, P. T. Cummings, Application of concepts from modeling integrated computing for the design of soft materials, TMS 2015 Annual Meeting & Exhibition, Orlando Fl, March 17th 2015.
79. G. Das, S. Hlushak, M. C. dos Ramos, and C. McCabe, "Thermodynamic properties of mixed solvent electrolyte solutions from the SAFT-VR+DE equation of state," SAFT 2015, Houston TX, May 18th 2015.
80. C. McCabe, "Understanding the Self-Assembly and Phase Behavior of Skin Lipids," MTMS 2015, Fukuoka, Japan, August 8th 2015.
81. C. McCabe, "Understanding the Self-Assembly and Phase Behavior of Skin Lipids," Thermodynamics 2015, Copenhagen, Denmark, September 16th 2015.
82. C. McCabe, "Understanding the Self-Assembly and Phase Behavior of Skin Lipids," Thermodynamics 2015, North Carolina State University, Raleigh NC, November 2nd 2015.
83. P.T. Cummings, C. McCabe, C. Klein, C.R. Iacovella. "Slip Slidin' Away: Three Decades of Adventures in Computational Rheology and Lubrication," AIChE 2016 Annual Meeting, San Francisco CA, November 14th 2016.
84. C. McCabe, "Molecular Dynamics Study of the Degradation of Alkylsilane Monolayers Under Shear," NESC16: Advances in theory and simulation of non-equilibrium systems, Sheffield, UK, July 27th 2016.
85. C. McCabe, "Understanding the Self-Assembly and Phase Behavior of Skin Lipids," 4th International Conference on Molecular Simulation (ICMS-2016), Shanghai, China, October 24th 2016.

86. C. McCabe, "Understanding the Self-Assembly and Phase Behavior of Skin Lipids," *Insights into Skin Permeation: from Theory to Practice* CECAM workshop, Lausanne, Switzerland, October 17th 2017.
87. C. McCabe, "Understanding the Self-Assembly and Phase Behavior of Skin Lipids," Institut für Chemie, Technische Universität Berlin, October 19th 2017.
88. C. McCabe, "Molecular Simulation of Skin Lipids: Insights into barrier function?" 14th National Computer Chemistry Conference of China and International Workshop on Molecular Simulations, Nanjing University International Conference Center, Nanjing, China, November 19th 2017.
89. C. McCabe, "Self-Assembly of Skin Lipids: Insights into barrier function?" Institute of Process Engineering, Chinese Academy of Sciences, Beijing, China, November 20th 2017.
90. C. McCabe, "Understanding the Self-Assembly and Phase Behavior of Skin Lipids," Department of Chemical Engineering, Tulane University, New Orleans LA, February 2nd 2018.
91. C. McCabe, "Understanding the Self-Assembly and Phase Behavior of Skin Lipids," Department of Chemical Engineering, Emory University, Atlanta GA, April 9th 2018.
92. C. McCabe, "Understanding the Self-Assembly and Phase Behavior of Skin Lipids," Department of Chemical Engineering, Syracuse University, Syracuse NY, April 20th 2018.
93. C. McCabe, "Structure and Permeability of Multi-Component, Gel-Phase Phospholipid Bilayers from Molecular Dynamics Simulation," College of Industrial Technology, Nihon University, Tsudanuma campus, Narashino, Chiba, Japan, September 4th 2018.
94. C. McCabe, "Examining the Self-Assembly of Stratum Corneum Lipid Mixtures," 8th international symposium on Molecular Thermodynamics and Molecular Simulation (MTMS '18), Chiba, Japan, September 5th 2018.
95. C. McCabe and P. Westmoreland, "25 by 25: Chemical Engineering in the Next 25 Years," AIChE's 110 Year Celebration, AIChE Annual Meeting, Pittsburgh, October 30th 2018.
96. C. McCabe, "Molecular Dynamics Simulations of Stratum Corneum Lipid Mixtures: A Multiscale Perspective," 31st annual Midwest Thermodynamics and Statistical Mechanics (MTSM) conference, Beckman Institute at the University of Illinois at Urbana-Champaign, June 3rd 2019.
97. C. McCabe, "Utilizing the Molecular Simulation Design Framework (MoSDeF) to Screen Soft Matter Systems," Midwest Theoretical Chemistry Conference (MWTCC), University of Notre Dame, June 6th 2019.
98. C. McCabe, "Molecular Dynamics Simulations of Stratum Corneum Lipid Mixtures: A Multiscale Perspective," GRC Barrier Function of Mammalian Skin, Waterville Valle NH, August 12th 2019.
99. C. McCabe, "Molecular Dynamics Simulations of Stratum Corneum Lipid Mixtures: A Multiscale Perspective," East China University of Science and Technology, Shanghai China, October 10th 2019.
100. A. Yang, C. Iacovella and C. McCabe, " Depth and Interfacial Fluctuations in Multi-Component Gel-Phase Lipid Bilayers, 2019 International Workshop on Molecular Simulation, Hangzhou, China, October 12th 2019.
101. C. McCabe, "Utilizing the Molecular Simulation Design Framework (MoSDeF) to Screen Soft Matter Systems," Huazhong University of Science and Technology. Wuhan, China, October 14th 2019.
102. C. McCabe, "Molecular Dynamics Simulations of Stratum Corneum Lipid Mixtures: A Multiscale Perspective," Dept. of Chemical Engineering, Colorado School of Mines, Golden CO, November 22nd 2019.
103. C. McCabe, "Molecular Dynamics Simulations of Stratum Corneum Lipid Mixtures: A Multiscale Perspective," XLIX Winter Meeting on Statistical Physics, Taxaco, Mexico, January 16th 2020.
104. C. McCabe, "Utilizing the Molecular Simulation Design Framework (MoSDeF) to Screen Soft Matter Systems," ACS Research Conference: Chemistry and Chemical Engineering, WuDoha Doha, Qatar, March 11th 2020. [Cancelled due to COVID-19]

Papers Presented

1. A. Galindo, A. Gil-Villegas, G. Jackson, C. McCabe, P. J. Whitehead, and A. N. Burgess, "Statistical Associating Fluid theory for Chain Molecules with Variable Attractive Potential Range (SAFT-VR)," European Physical Society (EPS), 3rd Liquid Matter Conference, Norwich, July 7th 1996.
2. A. Gil-Villegas, C. McCabe, L. A. Davies, G. Jackson, A. Galindo and A. N. Burgess, "Statistical Associating Fluid theory for Chain Molecules with Attractive Potential's of Variable Range," XXVI Winter Meeting on Statistical Physics, Cuernavaca, Mexico, January 16th 1997.
3. A. Gil-Villegas, A. Galindo, C. McCabe, P. J. Whitehead, G. Jackson, and A. N. Burgess, "Statistical Associating Fluid theory for Chain Molecules with Attractive Potential's of Variable Range (SAFT-VR)", 15th European Seminar on Applied Thermodynamics, Runcorn/Liverpool, June 13th 1996.
4. C. McCabe, A. Galindo, A. Gil-Villegas, and G. Jackson, "Predicting the High-Pressure Phase Equilibria of Binary Mixtures of Alkanes and Perfluoroalkanes", 13th Symposium on thermophysical Properties, Boulder, Colorado, June 26th 1997.
5. M. N. Garcia-Lisbona, G. Jackson, and C. McCabe, "Prediction of Phase Equilibria in Complex Fluids and Mixtures with the SAFT Approach", BP Chemicals, Sunbury, March 24th 1998.
6. M. N. Garcia-Lisbona, G. Jackson, and C. McCabe, "SAFT Predictions of Thermodynamic Properties of Fluids of Interest to BP," BP Chemicals, Lavera, France, June 24th 1998.
7. C. McCabe, L.A. Davies, A. Gil-Villegas, G. Jackson, S. Calero, and S. Lago, "Simulation of the Phase Equilibria of Monomer-Dimer Mixtures," XXth IUPAP International Conference on Statistical Physics, Paris, July 20th – 21st 1998.
8. S. Burton, A. Galindo, C. McCabe, G. Jackson, and A. N. Burgess, "Predicting the Phase Behavior of Complex Fluids For Industrial Applications," XXth IUPAP International Conference on Statistical Physics, Paris, July 20th – 21st 1998.
9. C. McCabe, A. Gil-Villegas, L.A. Davies, and G. Jackson, "Recent Developments in SAFT for Homo and Hetero-Nuclear Molecules," 15th International Conference on Chemical Thermodynamics ICCT-98, Porto, Portugal, July 27th 1998.
10. E. J. M. Filipe, L. M. B. Dias, J. C. G. Calado, C. McCabe, and G. Jackson, "Xenophobia and Xenophilia'', 15th International Conference on Chemical Thermodynamics ICCT-98, Porto, Portugal, July 28th 1998.
11. E. J. M. Filipe, L. M. B. Dias, J. C. G. Calado, C. McCabe, and G. Jackson, "Mixtures of Xenon, Alkanes and Perfluoroalkanes," 1st Workshop on Global Phase Diagrams, Walberberg, Cologne, Germany, March 22nd –24th 1999.
12. L. M. B. Dias, E. J. M. Filipe, J. C. G. Calado, C. McCabe, and G. Jackson, "Thermodynamics of Liquid Boron Trifluoride and Butane'', 16th Thermodynamics Conference, Imperial College, London, July 14th –16th 1999.
13. M. N. Garcia-Lisbona, A. Galindo, C. McCabe, and G. Jackson, "the Phase Equilibria of Binary and Ternary Mixtures of Non-Ionic Surfactants, Oligomers and Polymers," 16th Thermodynamics Conference, Imperial College, London, July 14th –16th 1999.
14. C. McCabe, M. N. Garcia-Lisbona, A. Galindo, and G. Jackson, "The Phase Equilibria of Binary and Ternary Mixtures of Non-Ionic Surfactants, Oligomers and Polymers," 4th Liquid Matter Conference, University of Granada, Spain, July 3rd –7th 1999.
15. C. McCabe, M. N. Garcia-Lisbona, and G. Jackson, "Phase Equilibria of Binary Mixtures of Oligomers and Polymers," AIChE Annual Meeting, Dallas, November 2nd 1999.
16. C. McCabe, J. D. Moore, S. T. Cui, P. T. Cummings, and H. D. Cochran, "Molecular Dynamics Simulations of the Rheological Properties of Linear and Branched Alkanes in the C20-C40 range," AIChE Annual Meeting, Dallas, November 2nd 1999.
17. C. McCabe, S. T. Cui, and P. T. Cummings, "Molecular Dynamics Simulation of the Rheology of 9-Octyldocosane," 14th Symposium on thermophysical Properties, Boulder, Colorado, June 25th 2000.

18. C. McCabe, S. T. Cui, and P. T. Cummings, "Examining the Rheology of 9-Octylheptadecane by Molecular Simulation", Foundations of Molecular Modeling and Simulation (FOMMS 2000), Keystone, Colorado, July 26th 2000.
19. P. T. Cummings, J. D. Moore, S. T. Cui, H. D. Cochran and C. McCabe, "Transient Rheology of a Polyethylene Melt Under Shear", Rheology 2000, Cambridge, August 23rd 2000.
20. C. McCabe, D. Bedrov, G. D. Smith, and P. T. Cummings, "A Molecular Dynamics Study of the Rheology of Perfluoroalkanes: Comparing A Fully Atomistic and United Atom Model" AIChE Annual Meeting, Los Angeles, November 16th 2000.
21. C. McCabe, D. Bedrov, G. D. Smith, and P. T. Cummings, "Examining the Rheology of Flourinated Molecules by Molecular Simulation", Thermodynamics 2001, Bristol, UK, April 5th 2001.
22. S. T. Cui, C. McCabe, H. D. Cochran and P. T. Cummings, "Structure and Rheology of Linear and Branched Alkane Fluids Confined To Nanoscale Gaps", Thermodynamics 2001, Bristol, UK, April 5th 2001.
23. C. McCabe, Y. V. Kalyuzhnyi and P. T. Cummings, "thermodynamic Properties of Freely-Jointed Hard-Sphere Multi-Yukawa Chain Fluids," PPEPPD, Kurashiki, Japan, 2001.
24. S. Furukawa, C. McCabe, P. T. Cummings, T. Nitta, "Non-Equilibrium Molecular Dynamics Simulation Studies On the Behavior of Hydrocarbon-Isomers in Silicalite," PPEPPD, Kurashiki, Japan, 2001.
25. E. J. M. Filipe, L. M. B. Dias, J. C. G. Calado, C. McCabe, and G. Jackson, "Is Xenon an "ennobled" alkane?" 76th International Bunsen Discussion Meeting: Global Phase Diagrams," Walberberg, Germany, August 21st 2001.
26. C. McCabe and P. T. Cummings, "Characterizing Lubricant Properties by Molecular Simulation," 6th World Congress of Chemical Engineering, Melbourne, Australia, September 27th 2001.
27. C. McCabe, E. J. M. Filipe and L. M. B. Dias, "Mixtures of Xenon, Alkanes and Perfluorocompounds: theory and Experiment," AIChE Annual Meeting, Reno, Nevada, November 7th 2001.
28. H-C. Li, C. McCabe, S. T. Cui, P. T. Cummings and H. D. Cochran, "Development of A Force Field For Molecular Simulation of the Phase Equilibria of Perfluoroethers," AIChE Annual Meeting, Reno, Nevada, November 7th 2001.
29. S. T. Cui, C. McCabe, P. T. Cummings, H. D. Cochran, Y. Zhu and S. Granick "Rheology of Thin Confined Films: Coordinated Molecular Simulations and Surface Force Apparatus Experiments," AIChE Annual Meeting, Reno, Nevada, November 7th 2001.
30. C. McCabe, P. T. Cummings, C. Manke, P. A. Gordon, R. B. Saeger, "Characterizing the High Pressure Behavior of Lubricant Basestocks," AIChE Annual Meeting, Reno, Nevada, November 9th 2001.
31. C. McCabe, P. T Cummings, S. Bair, and C. Manke, Characterizing the High Pressure Behaviour of Lubricant Basestocks, ", ACS National meeting, Orlando, FL, April 10th 2002.
32. J. C. Pàmies, C. McCabe, P. T. Cummings, and L. F. Vega, "Comparison of Gibbs Ensemble Monte Carlo and Quench Molecular Dynamics phase equilibrium results for short n-alkane chains", XI Congreso de Física Estadística FisEs, Tarragona, May 23rd – 25th 2002.
33. C. McCabe, Y. V. Kalyuzhnyi and P. T. Cummings, "Thermodynamic Properties of Freely-Jointed Hard-Sphere Multi-Yukawa Chain Fluids: Theory and Simulation", 6th Liblice Conference on the Statistical Mechanics of Liquids, Spindleruv Mlyn, Czech Republic, June 12th 2002.
34. C. McCabe, A. Galindo and P. T. Cummings, "Anomalies in the Solubility of Alkanes in Near Critical Water," 16th European Conference on Thermophysical Properties, Imperial College, London, September 2nd 2002.
35. C. McCabe, P. T. Cummings, S. Bair and C. W. Manke, "Characterizing the High Pressure Behaviour of Lubricant Basestocks Using High Performance Parallel Supercomputers," 16th European Conference on Thermophysical Properties, Imperial College, London, September 3rd 2002.

