Jonathan K. Whitmer

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Chemical and Biomolecular Engineering
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Education

Ph.D. Physics, University of Illinois, 2011
Dissertation: Dynamics and Assembly of Colloidal Particles
Advisor: Erik Luijten

M.S. Physics, University of Illinois, 2009

B.S. Physics and B. S. Mathematics, *Summa Cum Laude*, Kansas State University, 2005

Professional Experience

- Chemical and Biomolecular Engineering, University of Notre Dame
  - Assistant Professor (2014–present)
- Materials Science Division, Argonne National Laboratory
  - Postdoctoral Scientist (2013–2014)
- Institute for Molecular Engineering, University of Chicago
  - Visiting Scientist (2013–2014)
- Department of Chemical and Biological Engineering, University of Wisconsin
  - Postdoctoral Research Associate (2011–2013)
- Department of Physics, University of Illinois (2006–2011)
  - Graduate Research Assistant (2006–2011)
  - Graduate Teaching Assistant (2005–2006, 2011)
  - Undergraduate Research Assistant (2002)
- Department of Physics, Kansas State University
  - Undergraduate Research Assistant (2002–2005)

Publications

Citations in the electronic version of this CV contain clickable web links to the journal or proceedings, if available. The following key applies to authors, and refers to their rank at the time of their contribution: (*) undergraduate student, (°) graduate student, (+) postdoctoral researcher. All unlabeled authors hold the rank of assistant professor or above. Citation statistics are from the ISI Web of Science.

Submitted Publications

35. "Dynamics and structure of colloidal aggregates under microchannel flow," °Ming Han, **Jonathan K. Whitmer** and Erik Luijten. *Submitted to ACS Nano* (2018).
Contribution: Wrote simulation code, designed initial simulations, and wrote the paper.

Refereed Publications–Notre Dame

34. "Hierarchical Coupling of First Principles Molecular Dynamics with Advanced Sampling Methods," °Emre Sevgen, $^{+}$Federico Giberti, °Hythem Sidky, **Jonathan K. Whitmer**, François Gygi, Giulia Galli and Juan J. de Pablo. The Journal of Chemical Theory and Computation, *Accepted* (2018).
Contribution: Co-Lead PI. Designed the project, directed research contributions of HS, and wrote the paper.

33. "Adaptive Enahnced Sampling with FUNN: Force-bias Using Neural Networks." °Ashley Guo, °Emre Sevgen, °Hythem Sidky, **Jonathan K. Whitmer** and Juan J. de Pablo. Journal of Chemical Physics **148**, 134108 (2018).
Contribution: Co-PI. Directed research contributions of HS and wrote the paper.

32. "Weak Polyelectrolyte Complexation Driven by Associative Charging." °Vikramjit S. Rathee, *Aristotle J. Zervoudakis, °Hythem Sidky $^{+}$Benjamin J. Sikora and **Jonathan K. Whitmer**. The Journal of Chemical Physics, **148**, 114901 (2018).
Contribution: Lead PI. Designed the project, directed the research, and wrote the paper.

31. "*In Silico* Measurement of Elastic Moduli of Nematic Liquid Crystals," °Hythem Sidky, Juan J. de Pablo and **Jonathan K. Whitmer**. Physical Review Letters **120**, 107801 (2018).
Contribution: Lead PI. Designed the project, directed the research, and wrote the paper.

30. "Learning Free Energy Landscapes with Artificial Neural Networks," °Hythem Sidky and **Jonathan K. Whitmer**. The Journal of Chemical Physics **148**, 104111 (2018). arXiv preprint: 1712.02840.
Contribution: Lead PI. Designed the project, directed the research, and wrote the paper.

29. "SSAGES: A Comprehensive Platform for Enhanced Sampling Simulations." °Hythem Sidky, $^{+}$Yamil J. Colón, $^{+}$Benjamin J. Sikora, °Cody Bezik, $^{+}$Federico Giberti, °Ashley Guo, $^{+}$Julian Helfferich, Xikai Jiang, °Joshua Lequieu, Jiyuan Li, °Joshua Moller, °Michael Quevillon, $^{+}$Mohammad Rahimi, $^{+}$Hadi Ramezani-Dakhel, °Vikramjit Rathee, °Daniel Reid, °Emre Sevgen, $^{+}$Vikram Thapar, $^{+}$Michael Webb, Justin Wozniak, Xujun Zhao, Nicola J. Ferrier, Olle G. Heinonen, Giulia Galli, Franois Gygi, Juan de Pablo and **Jonathan K. Whitmer**. The Journal of Chemical Physics **148**, 044104 (2018).
Contribution: Co-Lead PI. Designed the project, directed the research, developed and tested software, and wrote the paper.

28. "Charge Transport and Phase Behavior of Imidazolium-Based Ionic Liquid Crystals from Fully Atomistic Simulations." Part of themed issue