36. C. McCabe, A. Galindo and P. T. Cummings, "Anomalies in the Solubility of Alkanes in Near Critical Water," 9th Asian Pacific Confederation of Chemical Engineering Congress, ChristChurch, New Zealand, 30th September 2002.
37. S. Bair, C. McCabe, P. T. Cummings, "Calculation of EHL Traction for a Model Hydrocarbon Using Molecular Simulation and Rheometry, " 2nd ASIATRIB International Conference, Cheju Island, Korea, October 22nd 2002.
38. H-C. Li, C. McCabe and P. T. Cummings, "Ab Initio Calculations on Tethered Polyhedral Oligomeric Silsesquioxanes," AIChE Annual Meeting, Indianapolis, Indiana, November 4th 2002.
39. H-C. Li, C. McCabe, S. T. Cui, P. T. Cummings and H. D. Cochran, "Development of a Force Field for Molecular Simulation of the Phase Equilibria of Perfluoroethers Ab Initio Calculations," AIChE Annual Meeting, Indianapolis, Indiana, November 5th 2002.
40. J. L. Rivera-Rojas, C. McCabe and P. T. Cummings, "Molecular Simulations of Liquid-Liquid Interfacial Properties: Water/n-Alkane and Water/n-Alkane/Methanol Systems," AIChE Annual Meeting, Indianapolis, Indiana, November 6th 2002.
41. J. L. Rivera-Rojas, C. McCabe and P. T. Cummings, "Molecular Simulation of the Sliding Behavior of Multiwall Carbon Nanotubes," AIChE Annual Meeting, Indianapolis, Indiana, November 6th 2002.
42. M.-J. Lee, C. McCabe and P. T. Cummings, "Equation of State for Square-Well Chain Molecules," AIChE Annual Meeting, Indianapolis, Indiana, November 7th 2002.
43. C. McCabe, A. Galindo and P. T. Cummings, "Anomalies in the Solubility of Alkanes in Near Critical Water," AIChE Annual Meeting, Indianapolis, Indiana, November 7th 2002.
44. C. McCabe, S. Kiselev, J. F. Ely, "Application of Crossover Theory to the SAFT-VR Equation of State," AIChE Annual Meeting, Indianapolis, Indiana, November 8th 2002.
45. J. L. Rivera-Rojas, C. McCabe and P. T. Cummings, "Molecular Modeling of the Oscillatory Damped Behavior in the Separation of Double-Wall Carbon Nanotubes," Pan-American Workshop on Molecular and Materials Sciences: Theoretical and Computational Aspects, Cuernavaca, México, February 17th – 19th 2003.
46. T. Rignall, C. McCabe and M. E. Himmel, "Molecular Modeling of the *T. Reesei* CBH 1 Linker," NCS 2003 – NREL Workshop on Computational Science in Material Science, Chemistry and Biology, April 3rd 2003.
47. J. L. Rivera-Rojas, C. McCabe and P. T. Cummings, "Molecular Simulation of the Sliding Behavior of Double-Wall Carbon Nanotubes," Thermodynamics 2003, Cambridge, England, April 11th 2003.
48. T. Rignall, C. McCabe, D. Woods, J. W. Brady, and M. E. Himmel, "Molecular modeling of the T. reesei CBH I linker," 25th Symposium on Biotechnology for Fuels and Chemicals, Breckenridge, CO, May 4th 2003.
49. C. Skopec, J. W. Brady, T. Rignall, C. McCabe, and M. E. Himmel, "Computer Simulations of Water Structuring Adjacent to Microcrystalline Cellulose Iβ Surfaces," 25th Symposium on Biotechnology for Fuels and Chemicals, Breckenridge, CO, May 5th 2003.
50. C. McCabe, S. B. Kiselev, and J. F. Ely, "Molecular Modeling of Fluids Near to and Far from the Critical Region: Application of SAFT-VRX," 15th Symposium of Thermophysical Properties, Boulder CO, June 25th 2003.
51. T. Rignall, C. McCabe, C. Skopec, D. Woods, J. W. Brady, and M. E. Himmel, "Molecular Modeling of Cellulose Hydrolysis," Foundations of Molecular Modeling and Simulation, Keystone Resort, Keystone, CO, July 6th-11th 2003.
52. C. McCabe, S. B. Kiselev, and J. F. Ely, "SAFT-VRX Modeling of Fluids Near to and Far from the Critical Region," Foundations of Molecular Modeling and Simulation, Keystone Resort, Keystone, CO, July 6th-11th 2003.
53. H. Barkley, E. Chan, A. Cochran, T. Ionescu, C.-Y. Lee, F. Qi, C. Zhang, J. Zhou, M. Durandurdu, J.-S. Filhol, M. Lamm, H.-C. Li, P. T. Cummings, S. C. Glotzer, J. Kieffer, C. McCabe, M. Neurock, "Multiscale Simulation of the Synthesis, Assembly and Properties of Nanostructured

Organic/Inorganic Hybrid Materials," Foundations of Molecular Modeling and Simulation, Keystone Resort, Keystone, CO, July 6th-11th 2003.

54. T. C. Ionescu, P. T. Cummings, H. Barkley, A. Cochran, C. McCabe, F. Qi, M. Durandurdu, J. Kieffer, "Molecular simulation of polyhedral oligomeric silsesquioxane systems," AIChE Annual Meeting, San Francisco, California, November 17th 2003.
55. C. McCabe, S. B. Kiselev, and J. F. Ely, "Application of Crossover Theory to the SAFT-VR Equation of State: Bulk Properties and Surface Tension," AIChE Annual Meeting, San Francisco, California, November 7th 2003.
56. H.-C. Li, C. McCabe, and P. T. Cummings, "Atomistic potential model developing for POSS," AIChE Annual Meeting, San Francisco, California, November 7th 2003.
57. P. Morgado, C. McCabe, F. J. Blas, E. J. M. Filipe, "An examination of the vapor-liquid phase behavior of perfluoroalkane-alkane diblock surfactants using the SAFT-VR approach," AIChE Annual Meeting, San Francisco, California, November 21st 2003.
58. C. McCabe, S. B. Kiselev, L. Sun and H. G. Zhao, "Predicting the Thermodynamic Properties and Surface Tension of Fluids using the SAFT-VRX Equation of State," Tenth International Conference on Properties and Phase Equilibria for Product and Process Design, Snowbird, Utah, May 17th 2004.
59. C. McCabe, A. Galindo and P. T. Cummings, "On the Infinite Dilution Properties of n-Alkanes in Near Critical Water and their Relation to Phase Equilibria," Tenth International Conference on Properties and Phase Equilibria for Product and Process Design, Snowbird, Utah, May 18th 2004.
60. P. Morgado, H. G. Zhao, C. McCabe, F. J. Blas, and E. J. M. Filipe, "An Examination of the Vapor-Liquid Phase Behavior of Perfluoroalkane-Alkane Diblock Surfactants: Theory and Experiment," Tenth International Conference on Properties and Phase Equilibria for Product and Process Design, Snowbird, Utah, May 18th 2004.
61. H. G. Zhao, L. Sun, S. B. Kiselev, and C. McCabe, "Predicting the Thermodynamic Properties of Fluids using the SAFT-VRX Equation of State," ACS-PRF Summer School on Green Chemistry, Carnegie Mellon University, Pittsburgh, PA, July 31 – August 7, 2004.
62. C. McCabe, L. Sun, H. G. Zhao and S. B. Kiselev, "Mixture Phase Equilibria and Critical Behavior of Alkanes and CO2 using the SAFT-VRX Equation," AIChE Annual Meeting, Austin, Texas, November 8th 2004.
63. C. McCabe, H. Barkley, T. Ionescu, A. Striolo and P. T. Cummings, "Molecular Simulations for Mono-Substituted Polyhedral Oligomeric Sislesquioxanes either Pure or Dissolved in Water and in Normal Hexane," AIChE Annual Meeting, Austin, Texas, November 8th 2004.
64. A. Striolo, P. T. Cummings and C. McCabe, "Thermodynamic and Transport Properties of Polyhedral Oligomeric Sislesquioxanes in Hexadecane and in Poly(Dimethyl Siloxane)," AIChE Annual Meeting, Austin, Texas, November 8th 2004.
65. T. Rignall, C. McCabe and M. E. Himmel, "Molecular Modeling of the Hydrated T. reesei Cel7A Linker Peptide," AIChE Annual Meeting, Austin, Texas, November 11th 2004.
66. G. Pan and C. McCabe, "Predicting the Shear Viscosity of n-Alkanes to Low Shear Rates," AIChE Annual Meeting, Austin, Texas, November 11th 2004.
67. T. Rignall, C. McCabe, and M. E. Himmel, "Energetics and Conformations of the Hydrated Cel7A Linker Peptide," 27th Symposium on Biotechnology for Fuels and Chemicals, Denver, CO, May 1 – 4 2005. **(Best Poster Award)**
68. A. Striolo, C. McCabe, and P. T. Cummings, "Polyhedral Oligomeric Sislesquioxanes in Organic Solutions: Thermodynamic Properties from Molecular Simulations," 7th Italian Conference on Chemical & Process Engineering, Giardini Naxos, Italy, May 18th 2005.
69. P. Morgado, H. G. Zhao, M. C. dos Ramos, C. McCabe, F. J. Blas, E. J. M. Filipe, "Phase equilibria behaviour of alkane, perfluoroalkane and perfluoroalkane-alkane diblock surfactants and their mixtures" 6th Liquid Matter Conference, Utrecht University, the Netherlands, July 2-6 2005.

70. L. X. Sun, H. G. Zhao and C. McCabe, "Mixture Phase Equilibria and Critical Behavior of Alkanes and CO_2 using the SAFT-VRX Equation," 6th Liquid Matter Conference, Utrecht University, the Netherlands, July 2-6 2005.
71. L. X. Sun, H. G. Zhao and C. McCabe, "Mixture Phase Equilibria and Critical Behavior of Alkanes and CO_2 using the SAFT-VRX Equation," 7th World Congress of Chemical Engineering, Glasgow, UK, July 11th 2005.
72. C. McCabe, S. C. Glotzer, J. Kieffer, M. Neurock and P. T. Cummings, "Multiscale Simulation of the Properties of Nanostructured Organic/Inorganic Hybrid Materials," Proceedings of the 7th World Congress of Chemical Engineering, Glasgow, UK July 11th 2005.
73. T. Rignall, C. McCabe, and M. E. Himmel, "Energetics and Conformations of the Hydrated Cel7A Linker Peptide," 2005 Gordon Research Conference on Cellulases and Cellulosomes, Proctor Academy, Andover, NH, August 10th 2005.
74. E. Chan, A. Striolo, C. McCabe, P. T. Cummings and S. C. Glotzer, "Multiscale modeling and simulation of polymer-tethered silsesquioxane assemblies," 230th ACS National Meeting, Washington, DC, August 28th, 2005.
75. T. Rignall, C. McCabe and M. E. Himmel, "Molecular Modeling of Cellulose Hydrolysis: The Hydrated Cel7A Linker Peptide," AIChE Annual Meeting, Cincinnati, Ohio, October 31st 2005.
76. Y. Peng, H. G. Zhao and C. McCabe, "On the Thermodynamics of Chain Fluids from Simulation and the Heteronuclear SAFT-VR Approach," AIChE Annual Meeting, Cincinnati, Ohio, October 31st 2005.
77. H. G. Zhao, C. M. Earnest and C. McCabe, "Phase Behavior of dipolar fluids from the SAFT-VR equation of state," AIChE Annual Meeting, Cincinnati, Ohio, November 1st 2005.
78. A. Striolo, C. McCabe, P. T. Cummings, "Polyhedral Oligomeric Sislesquioxanes in Solution: Insights from All-Atom Molecular Dynamics Simulations," AIChE Annual Meeting, Cincinnati, Ohio, November 1st 2005.
79. B. J. Schindler, C. McCabe, P. T. Cummings, M. D. LeVan, "Comparison of Adsorption of Spherical and Non-Spherical Nitrogen in Parallel Slit Pores Using Density Functional Theory: Density Profiles and Pore Size Distributions," AIChE Annual Meeting, Cincinnati, Ohio, November 1st 2005.
80. L. Sun, H. G. Zhao, C. McCabe, "Evaluation of the Phase Equilibria of Gas Condensates and Light Petroleum Fractions using the SAFT-VR approach," AIChE Annual Meeting, Cincinnati, Ohio, November 2nd 2005.
81. E. Chan, A. Striolo, C. McCabe, S. Glotzer, P. T. Cummings, "Development of Coarse-Grained Force Fields for Polymer-Tethered Silsesquioxanes," AIChE Annual Meeting, Cincinnati, Ohio, November 2nd 2005.
82. P. S. Redmill, A. Striolo, C. McCabe and P. T. Cummings, "Determining the Octanol-Water Partition Coefficient for POSS Systems," AIChE Annual Meeting, Cincinnati, Ohio, November 4th 2005.
83. M. C. Dos Ramos, F. J. Blas, P. Morgado, E. J. M. Filipe, H. G. Zhao and C. McCabe, "Phase Behavior of Binary and Ternary Mixtures of Alkane, Perfluoroalkane and Perfluoroalkylalkane Diblock Surfactants Using the SAFT-VR Approach" 7th Liblice Conference on the Statistical Mechanics of Liquids, Lednice, Czech Republic, June 12th 2006.
84. H. G. Zhao and C. McCabe, "A Statistical Associating Fluid Theory for Strong Electrolyte Solutions," 3rd Foundations of Molecular Modeling and Simulation Conference, Semiahmoo, Blaine, WA, July 9th -14th 2006.
85. A. Striolo, E. R. Chan, C. McCabe, S. C. Glotzer, P. T Cummings, "Multiscale Simulation of Organic-Inorganic Polyhedral Nano-Materials," 3rd Foundations of Molecular Modeling and Simulation Conference, Semiahmoo, Blaine, WA, July 9th -14th 2006.
86. Y. Peng, T. Ionescu, S. Capps and C. McCabe, "Molecular Simulation and Theoretical Modeling of Polyhedral Oligomeric Silsequioxanes," 3rd Foundations of Molecular Modeling and Simulation Conference, Semiahmoo, Blaine, WA, July 9th -14th 2006.

87. P. S. Redmill, C. McCabe and P. T. Cummings, "Determining Thermodynamic Solubility Parameters for Nanoscale Building Blocks," 3rd Foundations of Molecular Modeling and Simulation Conference, Semiahmoo, Blaine, WA, July 9th -14th 2006.
88. B. Schindler, C. McCabe, P. T. Cummings and M. D. LeVan, "Comparison of a SAFT-DFT Approach and Monte Carlo Simulations for Adsorption in Parallel Slit Pores," 3rd Foundations of Molecular Modeling and Simulation Conference, Semiahmoo, Blaine, WA, July 9th -14th 2006.
89. M. Castro, A. Martìnez, C. McCabe, A. Gil-Villegas, "Molecular Thermodynamics of Chemical Adsorption," XLIX Mexican Physical Society Congress, October 16-20 2006.
90. A. Striolo, E. R. Chan, C. McCabe, S. C. Glotzer and P. T. Cummings, "Multiscale Simulation of Organic-Inorganic Polyhedral Nano-Materials," 16th Symposium of Thermophysical Properties, Boulder, Colorado, July 30th 2006.
91. H. G. Zhao and C. McCabe, "A Statistical Associating Fluid Theory for Electrolyte Solutions," 16th Symposium of Thermophysical Properties, Boulder, Colorado, August 4th 2006.
92. S. Capps, P. S. Redmill, C. McCabe, "Determining Thermodynamic Solubility Parameters for Polyhederal Oligomeric Silsequioxanes," AIChE Annual Student Meeting, San Francisco, California, November 11th 2006.
93. M. Earnest, H. G. Zhao and C. McCabe, "Modeling Phase Equilibria of Dipolar Fluids with the SAFT-VR+D Equation," AIChE Annual Student Meeting, San Francisco, California, November 11th 2006. **(3rd place in undergraduate student poster competition)**
94. H. G. Zhao and C. McCabe, "A Statistical Associating Fluid Theory for Electrolyte Solutions," AIChE Annual Meeting, San Francisco, California, November 13th 2006.
95. P. S. Redmill, S. Capps, C. McCabe and P. T. Cummings, Probing Biologically Relevant Solubility Parameters for Selected Nanoscale Building Blocks Using Molecular Dynamics, Eleventh International Conference on Properties and Phase Equilibria for Product and Process Design, Hersonissos, Crete, Greece, May 21st 2007.
96. P. Morgado, F. Menezes, L. Martins, C. Laginhas, C. McCabe and E. J. M. Filipe, "Thermodynamic properties of Perfluoroalkylalkanes," Eleventh International Conference on Properties and Phase Equilibria for Product and Process Design, Hersonissos, Crete, Greece, May 23rd 2007.
97. H. G. Zhao, M. C. dos Ramos and C. McCabe, "A Statistical Associating Fluid Theory for Electrolyte Solutions," Eleventh International Conference on Properties and Phase Equilibria for Product and Process Design, Hersonissos, Crete, Greece, May 23rd 2007.
98. H. G. Zhao, M. C. dos Ramos and C. McCabe, "A Statistical Associating Fluid Theory for Electrolyte Solutions," 30th International Conference on Solution Chemistry, Perth, Australia, August 18th 2007.
99. K. R. Hadley and C. McCabe, "Molecular Modeling of Self-Assembling Human Skin Lipids," 10th Gordon Research Conference on Barrier Function of Mammalian Skin, Salve Regina University, August 5th-10th, 2007.
100. P. S. Redmill, S. Capps C. McCabe, and P. T. Cummings, "Determining thermodynamics solubility parameters for nanoscale building blocks," Fall Creek Falls 2007, Nashville TN, September 24th 2007.
101. A. Gil-Villegas, M. Castro, E. Buenrostro-González and C. McCabe, "Predicting Adsorption Isotherms Using a Two Dimensional Statistical Associating Fluid Theory," Thermodynamics 2007, Paris, France, September 26th 2007
102. K. D. Goff, M. C. dos Ramos, H. G. Zhao and C. McCabe, "Modelling the Phase Behaviour of H2S + n-Alkanes with the SAFT Equation of State," AIChE Annual Student Meeting, Salt Lake City, Utah, November 5th 2007. **(1st place in undergraduate student poster competition)**
103. M. C. dos Ramos, H. G. Zhao and C. McCabe, "Modeling the Thermodynamic Behavior of Systems Containing Charged and/or Dipolar Fluids," AIChE Annual Meeting, Salt Lake City, Utah, November 5th 2007.

104. Y. Peng, K. D. Goff, M. C. dos Ramos, and C. McCabe, "Developing a Group Contribution Based SAFT-VR," AIChE Annual Meeting, Salt Lake City, Utah, November 6th 2007.
105. O. A. Mazyar, A. Cione, B. Booth, G. Kane Jennings, and C. McCabe, "Ionic Liquids as Novel Lubricants: Application to Nano-Electromechanical Systems," AIChE Annual Meeting, Salt Lake City, Utah, November 7th 2007.
106. K. R. Hadley and C. McCabe, "Coarse Graining of Crystalline Free-Fatty Acids," AIChE Annual Meeting, Salt Lake City, Utah, November 7th 2007.
107. X. Zhao, C. McCabe and M. E. Himmel, " Conformational energies of cellobiohydrolase I linker on cellulose surface," AIChE Annual Meeting, Salt Lake City, Utah, November 8th 2007.
108. K. R. Hadley and C. McCabe, "Coarse-Grained Simulations of Stratum Corneum Lipids," Fifth Annual Tennessee Structural Biology Symposium: Vanderbilt University, Nashville, TN, June 20th 2008.
109. J. Westwood, M. C. dos Ramos and C. McCabe. "Application of the GC-SFAT-VR Equation of State to Predict Fluid Phase Behaviour", AIChE Annual Meeting, Philadelphia, Pennsylvania, November 17th 2008. **(3rd place in undergraduate student poster competition)**
110. O. A. Mazyar, G. K. Jennings, C. McCabe, "Molecular Dynamics Studies of Friction and Lubrication In Nanoelectromechanical Devices," AIChE Annual Meeting, Philadelphia, Pennsylvania, November 17th 2008.
111. K. R. Hadley and C McCabe, "Coarse-Grained Water Model for Multiple Waters Mapped to Single Sites," AIChE Annual Meeting, Philadelphia, Pennsylvania, November 17th 2008.
112. X. Zhao, E. O'Neal, W. S. Adney, M. E. Himmel, C. McCabe, "Using Molecular Modeling to Understand Enzymatic Cellulose Hydrolysis," AIChE Annual Meeting, Philadelphia, Pennsylvania, November 17th 2008.
113. M. C. dos Ramos, Y. Peng, K. Goff and C. McCabe. "Predicting the VLE for Polymer Systems with the GC-SAFT-VR Approach", AIChE Annual Meeting, Philadelphia, Pennsylvania, November 18th 2008.
114. B. D. Booth, G. K. Jennings, O. A. Mazyar, C. McCabe, "Tribometric Characterization and Simulations of Monolayer Films on Silicon and Gold," AIChE Annual Meeting, Philadelphia, Pennsylvania, November 20th 2008.
115. K. R. Hadley and C McCabe, "Retention of the Structural Properties of Cholesterol on the Coarse-Grained Level," AIChE Annual Meeting, Philadelphia, Pennsylvania, November 21st 2008.
116. S. G. Vilt, C. McCabe, and G. Kane Jennings, "Chain Mobility and Functional Group Effects in Micro-Scale Friction," 13th IACIS International Conference on Surface and Colloid Science and the 83rd ACS Colloid & Surface Science Symposium, Columbia University, New York, NY, June 19th 2009.
117. M. C. dos Ramos and C. McCabe, "Modeling the Thermodynamic Phase Behavior of Charged fluids using the SAFT-VR+DE EOS," 17th Symposium on Thermophysical Properties, Boulder, CO, June 21 - 26th 2009.
118. M. C. dos Ramos, Y. Peng, K. D. Goff, J. Westwood and C. McCabe, "A Group Contribution SAFT-VR Equation of State to Predict the Fluid Phase Behavior of Complex Systems," 17th Symposium on Thermophysical Properties, Boulder, CO, June 21 - 26th 2009.
119. K. R. Hadley and C. McCabe, "Developing Coarse Grained Models for Skin Lipids," 17th Symposium on Thermophysical Properties, Boulder, CO, June 21 - 26th 2009.
120. B. J. Lewis, J. L. Rivera, O. A. Mazyar, S. Vilt, G. K. Jennings and C. McCabe, "Novel Lubrication Schemes for Silicon-Based Microelectromechanical Devices," Foundations of Molecular Modeling and Simulation (FOMMS 2009), Blaine, WA, July 12 - 16th 2009.
121. J. L. Rivera, O. A. Mazyar, B. J. Lewis, G. K. Jennings and C. McCabe, "Molecular Dynamics Studies of Friction in Alkylsilane and Hydroxyalkylsilane Coated MEMs Devices," Foundations of Molecular Modeling and Simulation (FOMMS 2009), Blaine, WA, July 12 - 16th 2009.

122. K. R. Hadley, S. Guo and C. McCabe, "Studying the Self Assembly of Stratum Corneum Lipids via Molecular Simulation," 11th Gordon Research Conference on Barrier Function of Mammalian Skin, Waterville Valley Resort, Waterville NH, August 9th-14th, 2009.
123. B. J. Lewis, J. L. Rivera, O. A. Mazyar, S. Vilt, G. K. Jennings and C. McCabe, "Novel Lubrication Schemes for Silicon-Based Microelectromechanical Devices," Fall Creek Falls 2009 - Leadership Computing on Petascale Resources, Chatanooga, TN, September 22nd 2009.
124. K. R. Hadley, S. Guo and C. McCabe, "Studying the Self Assembly of Stratum Corneum Lipids via Molecular Simulation," Fall Creek Falls 2009 - Leadership Computing on Petascale Resources, Chatanooga, TN, September 22nd 2009.
125. J. D. Haley, M. C. Dos Ramos and C. McCabe, "Phase Behavior of Complex Systems Using the GC-SAFT-VR Equation of State," AIChE Annual Meeting, Nashville, Tennessee, November 9th 2009. **(3rd place in undergraduate student poster competition)**
126. J. Mikhail, G. Rouvelas, C. Taylor and C. McCabe, "Analyzing the Distribution of Water around the Cellobiohydrolase I Linker Peptide," AIChE Annual Meeting, Nashville, Tennessee, November 9th 2009. **(2nd place in undergraduate student poster competition)**
127. M. C. Dos Ramos and C. McCabe, "Modeling the Phase Behavior, Excess Enthalpies and Henry's Constants of the H2O + H2S Binary Mixture Using the SAFT-VR+D Approach," AIChE Annual Meeting, Nashville, Tennessee, November 9th 2009.
128. M. C. Dos Ramos, N. A. Aziz, J. R. Westwood, J. D. Haley and C. McCabe, "Application of the GC-SAFT-VR Equation to Predict Fluid Phase Behavior of Associating Systems," AIChE Annual Meeting, Nashville, Tennessee, November 10th 2009.
129. B. D. Booth, S. G. Vilt, C. McCabe and G. K. Jennings, "Tribometric Comparison of n-Alkanethiolate and n-Alkyl Trichlorosilane Monolayers," AIChE Annual Meeting, Nashville, Tennessee, November 10th 2009.
130. S. G. Vilt, J. B. Lewis, J. L. Rivera, C. McCabe and G. K. Jennings, "Characterization of Surface and Frictional Properties of Two-Component Alkyltrichlorosilane Monolayers," AIChE Annual Meeting, Nashville, Tennessee, November 11th 2009.
131. J. L. Rivera, G. K. Jennings and C. McCabe, "Molecular Dynamics Studies of Friction in Alkylsilane and Hydroxyalkylsilane Coated MEMS Devices," AIChE Annual Meeting, Nashville, Tennessee, November 12th 2009.
132. X. Zhao, C. Taylor, C. McCabe, W. S. Adney, and M. E. Himmel, "Investigating the Role of the Cel7A Linker Peptide in Enzymatic Hydrolysis of Cellulose Chains: A Simulation Study," AIChE Annual Meeting, Nashville, Tennessee, November 12th 2009.
133. M. C. Dos Ramos and C. McCabe, "Predicting the Phase Behavior of Charged and Polar Fluids Using the SAFT-VR+DE Approach," AIChE Annual Meeting, Nashville, Tennessee, November 13th 2009.
134. K. R. Hadley, S. Guo and C. McCabe, "Self-Assembly of Coarse-Grained Stratum Corneum Lipids," AIChE Annual Meeting, Nashville, Tennessee, November 13th 2009.
135. C. B. Taylor, X. Zhao, C. McCabe, W. S. Adney and M. E. Himmel, "Role of Cel7A Linker in Enzymatic Hydrolysis of Cellulose: A Molecular Simulation Study," Mardi Gras Conference 2010: Computational Materials and Methods, Cook Conference Center, Louisiana State University, Baton Rouge, LA, February 12th 2010. **(Poster award - resulting in oral presentation)**
136. M. C. dos Ramos, Y. Peng, K. D. Goff, J. D. Haley, C. McCabe, "Developing Predictive Tools for Modeling Complex Fluids within a SAFT-Based Approach," 12th International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD), Suzhou, Jiangsu, China, May 20th 2010.
137. K. R. Hadley, S. Guo and C. McCabe, "Molecular Simulation of the Self-assembly of Fatty Acids and Cholesterol into Bilayer Structures," 12th International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD), Suzhou, Jiangsu, China, May 20th 2010.

138. J. B. Lewis, J. L. Rivera, S. Vilt, G K. Jennings and C. McCabe, "On the Investigation of Frictional Properties in Pure and Mixed Fluorocarbon/Hydrocarbon Monolayers," Midwest Thermodynamics and Statistical Mechanics meeting, University of Notre dame, South Bend, IN, June 2nd 2010.
139. L. A. Strickland and C. McCabe, "On Oligomer Adsorption in Cylindrical Pores from Discontinuous Molecular Dynamics Simulation," Midwest Thermodynamics and Statistical Mechanics meeting, University of Notre dame, South Bend, IN, June 2nd 2010.
140. S. G. Vilt, N. Martin, C. McCabe, and G. K. Jennings, "Characterizing Rolling Friction at the Microscale," 84th ACS Colloid and Surface Science Symposium, University of Akron, Akron, OH, June 20th 2010.
141. S. G. Vilt, B. J. Lewis, C. McCabe, and G. K. Jennings, "Characterization of Surface and Frictional Properties of Two-Component Alkylsilane Monolayers on Silicon," 84th ACS Colloid and Surface Science Symposium, University of Akron, Akron, OH, June 22nd 2010.
142. B. Booth, S. G. Vilt, C. McCabe and G. K. Jennings, "Frictional Performance and Tribological Durability of Monolayer Films," 84th ACS Colloid and Surface Science Symposium, University of Akron, Akron, OH, June 23rd 2010.
143. M. C. dos Ramos, Y. Peng, K. D. Goff, J. D. Haley, and C. McCabe, "GC-SAFT-VR: A predictive tool for the Fluid Phase Behavior of non-Associating, Associating and Polymer Systems," 20 Years of the SAFT Equation: Recent Advances and Challenges, Barcelona, Spain, September 21st 2010.
144. L. G. Martins, F. Blas, M. C. dos Ramos, C. McCabe and E. J. M. Filipe, "Solubility of xenon in n-alkanes and cycloalkanes," 20 Years of the SAFT Equation: Recent Advances and Challenges, Barcelona, Spain, September 21st 2010.
145. P. Morgado, H. Rodrigues, L. G. Martins, F. Blas, M. C. dos Ramos, C. McCabe and E. J. M. Filipe, "SAFT Modeling of Perfluoralkanes," 20 Years of the SAFT Equation: Recent Advances and Challenges, Barcelona, Spain, September 21st 2010.
146. J. B. Lewis, S. G. Vilt, J. L. Rivera, G. K. Jennings and C. McCabe, "On the Investigation of Frictional Properties in Pure and Mixed Fluorocarbon/Hydrocarbon Monolayers," AIChE Annual Conference, Salt Lake City, Utah, November 9th 2010.
147. M. C. dos Ramos, and C. McCabe, "Examining the Thermodynamic Properties of Ionic Systems Using the SAFT-VR+DE Approach. From Simple Aqueous Electrolyte to Polar Mixed-Solvent Electrolyte Mixtures," AIChE Annual Meeting, Salt Lake City, Utah, November 10th 2010.
148. L. A. Strickland, S. Guo and C. McCabe, "Molecular Simulation of a Ceramide/Water Bilayer: On developing atomistic and coarse-grained models," AIChE Annual Meeting, Salt Lake City, Utah, November 15th 2010.
149. J. L. Rivera, G. K. Jennings and C. McCabe, "Frictional Forces in Mixed Hydrophobic-Hydrophilic Alkylsilane Monolayers", 2nd Meeting on Molecular Simulations: From simple fluids to Chemical Reactions, Mexico City, Mexico, December 9, 2010.
150. L. Gai, K. Maerzke, P. T. Cummings and C. McCabe, "Wang-Landau Monte Carlo simulation of Bilayer Formation in a 3D lattice model," 24th Annual CSP Workshop, Athens, Georgia, February 21st 2011.
151. M. F. Crowley, G. T. Beckham, L. Bu, Y. J. Bomble, J. F. Matthews, M. R. Nimlos, C. B. Taylor, C. McCabe, M. E. Himmel, W. S. Adney, "Molecular-level mechanisms of enzymatic deconstruction of cellulose," 33rd Symposium on Biotechnology for Fuels and Chemicals, Seattle, WA, May 5th 2011.
152. J. L. Rivera, G. K. Jennings and C. McCabe, "Tribological Behavior of Silica Surfaces Covered with Monolayers of Alcoxy Chains", Chemical Engineering Department, Universidad Michoacana de San Nicolas de Hidalgo, Michoacan, Mexico, June 2nd 2011.
153. P. Morgado, H. Rodrigues, F. Blas, L. G. Martins, C. McCabe and E. J. M. Filipe, "Thermodynamics of Perfluoroalkylalkanes: liquid, surface and transport properties," 25th European Symposium on Applied Thermodynamics, Saint Petersburg, Russia, June 24th-27th 2011.

154. C. B. Taylor, C. McCabe, L. Bu, M. E. Himmel, M. F. Crowley, and G. T. Beckham, "The impact of O-glycosylation and aromatic-carbohydrate interactions on the binding affinity of a Family 1 carbohydrate-binding module," 2011 Cellulosomes, Cellulases & Other Carbohydrate Modifying Enzymes Gordon Research Conference, Stonehill College, Easton, MA, July 24th-29th 2011.
155. L. E. Taylor, C. B. Taylor, L. Bu, J. Baker, C. McCabe, W. S. Adney, M. F. Crowley, M. E. Himmel, "Combined computational and experimental investigations of Cel7A for understanding and activity improvements," 2011 Cellulosomes, Cellulases & Other Carbohydrate Modifying Enzymes Gordon Research Conference, Stonehill College, Easton, MA, July 24th-29th 2011.
156. S. Guo, L. A. Strickland, K. R. Hadley and C. McCabe, "Understanding the Self-Assembly of Skin Lipids," 12th Gordon Research Conference on Barrier Function of Mammalian Skin, Waterville Valley Resort, Waterville NH, August 7th-12th 2011.
157. G. T. Beckham, C. M. Payne, D. W. Sammond, C. B Taylor, L. Bu, M. R. Nimlos, C. McCabe, M. E. Himmel, W. S. Adney, and M. F. Crowley, "Elucidating protein-carbohydrate interactions in cellulase enzymes with molecular simulation," 242nd ACS National Meeting & Exposition, Denver, Colorado, August 28th- September 1st 2011.
158. G. K. Jennings, S G. Vilt, C. Caswell and C. McCabe, "Effect of Surface Topography and Superhydrophobicity On Friction," AIChE annual meeting, Minneapolis, MN, October 18th 2011.
159. K. A. Maerzke, L. Gai, P. T. Cummings, and C. McCabe, "Wang-Landau simulations for self-assembling systems," AIChE Annual Meeting, Minneapolis, MN, October 17th 2011.
160. C. B. Taylor, M. F. Talib, C. McCabe, L. Bu, W. S. Adney, M. E. Himmel, M. F. Crowley, and G. T. Beckham, "Computational Investigation of Glycosylation Effects on a Family 1 Carbohydrate-binding Module," AIChE Annual Meeting, Minneapolis, MN, October 18th 2011.
161. C. McCabe, "Evolving the SAFT-VR Equation of State Into a General Modeling Platform for Complex Fluids," AIChE Annual Meeting, Minneapolis, MN, October 18th 2011.
162. S. Hlushak, C. McCabe and P. T. Cummings, "Fourier Space Based Approach to Classical Density Functional Theory," AIChE Annual Meeting, Minneapolis, MN, October 20th 2011.
163. M. C. dos Ramos and C. McCabe, "Predicting the Thermodynamic Properties of Mixed Solvent Electrolytes Using the SAFT-VR+DE Approach," AIChE Annual Meeting, Minneapolis, MN, October 20th 2011.
164. S. Guo, L. A. Strickland and C. McCabe, "On the Development of Coarse-Grained Models for Skin Lipids," AIChE Annual Meeting, Minneapolis, MN, October 21st 2011.
165. L. Gai, K. Maerzke, P. T. Cummings and C. McCabe, "A Wang-Landau Study of Bilayer Formation," 25th Annual CSP Workshop, Athens, Georgia, February 20th 2012.
166. C. B. Taylor, M. F. Talib, C. McCabe, M. E. Himmel, M. F. Crowley, and G. T. Beckham, "A simulation study on the impact of glycosylation patterns on a Family 1 carbohydrate-binding module's relative binding affinity," 34th Symposium on Biotechnology for Fuels and Chemicals, New Orleans, LA, April 30th 2012.
167. G. T. Beckham, L. Bu, C. M. Payne, C. B. Taylor, D. W. Sammond, M. Nimlos, C. McCabe, Y. Lin, J-W. Chu, C. J. Dibble, M. E. Himmel and M. F. Crowley," 34th Symposium on Biotechnology for Fuels and Chemicals, New Orleans, LA, Understanding fungal cellulases with molecular simulation," May 2nd 2012.
168. G. Das, M. C. dos Ramos and C. McCabe, "Phase Behavior of Aromatic Molecules and their Mixtures Using the GC-SAFT-VR Equation of State," 18th Symposium on Thermophysical Properties, boulder, CO, June 25th 2012.
169. K. Maerzke, L. Gai, P. T. Cummings and C. McCabe, "Wang-Landau Simulations for Self-Assembling Systems," 18th Symposium on Thermophysical Properties, Boulder, CO, June 27th 2012.
170. S. Guo and C. McCabe, "Molecular Dynamics Simulations of the Self-Assembly of Skin Lipids," Foundations of Molecular Modeling and Simulation (FOMMS 2012), The Resort at the Mountain, Mt. Hood, OR, July 22nd – 26th 2012.

171. L. Gai, K. Maerzke, P. T. Cummings and C. McCabe, "A Wang-Landau Study of Bilayer Formation," Foundations of Molecular Modeling and Simulation (FOMMS 2012), The Resort at the Mountain, Mt. Hood, OR, July 22nd – 26th 2012.
172. R. D. Chirico1, M. Frenkel, J. W. Magee, V. V. Diky, K. Kroenlein, C. D. Muzny, A. F. Kazakov, I. M. Abdulagatov, G. R. Hardin, T. W. de Loos, J. P. O'Connell, C. McCabe, J. F. Brennecke, P. M. Mathias, A. R. H. Goodwin, J. Wu, K. N. Marsh, R. D. Weir, W. E. Acree, Jr., A. Pádua, W. M Haynes, D. G. Friend, A. Mandelis, V. Rives, C. Schick, S. Vyazovkin, and E. Chen, "NIST-Journal Cooperation to Improve the Quality of Published Experimental Data: New On-line Tools and IUPAC Recommendations," ICCT 2012, Búzios, Brazil, August 5th - 10th 2012.
173. J. D. Haley and C. McCabe, "Predicting the Phase Behavior of Fluorinated Systems Using the GC-SAFT-VR Equation of State" CCP5 Methods in Molecular Simulations Summer School, University of Cardiff, Cardiff, UK, July 21st – 31st, 2012.
174. S. Guo and C. McCabe, "On the Self-Assembly of Skin Lipids Using Coarse-Grained Molecular Dynamics Simulation," American Institute of Chemical Engineers Annual Meeting, Pittsburgh, PA, October 29th 2012.
175. L. Gai, K. A. Maerzke, C. R. Iacovella, P. T. Cummings and C. McCabe, "Lipid Self Assembly by Statistical Temperature Monte Carlo and Molecular Dynamics," American Institute of Chemical Engineers Annual Meeting, Pittsburgh, PA, October 30th 2012.
176. S. Hlushak, C. McCabe, P. T. Cummings, "Accurate and robust classical density functional theory for the adsorption of fluids into nanoporous materials", American Institute of Chemical Engineers Annual Meeting, Pittsburgh, PA, October 31st 2012.
177. L. A. Mitchell, B. J. Schindler, M. C. dos Ramos, C. McCabe, P. T. Cummings and M. D. LeVan, "Using SAFT-FMT-DFT to Model the Adsorption of Light Gases and Hydrocarbons in Activated Carbon," American Institute of Chemical Engineers Annual Meeting, Pittsburgh, PA, October 31st 2012.
178. G. Das, J. D. Haley and C McCabe, "Predicting the Phase Behavior of Fluids with Multiple Polar Groups Using the GC-SAFT-VR Equation of State" American Institute of Chemical Engineers Annual Meeting, Pittsburgh, PA, October 31st 2012.
179. L. Gai, K. Maerzke, C. R. Iacovella, P. Cummings, C. McCabe, "Examining Phase Transition Behavior By Statistical Temperature Molecular Dynamics (STMD)," 26th Annual Workshop on Simulational Physics, University of Georgia, Athens, GA, 25th February 2013.
180. J. D. Haley and C. McCabe, "Predicting the Phase Behavior of Fluorinated Complex Systems Using the GC-SAFT-VR Equation of State," NSBE National Conference, Indianapolis, Indiana, 30th March 2013.
181. R. D. Chirico, M. Frenkel, J. W. Magee, V. V. Diky, K. Kroenlein, C. D. Muzny, A. F. Kazakov, I. M. Abdulagatov, G. R. Hardin, T. W. de Loos, J. P. O'Connell, C. McCabe, J. F. Brennecke, P. M. Mathias, A. R. H. Goodwin, J. T. Wu, K. N. Marsh, R. D. Weir, W. E. Acree, A. Padua, W. M. Haynes, D. G. Friend, A. Mandelis, V. Rives, C. Schick, S. Vyazovkin, and E. Chen, "NIST-journal cooperation to improve the quality of published experimental data: Pre-acceptance evaluation and on-line tools," American Chemical Society, Spring Meeting, New Orleans, LA, April 8th 2013.
182. G. Das, J. D. Haley and C. McCabe, "Modeling of complex fluids using the GC-SAFT-VR based equation of state," 13th International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD), Iguazu Falls, Argentina, Brazil, 27th May 2013.
183. A. Z. Summers, J. B. Lewis, J. Black, C. Klein, C. R. Iacovella, P. T. Cummings and C. McCabe, "Development of an Integrated Molecular Design Environment for Lubrication Systems (iMoDELS)," CCP5 Methods in Molecular Simulations Summer School, University of Manchester, Manchester, UK, July 21st – 30th, 2013.
184. T. Moore, S. Guo, C. R. Iacovella, and C. McCabe, "Understanding the Molecular Interactions of Skin Lipids from Molecular Dynamics Simulation," 13th Gordon Research Conference on Barrier Function of Mammalian Skin, Waterville Valley Resort, Waterville NH, August 18th-23rd 2013.

185. P. Morgado, G. Das, C. McCabe, and E. Filipe, "Interactions between Perfluoroalkylalkanes and Water: Solubilities and Interfacial Tensions," Thermodynamics 2013, University of Manchester. Manchester, UK, September 5th 2013.
186. T. Moore, S. Guo, C. Iacovella, and C. McCabe, "Coarse-grained Potential Derivation With Multi-State Iterative Boltzmann Inversion," Aachen Conference on Computational Engineering Science, RWTH Aachen University, 10th September 2013. (**1ST Place in conference poster competition**)
187. J. D. Haley, M. C. dos Ramos, and C. McCabe, "Predicting the Phase Behavior of Fluorinated Complex Systems Using the GC-SAFT-VR Equation of State," AIChE Annual meeting, San Francisco CA, November 4th 2013.
188. S. Mukherjee, J. D. Haley, C. R. Iacovella, C. McCabe, and P. T. Cummings, "Calculation of the Vapor-Liquid Phase Coexistence of Polymer-Grafted Nanoparticles," AIChE Annual meeting, San Francisco CA, November 4th 2013.
189. C. R. Iacovella, S. Guo, T. Moore, and C. McCabe, "A Comparative Study of GROMOS- and CHARMM-Based Force Fields for the Simulation of Non-Hydroxy Ceramide Bilayers," AIChE Annual meeting, San Francisco CA, November 5th 2013.
190. L. Gai, C. R. Iacovella, P. Cummings, C. McCabe, "Study of Phase Transitions By 2-D Density of States Simulation," AIChE Annual meeting, San Francisco CA, November 5th 2013.
191. J. Black, C. R. Iacovella, C. McCabe and P. T. Cummings, "Reactive Molecular Dynamics Study of Alkylsilane Monolayers On Realistic Amorphous Silica Substrates," AIChE Annual meeting, San Francisco CA, November 5th 2013.
192. S. Hlushak, C. McCabe, P. T. Cummings, "An Improved Classical Density Functional Theory for the Description of Adsorption Thermodynamics", AIChE Annual meeting, San Francisco CA, November 7th 2013.
193. S. Hlushak, M. D. LeVan, P. T. Cummings and C. McCabe, "Heats of adsorption and pore pressures predicted by classical density functional theory," ACS Spring National Meeting, Dallas TX, March 16th 2014.
194. G. Das; S. Hlushak; M.C. dos Ramos; C. McCabe, "Study of thermodynamic properties of aqueous electrolyte solutions using SAFT-VR+DE equation of state," SAFT Meeting 2014, Troia, Portugal, April 23rd 2014
195. P. Morgado; G. Das; C. McCabe, and E. Filipe, "SAFT modeling of Semifluorinated Alkanes- the Importance of Dipolar Interactions," SAFT Meeting 2014, Troia, Portugal, April 24th 2014.
196. C.R. Iacovella, S. Guo, T.C. Moore, C. McCabe "Simulation Study of the Morphology of Ceramide and Cholesterol Bilayers," Biomolecular Structure, Dynamics and Function: Membrane Proteins Conference, Vanderbilt University, Nashville TN, May 2nd 2014
197. T. C. Moore, C. R. Iacovella, and C. McCabe. "Derivation of coarse-grained potentials via multistate iterative Boltzmann inversion," Biomolecular Structure, Dynamics, and Function: Membrane Proteins, Vanderbilt University, Nashville TN, May 3rd 2014.
198. J. Sallai, G. Varga, S. Toth, C. R. Iacovella, C. Klein, C. McCabe, A. Ledeczi, and P. T. Cummings, "Web- and Cloud-based Software Infrastructure for Materials Design", International Conference on Computational Science (ICCS) 2014, Cairns, Queensland, Australia, June 10th 2014.
199. G. Varga, J. Sallai, A. Ledeczi, C. R. Iacovella, C. McCabe, P. T. Cummings, "Enabling Cross-Domain Collaboration in Molecular Dynamics Workflows," Fourth International Conference on Advanced Collaborative Networks, Systems and Applications (COLLA 2014), June 22 – 26 2014, Seville, Spain.
200. U. Kumar, L. Gai, C. R. Iacovella, P. T. Cummings and C. McCabe, "Application of Statistical Temperature Molecular Dynamics (STMD) Simulation To Study Phase Behavior of Nano-Confined Fluids", CCP5 Summer School 2014, University of Manchester, Manchester, UK, July 16th 2014.

201. J. D. Haley, C. R. Iacovella, P. T. Cummings and C. McCabe, "Examination of the Aggregation Behavior of Polymer Grafted Nanoparticles using Molecular Simulation and Theory," P&G FIRST Conference, Cincinnati OH, September 22nd 2014.
202. J. D. Haley, C. R. Iacovella, P. T. Cummings and C. McCabe, "Examination of the Aggregation Behavior of Polymer Grafted Nanoparticles using Molecular Simulation and Theory," National Organization for the Professional Advancement of Black Chemists and Chemical Engineers (NOBCChE) Conference 2014, New Orleans LA, September 25th 2014
203. T. C. Moore, C. R. Iacovella, and C. McCabe. "Dervation of coarse-grained potentials via multistate iterative Boltzmann inversion," SERMACS 2014, Nashville TN, October 16th 2014.
204. A. Z. Summers, M. R. Billingsley, C. R. Iacovella, P. T. Cummings, C. McCabe, "Investigating the Shear-Induced Wear of Alkylsilane Monolayers through Molecular Dynamics Simulation," SERMACS 2014, Sheraton Music City Hotel, Nashville TN, October 16th 2014.
205. J. E. Black, C. R. Iacovella, P. T. Cummings and C. McCabe, "Reactive Molecular Dynamics Study of Alkylsilane Monolayers on Realistic Amorphous Silica Surfaces," SERMACS 2014, Nashville TN, October 16th 2014.
206. C. Klein, J. Sallai, C. R. Iacovella, A. Ledeczi, C. McCabe and P. T. Cummings, "mBuild: A Hierarchical, Component Based Molecule Builder," SERMACS 2014, Nashville TN, October 17th 2014.
207. A. Z. Summers, C. R. Iacovella, M. R. Billingsley, S. T. Arnold, P. T. Cummings, C. McCabe, "Investigating the Shear-Induced Wear of Alkylsilane Monolayers through Molecular Dynamics Simulation," Poster presented at the 15th Annual Nanoscience and Nanotechnology Forum, Vanderbilt University, Nashville TN, November 12th 2014.
208. N. Nordin, C. Klein, C. R. Iacovella, P. T. Cummings, C. McCabe, "Frictional study of polyethylene glycol monolayers on silica substrate," AIChE Annual Meeting, Atlanta, GA, November 17th 2014.
209. C. Klein, J. Sallai, C. R. Iacovella, A. Ledeczi, C. McCabe, and P. T. Cummings, "mBuild: A Hierarchical, Component Based Molecule Builder," AIChE Annual Meeting, Atlanta GA, November 17th 2014.
210. P. Morgado, G. Das, C. McCabe and E. Filipe, "Solubility of Water in Alkanes, Perfluoroalkanes and Perfluoroalkylalkanes: Experimental Results and SAFT Modeling" AIChE Annual Meeting, Atlanta GA, November 17th 2014.
211. L. A. Mitchell, B. J. Schindler, G. Das, M. Carolina dos Ramos, C. McCabe, M. D. LeVan, "Development and Application of the SAFT-FMT-DFT Approach for Adsorption Equilibrium," AIChE Annual Meeting, Atlanta GA, November 17th 2014.
212. J. D. Haley, C. R. Iacovella, C. McCabe, and P. T. Cummings, "Examination of the Aggregation Behavior of Polymer Grafted Nanoparticles using Molecular Simulation and Theory," AIChE Annual Meeting, Atlanta GA, November 17th 2014.
213. T. C. Moore, C. R. Iacovella, S. Guo, and C. McCabe. "Derivation of Coarse-Grained Lipid Potentials Using Multi-State Iterative Boltzmann Inversion," AIChE Annual Meeting 2014, Atlanta GA, November 18th 2014.
214. C.R. Iacovella, T.C. Moore, S. Guo, and C. McCabe, "Simulation Study of the Impact of Cholesterol on Ceramide-Based Lipid Bilayers," AIChE Annual Meeting, Atlanta GA, November 18th 2014.
215. C. Klein, C. R. Iacovella, C. McCabe, P. T. Cummings, "Determination of Hydration Lubrication Regime in Sparse Zwitterionic Monolayers," AIChE Annual Meeting, Atlanta GA, November 18th 2014.
216. A. Z. Summers, C. R. Iacovella, P. T. Cummings, and C. McCabe, "Characterizing Tip-Surface Contact between Monolayer Functionalized Silica Surfaces through Molecular Dynamics Simulation," AIChE Annual Meeting, Atlanta GA, November 19th 2014.

217. J. E. Black, C. R. Iacovella, P. T. Cummings, and C. McCabe, "Atomistic Molecular Dynamics Study of Thin-Film Based Nanoscale Lubrication Schemes," AIChE Annual Meeting, Atlanta GA, November 19th 2014.
218. J.D. Haley, G. Das and C. McCabe, "Developing a Model for Carbon Dioxide using the modified Group Contribution-SAFT-VR with Dipole Theory" AIChE Annual Meeting, Atlanta GA, November 2014.
219. G. Das, S. Hlushak, M. C. dos Ramos, and C. McCabe, "Study of thermodynamic properties of mixed electrolyte solutions using SAFT-VR+DE equation of state," AIChE Annual Meeting, Atlanta GA, November 19th 2014.
220. J. D. Haley, G. Das, and C. McCabe, "Developing a Molecular Model for Carbon Dioxide Using the Group Contribution - SAFT-VR Equation," AIChE Annual Meeting, Atlanta GA, November 20th 2014.
221. V. M. Trejos, G. Das, L. A. Mitchell, M. D. LeVan, P. T. Cummings and C. McCabe, "Theoretical modeling of n-alkane adsorption on different porous materials using the SAFT-FMT-DFT approach," 19th Symposium on Thermophysical Properties, Boulder CO, June 22nd 2015.
222. T. C. Moore, C. R. Iacovella, and C. McCabe. "Self-Assembly Studies of Coarse-Grained Skin Lipids," Foundations of Molecular Modelling and Simulation (FOMMS) 2015, Welches OR, July 14th 2015.
223. C. Klein, C. R. Iacovella, C. McCabe, and P. T. Cummings, "Hydration Lubrication in Sparse Zwitterionic Monolayers," Foundations of Molecular Modelling and Simulation (FOMMS) 2015, Welches OR, July 15th 2015.
224. J. E. Black, C. R. Iacovella, P. T. Cummings and C. McCabe, "Molecular Dynamics Study of Alkylsilane Monolayers on Realistic Amorphous Silica Surfaces," Foundations of Molecular Modelling and Simulation (FOMMS) 2015, Welches OR, July 15th 2015.
225. A. Z. Summers, M. R. Billingsly, S. A. Arnold, C. R. Iacovella, P. T. Cummings and C. McCabe, "Molecular Dynamics Study of the Degredation of Alkylsilane Monolayers Under Shear" Foundations of Molecular Modelling and Simulation (FOMMS) 2015, Welches OR, July 15th 2015.
226. C. R. Iacovella, C. Klein, J. Sallai, T. J. Jones, N. Nordin, A. Ledezci, C. McCabe and P. T. Cummings, "mBuild: A Hierarchical, Component Based Molecule Builder," Foundations of Molecular Modelling and Simulation (FOMMS) 2015, Welches OR, July 15th 2015.
227. T. C Moore, C. R. Iacovella, and C. McCabe. "Understanding Stratum Corneium Lipid Morphology Through Molecular Dynamics Simulations." Barrier Function of Mammalian Skin, Gordon Research Conference, Waterville Valley NH, August 19-20th 2015.
228. A. Z. Summers, C. R. Iacovella, M. R. Billingsly, S. A. Arnold, P. T. Cumminggs and C. McCabe, "Molecular Dynamics Study of the Degradation of Alkylsilane Monolayers Under Shear," MTMS 2015, Fukuoka, Japan, August 8th 2015.
229. G. Das, S. Hlushak, M. C. dos Ramos, and C. McCabe, "Thermodynamic properties of mixed electrolyte solutions from the SAFT-VR+DE equation of state," Thermodynamics 2015, Copenhagen, Denmark, September 17th 2015.
230. C. Klein, C.R. Iacovella, C. McCabe, P.T. Cummings. "Hydration Structure and Dynamics of Poly(2-methacryloyloxyethyl phosphorylcholine)," AIChE, Salt Lake City, UT, November 10th 2015.
231. T. J. Jones, C. Klein, J. Sallai, C.R. Iacovella, P.T. Cummings, C. McCabe. "A Software Pipeline for the Rational Design of Soft Materials", AIChE, Salt Lake City, UT, November 9th 2015.
232. T. C Moore, C. R. Iacovella, and C. McCabe, "Understanding the Structural Arrangements of Stratum Corneum Lipids through Coarse-Grained and Fully Atomistic Molecular Dynamics Simulations" AIChE Annual meeting, Salt Lake City UT, November 11th 2015.
233. R. Hartkamp, T. C. Moore, C. R. Iacovella, M. Thompson, P. Bulsara, D. J. Moore and C. McCabe, "A Computational Study of the Molecular Structure and Permeability of Multi-Component Gel Phase Lipid Membranes" AIChE Annual meeting, Salt Lake City UT, USA, November 12th, 2015.

234. A. Z. Summers, C. R. Iacovella, M. R. Billingsley, S.T. Arnold, P. T. Cummings, C. McCabe, "Molecular Dynamics Study of the Degradation of Alkylsilane Monolayers Under Shear," AIChE 2015 Annual Meeting, Salt Lake City UT, November 12th 2015.
235. T. J. Jones, P.T. Cummings and C. McCabe, " A software pipeline for the rational design of soft materials", Tennessee Louis Stokes Alliance for Minority Participation 13th Annual Research Conference, Knoxville TN, February 25th 2016.
236. T. C. Moore, S. Guo, C. R. Iacovella, and C. McCabe, "Understanding the Self-Assembly and Phase Behavior of Skin Lipids," 14th Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD), Porto, Portugal, May 24th 2016.
237. C. Klein, C.R. Iacovella, C. McCabe, P.T. Cummings. "Hydration Structure and Dynamics of Poly(2-methacryloyloxyethyl phosphorylcholine)," 14th Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD), Porto, Portugal, May 25th 2016.
238. A. L. Bunge, T. C. Moore, C. R. Iacovella and C. McCabe "Molecular Simulations of Stratum Corneum Lipids: The Promise and Challenges," Occupational and Environmental Exposure of Skin to Chemicals Conference, Manchester, UK, September 21ST 2016.
239. A. Z. Summers, C. R. Iacovella, K. Mancini, O. M. Cane, P. T. Cummings, C. McCabe, "A Transferable Multi-Resolution Coarse-Grained Model for Amorphous Silica Nanoparticles," 17th Annual Nanoscience and Nanotechnology Forum, Vanderbilt University, Nashville, TN, October 19th, 2016.
240. C. Klein, J. Sallai, T.J. Jones, L. Williams, C.R. Iacovella, C. McCabe, and P.T. Cummings. " MoSDeF: A General Tool Chain for Screening of Soft Materials," 4th International Conference on Molecular Simulation (ICMS-2016), Shanghai, China, October 24th 2016.
241. C. Klein, W.L. Roussell, C.R. Iacovella, C. McCabe, and P.T. Cummings. "Choline and Phosphoryl Contributions to Hydration Structure and Dynamics of Poly(2-methacryloyloxyethyl phospho-rylcholine)", AIChE Annual Meeting, San Francisco CA, November 14th 2016.
242. C. Klein, J. Sallai, T.J. Jones, C.R. Iacovella, C. McCabe, P.T. Cummings. "A General Tool Chain for Screening of Soft Materials", AIChE 2016 Annual Meeting, San Francisco CA, November 14th 2016.
243. C. Klein, C. McCabe, P.T. Cummings, J. Sallai, and C.R. Iacovella, "A Logic-Based Framework for Defining Force Field Usage Semantics and Atom-Typing Molecular Systems "AIChE Annual Meeting, San Francisco CA, November 14th 2016.
244. A. Z. Summers, C. R. Iacovella, K. Mancini, O. M. Cane, P. T. Cummings, and C. McCabe, "A Transferable Multi-Resolution Coarse-Grained Model for Amorphous Silica Nanoparticles," Poster presented at the AIChE Annual Meeting, San Francisco CA, November 14th 2016.
245. T. C. Moore, C.R. Iacovella, and C. McCabe, "Development of Transferable Coarse-Grained Force Fields Via Multistate Iterative Boltzmann Inversion", AIChE Annual Meeting, San Francisco CA, November 14th 2016.
246. A. C. Leonhard, T. C. Moore, C.R. Iacovella, and C. McCabe, "Coarse-Grained Simulations of the Self-Assembly of Skin-Relevant Lipid Structures", AIChE Annual Meeting, San Francisco CA, November 14th 2016.
247. T. J. Jones, C. Klein, J. Sallai, P.T. Cummings and C. McCabe, "Screening Chemical Parameter Space of Self Assembling Monolayers", AIChE Annual Meeting, San Francisco CA, November 14th 2016. **(1st place in undergraduate student poster competition)**
248. R. Hartkamp, T.C. Moore, C.R. Iacovella, M.A. Thompson, P.A. Bulsara, D.J. Moore, and C. McCabe, "Molecular Dynamics Simulations of Permeability in Gel Phase Mixed Lipid Bilayers" AIChE Annual Meeting, San Francisco CA, November 15th 2016.
249. T. C. Moore, C. R. Iacovella, R. H. Hartkamp, and C. McCabe, "Development and Self-Assembly of Coarse-Grained Skin Lipid Models Derived Via Multistate Iterative Boltzmann Inversion," AIChE Annual Meeting, San Francisco CA, November 16th 2016.

250. C. Klein, C.R. Iacovella, J. Sallai, Á. Lédeczi, C. McCabe, and P.T. Cummings. "Application of Concepts from Modeling Integrated Computing for Molecular Simulation for Workflow Encapsulation", AIChE Annual Meeting, San Francisco CA, November 16th 2016.
251. C. R. Iacovella, T.C. Moore, R. Hartkamp, and C. McCabe "The Influence of Lipid Tail Length and Cholesterol Content on the Structure of Model Stratum Corneum Bilayers," AIChE Annual Meeting, San Francisco CA, November 17th 2016.
252. A. Z. Summers, C. R. Iacovella, P. T. Cummings, and C. McCabe, "Friction and Wear of Alkylsilane Monolayers at a Single Asperity Contact," AIChE Annual Meeting, San Francisco CA, November 18th 2016.
253. C. Klein, J. Sallai, T.J. Jones, C.R. Iacovella, C. McCabe, P.T. Cummings. "A General Tool Chain for Screening of Soft Materials", AIChE Annual Meeting, San Francisco CA, November 14th 2016.
254. T. J. Jones, P.T. Cummings and C. McCabe, " A software pipeline for the rational design of soft materials", Tennessee Louis Stokes Alliance for Minority Participation 14th Annual Research Conference, Nashville TN, February 23rd 2017.
255. K. G. Stassun, M. S. Hutson, C. McCabe, R. Pitt, W. H. Robinson, "AGEP Transformation Alliance: Bridging the PhD to Postdoc to Faculty Transitions for Women of Color", AGEP National Forum, Washington DC, February 23rd 2017.
256. C. Klein, C.R. Iacovella, C. McCabe, and P.T. Cummings, "Towards a Molecular Level Understanding Hydration Lubrication: Structure and Dynamics of 2-Methacryloyloxyethyl Phosphorylcholine," SIAM Conference on Computational Science and Engineering, Atlanta, GA, March 2nd 2017.
257. A. Yang, T.C. Moore, C.R. Iacovella, M.A. Thompson, P.A. Bulsara, D.J. Moore, and C. McCabe, "Structure of Phospholipid Bilayers with Alcohol and Free Fatty Acid Molecules," 2017 CCP5 Summer School for Molecular Simulation. Lancaster, UK. July 2017.
258. A. Yang, T. C. Moore, C.R. Iacovella, M. A. Thompson, P. A. Bulsara, D. J. Moore, and C. McCabe, "Structure and Permeability of Gel-Phase, Phospholipid Bilayers," 2017 Gordon Research Conference: Barrier Function of Mammalian Skin, Waterville Valley NH. August 15th 2017.
259. T. C. Moore, C. R. Iacovella, R. Hartkamp, A. L. Bunge, and C. McCabe, "The Effect of Composition and Ceramide Chain Length on Stratum Corneum Lipid Bilayer Structure," Gordon Research Conference on the Barrier Function of Mammalian Skin, Waterville Valley NH, August 15th 2017.
260. T. C. Moore, A. C. Leonhard, C. R. Iacovella, R. Hartkamp, A. L. Bunge, and C. McCabe, "Self-Assembly of Model Stratum Corneum Lipid Mixtures," Gordon Research Conference on the Barrier Function of Mammalian Skin, Waterville Valley NH, August 15th 2017.
261. J. Gilmer, C. Klein, J. Sallai, A. Z. Summers, C.R. Iacovella, A. Ledeczi, C. McCabe, and P.T. Cummings, Mosdef, a Python-Based Molecular Simulation and Design Framework," AIChE Annual Meeting, Minneapolis, October 30th 2017.
262. C. R. Iacovella, C. Klein, T.J. Jones, C. McCabe and P.T. Cummings, "Screening Self-Assembled Monolayers for Lubrication Properties: Trends and Pitfalls," AIChE Annual Meeting, Minneapolis, October 30th 2017.
263. C. Klein, W.L. Roussell, C.R. Iacovella, C. McCabe, and P.T. Cummings, "Hydration Structure and Dynamics of Poly(2-methacryloyloxyethyl phosphorylcholine), AIChE Annual Meeting, Minneapolis, October 30th 2017.
264. A. Yang, T. C. Moore, C. R. Iacovella, M.A. Thompson, P. A. Bulsara, D.J. Moore, and C. McCabe, "Structure of Multi-Component, Gel-Phase Lipid Bilayers," AIChE Annual Meeting, Minneapolis, November 1st 2017.
265. T. C. Moore, D. Xia, A. C. Leonhard, C. R. Iacovella, A. L. Bunge, C. McCabe, "Self-Assembly Simulations of Stratum Corneum Lipid Mixtures," AIChE Annual Meeting, Minneapolis, November 2nd 2017.

266. A. Z. Summers, C. R. Iacovella, P. T. Cummings, and C. McCabe, "Identifying Relationships between Terminal Group Chemistry and Interfacial Friction in Monolayer-Based Lubrication through a Molecular Dynamics Screening Approach," AIChE Annual Meeting, Minneapolis, November 2nd 2017.
267. C. Klein, A. Z. Summers, P.T. Cummings, J. Sallai, C.R. Iacovella, C. McCabe, "Foyer: A Framework for Defining Force Field Usage Semantics and Atom-Typing Molecular Systems," AIChE Annual Meeting, Minneapolis, November 2nd 2017.
268. C. Klein, J. Sallai, A. Z. Summers, C.R. Iacovella, A. Ledeczi, C. McCabe, and P.T. Cummings, "Mosdef: Molecular Simulation and Design Framework," AIChE Annual Meeting, Minneapolis, November 2nd 2017.
269. A. Z. Summers, C. R. Iacovella, P. T. Cummings, C. McCabe, "Screening Structure-Property Relationships in Lubricating Monolayer Films through Molecular Dynamics Simulation," Vanderbilt Data Science Symposium, Vanderbilt University, Nashville, March 30th 2018
270. P. Shamaprasad, T. C. Moore, C. R. Iacovella, and C. McCabe, "Development of Transferable Coarse- Grained Force Fields Via Multistate Iterative Boltzmann Inversion," CCP5 Summer School, Lancaster, U.K., July 9th 2018.
271. A. Yang, T. C. Moore, C. R. Iacovella, M. A. Thompson, P. A. Bulsara, D. J. Moore, C. McCabe "Depth and Interfacial Fluctuations in Multi-Component, Gel-Phase Lipid Bilayers," Foundations of Molecular Modeling and Simulation (FOMMS) Conference, Lake Delavan, July 16th 2018.
272. T. C. Moore, R. Hartkamp, C. R. Iacovella, Q. Zhang, and C. McCabe, "Influence of DNA Coating on the Interaction Between Graphene Nanoflakes and Lipid Bilayers," Foundations of Molecular Modeling and Simulation (FOMMS) 2018, Delevan, WI, July 16th 2018.
273. J. Gilmer, C. Klein, J. Sallai, A. Z. Summers, C. Iacovella, A. Lédeczi, P. Volgyesi, P. T. Cummings, C. McCabe, "MoSDeF: A Python-Based Molecular Simulation and Design Framework," Foundations of Molecular Modeling and Simulation (FOMMS) 2018, Delevan, WI, July 18th 2018.
274. A. Z. Summers, C. R. Iacovella, P. T. Cummings, C. McCabe, "Screening Structure-Property Relationships in Lubricating Monolayer Films through Molecular Dynamics Simulation," Foundations of Molecular Modeling and Simulation (FOMMS), Lake Delavan, July 18th 2018
275. A. Z. Summers, C. R. Iacovella, P. T. Cummings, C. McCabe, "Screening Structure-Property Relationships in Lubricating Monolayer Films through Molecular Dynamics Simulation," 19th Annual Nanoscience & Nanotechnology Forum, Vanderbilt University, Nashville, October 3rd 2018.
276. A. Z. Summers, C. R. Iacovella, P. T. Cummings, C. McCabe, "Screening Structure-Property Relationships in Lubricating Monolayer Films through Molecular Dynamics Simulation," AIChE Annual Meeting, Pittsburgh, October 28th 2018.
277. J. Gilmer, C. Klein, J. Sallai, A. Z. Summers, C. Iacovella, A. Lédeczi, P. Volgyesi, P. T. Cummings, C. McCabe, "MoSDeF: A Python-Based Molecular Simulation and Design Framework," 2018 AIChE Annual Meeting, Pittsburgh, PA, October 29th 2018.
278. J. Gilmer, C. Klein, J. Sallai, A. Z. Summers, C. Iacovella, A. Lédeczi, P. Volgyesi, P. T. Cummings, C. McCabe, "MoSDeF: Molecular Simulation and Design Framework for Transparent, Reproducible, Usable by Others, Extensible Simulations (TRUE)," 2018 AIChE Annual Meeting, Pittsburgh, PA, October 29th 2018.
279. C. Klein, J. Gilmer, A. Z. Summers, J. Black, J. Sallai, C. Iacovella, A. Lédeczi, P. Volgyesi, P. T. Cummings, C. McCabe, "Foyer: A Framework for Defining Force Field Usage Semantics and Atom-Typing Molecular Systems," 2018 AIChE Annual Meeting, Pittsburgh, PA, October 29th 2018.
280. A. J. Witte, J. B. Gilmer, A. H. Yang, C. McCabe, "Expanding crystalline material support in the Molecular Simulation and Design Framework (MoSDeF)," 70th Southeastern Regional meeting of the ACS (SERMACS), November 3rd 2018.

281. J. Gilmer, C. Klein, A. Z. Summers, C. Iacovella, P. T. Cummings, C. McCabe, "Zwitterionic Contribution to the Hydration Lubrication Dynamics of Poly(2-methacryloyloxyethyl phosphorylcholine)," 2018 AIChE Annual Meeting, Pittsburgh, PA, November 1st 2018.
282. O. Ogngbesan, A. Yang, C. R. Iacovella, and C. McCabe, "Using Molecular Simulation to Understand the Interactions Between DNA-Coated Graphene Sheets and Phospholipid Bilayers," Annual Biomedical Research Conference for Minority Students (ABRCMS), November 14th 2018.
283. A. Yang, T. C. Moore, C. R. Iacovella, M. A. Thompson, D. J. Moore, and C. McCabe, "Depth and Interfacial Fluctuations in Multi-Component Gel-Phase Lipid Bilayers," Thermodynamics 2019, Punta Umbria, Spain, June 27th 2019.
284. A. Yang, T. C. Moore, C. R. Iacovella, M. A. Thompson, P. A. Bulsara, D. J. Moore, C. McCabe "The Interfluence of Gel-Phase Bilayer Packing, order and Interfacial Behavior on Water Permeability," Properties and Phase Equilibria for Product and Process Design (PPEPPD) Conference, Vancouver Canada, May 12th - 16th 2019.
285. C. R. Iacovella, A. Summers, P. T. Cummings and C. McCabe, "Screening Structure-Property Relationships in Lubricating Monolayer Films through Molecular Dynamics Simulation, Properties and Phase Equilibria for Product and Process Design (PPEPPD) Conference, Vancouver Canada, May 12th - 16th 2019.
286. P. K. Shamaprasad, T. C. Moore, C. R. Iacovella, A. L. Bunge, and C. M. McCabe, "Transferability of Coarse-Grained Stratum Corneum Model," GRC Barrier Function of Mammalian Skin, Waterville Valley NH, August 14th 2019.
287. C. R. Iacovella, T. C. Moore, A. L. Bunge, and C. M. McCabe, "Examination of the role of ceramide headgroup chemistry and chain length on stratum corneum lipid bilayers," GRC Barrier Function of Mammalian Skin, Waterville Valley NH, August 14th 2019.
288. J. Gilmer, A. Z. Summers, C. Iacovella, P. T. Cummings, and C. McCabe, "Accelerating Large-Scale Screening of Tribological Properties and Chemistries," 2019 AIChE Annual Meeting, Orlando, FL, November 11th 2019.
289. J. Gilmer, C. Klein, A. Z. Summers, M. Thompson, C. Iacovella, P. Volgyesi, J. Sallai, P. T. Cummings, C. McCabe and C. R. Iacovella, "Foyer: A Framework for Defining Force Field Usage Semantics and Atom-Typing Molecular Systems," 2019 AIChE Annual Meeting, Orlando, FL, November 12th 2019
290. J. Gilmer, C. Klein, M. Thompson, J. Sallai, A. Z. Summers, C. R. Iacovella, A. Ledeczi, P. Volgyesi, C. McCabe and P. T. Cummings,, "MoSDeF: A Python-Based Molecular Simulation and Design Framework," 2019 AIChE Annual Meeting, Orlando, FL, November 12th 2019
291. P. T. Cummings, J. Gilmer, C. Klein, M. Thompson, J. Sallai, A. Z. Summers, C. R. Iacovella, A. Ledeczi, P. Volgyesi, and C. McCabe, "Molecular Simulation and Design Framework (MoSDef) for Transparent, Reproducible, Usable by Others, Extensible Simulations (TRUE)," 2019 AIChE Annual Meeting, Orlando, FL, November 14th 2019.
292. C. R. Iacovella, A. Summers, J. Gilmer, P. T. Cummings and C. McCabe, "Examination of the Relationships between Terminal Group Chemistry and Tribological Properties in Monolayer Films through Molecular Dynamics Screening," 2019 AIChE Annual Meeting, Orlando, FL, November 14th 2019.
293. P. K. Shamaprasad, T. C Moore, C. R. Iacovella, A. L. Bunge, C. McCabe, "Transferable Multiscale Model for Simulating Self-Assembled Skin Lipid Mixtures," AIChE 2019 Annual Meeting. Orlando, FL, November 15th 2019.
294. A. Yang, T. C. Moore, C. R. Iacovella, M. A. Thompson, P. A. Bulsara, D. J. Moore, C. McCabe "The Packing, Order and Interfacial Influences on Water Permeability through Gel-Phase Lipid Bilayers," 2019 AIChE Annual Meeting, Orlando, FL, November 15th 2019.
295. T. C. Moore, A. Yang, O. Ogungbesan, R. Hartkamp, C. R. Iacovella, Q. Zhang and C. McCabe, "Influence of Single-Stranded DNA Coatings on the Interaction between Graphene Nanoflakes and Lipid Bilayers," 2019 AIChE Annual Meeting, Orlando, FL, November 15th 2019.

296. C. D. Quach, M. W. Thompson, U. Timalsina, J. B. Gilmer, R. M. Matsumoto, P. Shamaprasad, A. Summers, C. R. Iacovella, C. McCabe, and P. T. Cummings, "MoSDeF: Molecular Simulation Design Framework, Open-source Software toward Reproducible Computational Simulation," Scipy2020. July 6-12, 2020.
297. C. D. Quach, M. W. Thompson, U. Timalsina, J. B. Gilmer, R. M. Matsumoto, P. Shamaprasad, A. Bansal, C. R. Iacovella, C. McCabe, and P. T. Cummings, "GMSO: A Flexible, Python-Based Representation of Chemical Topologies for Molecular Simulation," American Institute of Chemical Engineers Annual Meeting, November 17th 2020.
298. C. D. Quach, J. B. Gilmer, S. Dubose, C. R. Iacovella, P. T. Cummings, and C. McCabe, "Investigating the Tribological Properties of Monolayer Films through High-Throughput Screening and Machine Learning," American Institute of Chemical Engineers Annual Meeting, Online November 18th 2020.
299. C. R. Iacovella, P. Shamaprasad, C. Frame, A. L. Bunge, and C. McCabe, "Multiscale Modeling of Stratum Corneum Lipid Membranes," American Institute of Chemical Engineers Annual Meeting, November 18th 2020.
300. P. Shamaprasad, T. C. Moore, C. R. Iacovella, A. L. Bunge, and C. McCabe, "Exploring the Effect of Cholesterol on the Structure of Stratum Corneum Model Lamella Via Coarse-Grained Molecular Dynamics Simulations," American Institute of Chemical Engineers Annual Meeting, November 20th 2020.

Externally Funded Research Projects

1. Multiscale Simulation of the Synthesis, Assembly and Properties of Nanostructured Organic/Inorganic Hybrid Materials, coPI
   $1,950,000 (CMC share $80K) NSF, June 2002 – May 2005.
2. NSF REU Supplement to #1.
3. Molecular Modeling and Simulation of Aqueous Electrolyte Systems, co-PI
   $495,000 (CMC share $60K) DOE, June 2002 – May 2005.
4. Colorado School of Mines High Performance Network Connection, co-PI
   $150,000 NSF, October 2002 – September 2004.
5. NSF REU Supplement to #4.
6. High Pressure Computational Rheology, PI
   $35,000 Petroleum Research Fund, January 2003 – August 2005.
7. Impact of Water Structure Modifying Agents on Cellulose Water Boundary Layer, PI
   $113,000 DOE (subcontract from National Renewable Energy Laboratory), June 2002 – May 2004.
8. Molecular Modeling of Environmentally Benign Solute-Solvent Systems, PI
   $100,000 NSF, April 2003 – March 2004.
9. NSF REU Supplement to #8.
10. Molecular Modeling of Phase Equilibria in Porous Media: Application to Enhanced Oil and Gas Recovery, PI
    $99,935 NSF, August 2003 – July 2005.
11. Impact of Water Structure Modifying Agents on Cellulose Water Boundary Layer, PI
    $113,000 DOE (subcontract from NREL), June 2004 – May 2006.
12. Development of Predictive Methods for Thermodynamic Properties Relevant to Environmentally Benign Processes, PI
    $300,067 NSF, August 2004 – July 2009.
13. Molecular Modeling of Human Skin Lipids, PI

$50,000 VU Discovery Program, June 2005 – June 2008.

14. NSF REU Supplement to #1.
15. A Combined Computational and Experimental Study of Nanoscale Lubrication: Application to Micro- and Nano-Electromechanical Systems, PI
    $999,937 DoD/ONR 07/01/06 – 06/30/12
16. Molecular Modeling of Self-Assembling Human Skin Lipids, PI
    $374,192 Department of Health and Human Services R21 08/01/2007 – 07/31/2009
17. NSF REU Supplement to #12.
18. Acquisition of a Nanotribometer to Determine the Effectiveness of Novel Lubrication Strategies for Micro- and Nano- Electromechanical Systems, coPI
    $90,300 DoD - ONR 04/03/07 – 04/02/08
19. Molecular Modeling Studies of Linker Peptides to Aid in the Elucidation of Possible Enzymatic Mechanisms, PI
    $434,464 DOE (subcontract from National Renewable energy Laboratory) 09/1/2007 – 12/31/2011
20. A Molecular-Based Framework for Studying the Thermodynamic Properties of Ionic Liquids, PI
    $99,976, NSF - CBET 09/01/2008 – 08/31/2011
21. DURIP: Acquisition of a Computational Cluster for Simulation of Novel Lubrication Strategies for Micro- and Nano-Electromechanical Systems, PI
    $114,754 DoD - ONR 04/15/09 – 03/14/11
22. Combined Computational and Experimental Study of Nanoscale Lubrication: Application to Micro- and Nano- Electromechanical Systems, PI
    $150,000 DoD - ONR 01/01/09 – 12/31/10
23. NSF REU Supplement to #20.
24. Chemical Engineering Graduate Program for GAANN Fellows in Advanced Materials, PI
    $919,814, U.S. Department of Education GAANN program 08/15/09 - 08/14/2014
25. A Petaflop Cyberinfrastructure for Computing Free Energy Landscapes of Macro- and Biomolecular Systems, PI
    $1.5 M ($584,488 at VU) NSF-OCI 09/01/2009 - 08/31/2015
26. Using Molecular Modeling to Determine Structure and Organization in Skin Lipids, PI
    $685,987 Department of Health and Human Services R01 04/01/2010 – 03/31/2015
27. A GPU-based computing cluster for simulating n-body problems in the sciences and engineering, coPI
    $390,423 NSF-OCI 04/01/2010 – 03/31/2013
28. TurboComputing with Graphics Card Supercomputers, coPI
    $138,499 Vanderbilt IDEAS Program 07/01/2010 – 06/30/2013
29. REU Site: Nanoscale Materials Science and Engineering at Vanderbilt, PI
    $342,000 NSF - DMR 09/01/2010 – 08/31/2013
30. Developing a Molecularly Detailed Theoretical Framework for Predicting the Thermodynamic Properties of Ionic Liquids, PI
    $185,002 NSF - CBET 05/01/2011 – 04/30/2014
31. SI2-SSI: Development of an Integrated Molecular Design Environment for Lubrication Systems (iMoDELS), coPI
    $2,542,682 NSF-OCI 10/01/11 - 09/30/18
32. Multiscale and Multimodal Characterization of the Dynamics at Fluid Interfaces, coPI
    $25,000, Melbourne - Vanderbilt Partnership Grant, 01/01/2012 – 12/31/2013

33. Recruitment of Under-Represented Graduate Students in Engineering, Physical Sciences and Mathematics, PI
    $90,000 Vanderbilt University Enhancing Graduate Education Grant, 03/01/2012 – 06/30/2015
32. Molecular simulation and theory of adsorption and transport in nanoscale mineral pores, coPI
    $375,000, UT/Battelle, LLC, 10/1/2012 - 9/30/2015
34. REU Site: Nanoscale Materials Science and Engineering at Vanderbilt, PI
    $359,132 NSF - DMR 09/01/2013 - 08/31/2016
36. Modeling and Simulation Studies of Lipid Bilayers to Understand and Visualize Physiogel Lipid Behavior and Interactions with Skin Barrier Lipids, PI
    $249,280 GSK 12/01/2014 – 11/30/2016
37. REU Site: Nanoscale Materials Science and Engineering at Vanderbilt, PI
    $358,534 NSF - DMR 05/01/2016 - 04/30/2019
38. AGEP: AGEP Transformation Alliance: Bridging the PhD to Postdoc to Faculty Transitions for Women of Color in STEM, coPI
    $1,323,416 NSF – HRD 10/01/2016 – 09/30/2021
39. Modeling and Simulation Studies of Lipid Bilayers to Understand and Visualize Physiogel Lipid Behavior and Interactions with Skin Barrier Lipids, PI
    $220,000 GSK 01/01/2017 – 12/31/2018
40. NSF INCLUDES DDLP: Southeastern Compact for Inclusive Student Transitions in Engineering and Physical Sciences (SCI-STEPS), SI
    $298,416 NSF – OMA 09/15/2017 – 08/31/2019
41. Insights into Skin Barrier Function: In Silico and Experimental Studies of Healthy and Diseased Stratum Corneum Lipid Models, PI
    $1,725,488 NIH – NIAMS 08/10/2018 – 30/07/2023
42. Designing Deep Eutectic Solvents for Sustainable Separations, PI
    $308,040 NSF – CBET 08/15/2018 – 08/14/2021
43. Collaborative Research: NSCI Framework: Software for Building a Community-Based Molecular Modeling Capability Around the Molecular Simulation Design Framework (MoSDeF), coPI
    $3,000,000 NSF – OAC 10/1/2018 – 09/30/2021
44. Modeling and Simulation Studies of Lipid Bilayers to Understand and Visualize Physiogel Lipid Behavior and Interactions with Skin Barrier Lipids, PI
    $110,151 GSK 12/01/2018 – 11/30/2019
45. REU Site: Nanoscale Materials Science and Engineering at Vanderbilt, PI
    $359,933 NSF - DMR 05/01/2019 - 04/30/2022
46. Open Data-driven Infrastructure for Building Biomolecular Force Fields for Predictive Biophysics and Drug Design, coPI
    $242,679 NIH – NIGMS 09/01/2020 – 08/31/2021

Current Graduate Students and Post-Doctoral Researchers

Justin Gilmer	Materials Science Ph.D. student, co-supervised with Peter Cummings	Aug. 2016 - Present
Parashara Shamaprasad	ChBE Ph.D. student	Aug. 2017 - Present
Alyssa Nelson	ChBE Ph.D. student	Aug. 2018 - Present
Co Quatch	ChBE Ph.D. student, co-supervised with Peter Cummings	Aug. 2018 - Present

Chloe Frame	ChBE Ph.D. student	Aug. 2019 - Present
Duncan Stewart	ChBE Ph.D. student	Aug. 2019 - Present
Cal Craven	Materials Science Ph.D. student	Aug. 2019 - Present
Chris Iacovella	Research Assistant Professor	June 2012 - Present

Previous Graduate Student Research Supervision

Tauna R. Rignall	ChE M.S. Student Thesis Title: Molecular Modeling of Cellulose Hydrolysis: Energetics and Conformations of Hydrated Cel7a And Cel7b Linker Peptides	Sept. 2002 - Aug. 2006
Honggang Zhao	ChE Ph.D. student Thesis Title: A Statistical Associating Fluid Theory for Polar and Electrolyte Fluids	Aug. 2002 - Dec. 2006
Yun Peng	ChE Ph.D. student Thesis Title: Development and Applications of a Hetero-Based Statistical Associating Fluid Theory	Aug. 2002 - Sept. 2007
Patrick Redmill	ChE Ph.D. student, co-supervised with Peter Cummings Thesis Title: Probing the Solubility of Selected Nanoscale Building Blocks Using Molecular Simulation	Aug. 2003 - Dec. 2008
Kevin Hadley	ChBE Ph.D. student Thesis Title: A Molecular Dynamics Study of the Self-Assembly of Human Skin Lipids	Aug. 2004 - Aug. 2009
Brandon Booth	ChBE Ph.D. student, co-supervised with G. Kane Jennings Thesis Title: Tribometric Schemes for the Reduction of Friction in Microscale Devices	Aug. 2006 - Mar. 2011
Steve Vilt	ChBE Ph.D. student, co-supervised with G. Kane Jennings Thesis Title: Investigation of Interfacial Composition, Structure and Topography on Tribometric Friction	Aug. 2007 - Aug. 2011
Courtney Taylor	ChBE Ph.D. student Thesis Title: Investigating Structure-Function Relationships In Family 7 Cellulases By Molecular Simulation	Aug. 2008 - Aug. 2012
J. Ben Lewis	ChBE Ph.D. student Thesis Title: Investigation of Frictional Properties in Pure and Mixed Fluorocarbon/Hydrocarbon Monolayers by Molecular Simulations	Aug. 2007 Dec. 2012
Lili Gai	ChBE Ph.D. student Thesis Title: Examining the Phase Behavior of Complex Fluids with Free Energy Methods by Computer Simulation	Aug. 2009 - Aug. 2014
Jessica D. Haley	ChBE Ph.D. student Thesis Title: Predicting the Thermodynamic Properties of Complex Molecular Systems for Environmental Applications	May 2011 - May 2015
Gaurav Das	ChBE Ph.D. student Thesis Title: Theoretical Study of Complex Systems Using Statistical Associating Fluid Theory Based Equation of State	Aug. 2009 - June 2015
Christoph Klein	ChBE Ph.D. student, co-supervised with Peter Cummings Thesis Title: Towards Rational Design Of Nanoscale Lubricants And Elucidation Of The Hydration Lubrication Mechanism Using Molecular Simulation	Aug. 2012 - Aug. 2017
Tim Moore	ChBE Ph.D. student	Aug. 2011 - Dec. 2017

	Exploring the Structure of the Stratum Corneum Lipid Matrix via Molecular Dynamics Simulations	
Andrew Summers	ChBE Ph.D. student, co-supervised with Peter Cummings Tribological Examination of Alkylsilane Monolayer Films via Molecular Dynamics Simulation	Aug. 2012 - Dec. 2018
Alex Yang	ChBE Ph.D. student Thesis Title: Molecular Simulation Studies of Lipid Bilayers and Biomolecular Coatings for Water Barrier and Biocompatibility Purposes	Aug. 2016 - Dec. 2019

Previous Post-Doctoral Research Supervision

Hung-Chih Li	Project: Ab-inito investigation and Molecular Simulation of the Properties of Nanostructured Organic/Inorganic Hybrid Materials.	May 2002 - June 2004
Guoai Pan	Project: Computational Molecular Rheology	May 2003 - Nov. 2004
Lixin Sun	Project: Molecular Modeling of Environmentally Benign Solute-Solvent Systems	Sept. 2003 - Aug. 2004
Alberto Striolo	Project: Molecular Simulation of the Properties of Nanostructured Organic/Inorganic Hybrid Materials	Sept. 2003 - July 2005
Oleg Mazyar	Project: Using Molecular Simulation to Study Micro- and Nano-Electromechanical Systems Lubrication	Sept. 2006 - Dec. 2008
Leonardo Lenoci	Project: Molecular Modeling of the Self-Assembly of Human Skin Lipids	Apr. 2008 - Mar. 2009
Jose L. Rivera	Project: Using Molecular Simulation to Study Micro- and Nano-Electromechanical Systems Lubrication	Jan. 2009 - Nov. 2010
M. Carolina Dos Ramos	Project: Development of Predictive Methods for Thermodynamic Properties Relevant to Environmentally Benign Processes	Feb. 2007 - Oct. 2010
L. Anderson Strickland	Project: Molecular Modeling of the Self-Assembly of Human Skin Lipids	Sept. 2009 - Sept. 2011
Katie Maerzke	Project: Computing Free Energy Landscapes in Biomolecular Systems	July 2010 - June 2012
Stepan Hlushak	Project: Molecular simulation and theory of adsorption and transport in nanoscale mineral pores	Sept. 2012 - May 2014
Victor Montoya	Project: Molecular theory of adsorption in nanoscale mineral pores	Dec. 2014 - Feb. 2016
Remco Hartkamp	Project: Structure and Permeability of Multicomponent Lipid Bilayers in the Gel Phase	Dec. 2014 - Nov. 2016

Undergraduate Research Project Supervision

Jan. 2003 - Aug. 2003	Glenn Lau, honors undergraduate research and summer undergraduate research supported by NSF REU supplement. CSM[1] ChEN Class of 2004.
Jan. 2003 - May 2004	Heather Langmack, undergraduate student supported by NSF REU supplement and discretionary funds. CSM ChEN Class of 2004.

[1] Colorado School of Mines

May	2003	- Aug.	2004	Eric Whitebay, undergraduate student supported by NSF REU supplement. CSM ChEN Class of 2005.
Aug.	2003	- Jan.	2004	Pedro Morgado, visiting undergraduate student from IST, Lisbon Portugal. Supported by grant from the US-Portugal Fulbright Commission
May	2004	- Jan.	2005	Heather Barkley, undergraduate student supported by NSF REU supplement. CSM ChEN Class of 2005.
Jan.	2005	- May	2005	Becky Rutherford, independent study. VU ChE class of 2005.
Jan.	2005	- Dec.	2006	C. Matthew Earnest, honors independent study and summer student supported by VUSE summer research program and NSF REU supplement. VU ChE Class of 2007.
May	2005	- May	2007	Shannon Capps, honors independent study and summer student supported by VUSRP[2] program and NSF REU supplement. VU ChE Class of 2007. Shannon was awarded the Robert D. Tanner Undergraduate Research Award for her work with our group.
May	2005	- Aug.	2005	Justin Gregory, VINSE[3] IGERT REU Student.
May	2006	- Aug.	2006	Nurhikmah Mohd Hanifah, VUSE[4] summer research program. VU ChE Class of 2007.
Aug.	2006	- Dec.	2006	Josh Halperin, independent study. VU ChE Class of 2008.
Jan	2007	- May	2008	Kimberly Goff, NSF REU and VUSRP student. VU ChE Class of 2008. Kim was awarded the Robert D. Tanner Undergraduate Research Award for her work with our group.
June	2008	- Aug.	2008	Nurul Asyikin Aziz, summer session independent study. VU ChE Class of 2010.
Jan	2008	- May	2009	Everett O'Neal, honors independent study and summer undergraduate student supported by VUSRP program. VU ChE Class of 2009.
May	2008	- May	2009	Joel Westwood, VUSE summer research program and NSF REU supported student. VU ChBE Class of 2010.
Jan.	2009	- Aug.	2009	Craig Bullington, independent study and summer student supported by VUSE summer research program. VU ChBE Class of 2011.
Jan	2007	- May	2010	Jessica Haley, independent study and NSF REU supported student. VU ChBE Class of 2010.
Jan.	2009	- May	2010	Joseph Mikhail, honors independent study and summer undergraduate student supported by VUSRP program. VU ChBE Class of 2010.
June	2010	- Aug.	2010	Harry Watson, summer undergraduate student supported by VUSE summer program. VU ChBE Class of 2012.
Aug.	2009	- May	2011	Edward Buehler, honors independent study. VU ChBE Class of 2011.
June	2010	- May	2011	Nurbahirah Ibrahim, summer undergraduate student supported by VUSE summer program and an NSF REU supplement. VU ChBE Class of 2011.
June	2011	- Dec.	2011	Faiz Talib, summer undergraduate student supported by VUSRP program program. VU ChBE Class of 2012.
June	2011	- Aug.	2011	Eric Beiter, summer undergraduate student supported by VUSE summer program. VU ChBE Class of 2013.
June	2011	- Dec	2012	Jarrid Ristau, honors independent study and summer undergraduate student supported by VUSRP program. VU ChBE Class of 2013.

[2] Vanderbilt University Summer Research Program

[3] Vanderbilt Institute for Nanoscale Science and Education

[4] Vanderbilt University School of Engineering

June	2011	- May	2013	Matthew Claussen, honors independent study and summer undergraduate student supported by VUSE summer program. VU ChBE Class of 2013.
May	2013	- Aug.	2013	Nolan Smith, summer undergraduate student supported by VUSE summer program. VU CS Class of 2015.
May	2013	- April	2014	Phil Schapiro, independent study and summer undergraduate student supported by VUSE summer program. VU ChBE Class of 2015.
May	2014	- Dec.	2014	Monica Sowers, summer undergraduate student supported by VUSE summer program. VU ChBE Class of 2016.
May	2014	- Aug.	2014	Matthew Billingsly, VINSE NSF REU participant. Rose Hullman ChBE Class of 2015.
Aug.	2014	- Dec.	2014	Steven Arnold, independent study. VU ChBE Class of 2015.
May	2014	- Dec.	2014	Nadiah Nordin, independent study and summer undergraduate student supported by VUSRP program. VU ChBE Class of 2016.
May	2015	- May	2016	Eli McDonald, independent study and summer undergraduate student supported by VUSE summer program. VU ChBE Class of 2017.
May	2015	- Dec.	2016	Olivia Cane, independent study and summer undergraduate student supported by VUSE summer program. VU ChBE Class of 2017
May	2016	- Aug.	2016	Kristen Mancini, summer undergraduate student supported by VUSE summer program. VU ChBE Class of 2018.
May	2016	- Aug.	2016	Sobeen Park, summer undergraduate student supported by VUSRP program. VU ChBE Class of 2018.
May	2016	- Dec.	2016	Lily Williams, independent study and summer undergraduate student supported by VUSE summer program. VU ChBE Class of 2018.
May	2016	- May.	2017	Trevor Jones, independent study and summer undergraduate student supported by VUSRP program. VU ChBE Class of 2017
May	2016	- Aug.	2017	Anne Leonard, VINSE NSF REU participant. Rose Hullman ChBE Class of 2017.
May	2017	- Aug.	2017	Davy Yue, summer undergraduate student supported by VUSE summer program. VU ChBE Class of 2019.
May	2017	- Aug.	2017	Logan Guy, summer undergraduate student supported by VUSRP program. VU ChBE Class of 2018.
May	2017	- Aug.	2017	Donna Xia. VINSE NSF REU participant. University of Alabama ChBE Class of 2019.
May	2017	- May	2019	Adam Witte, summer undergraduate student supported by VUSE summer program (2017) and VUSRP (2018). VU ChBE Class of 2019.
May	2018	- Aug.	2018	Olu Ogungbesan. VINSE NSF REU participant. University of Maryland Baltimore County ChBE Class of 2021.
May	2018	- Aug.	2018	Katrina Luo. summer undergraduate student supported by VUSRP program. VU ChBE Class of 2020.
May	2019	- Aug.	2019	Anisha Matthew, summer undergraduate student supported by VUSE summer program.
May	2020	- Aug.	2020	Daniel Pert. Frist Center for Autism and Innovation REU participant. University of Michigan ChBE Class of 2023.
May	2020	- Aug.	2020	Caroline Spindel. Summer undergraduate student supported by VUSE summer program. Lehigh University ChBE Class of 2022.
May	2019	-		Savannah DuBose, independent study and summer undergraduate student supported by VUSE summer program (2019, 2020). VU ChBE Class of 2021.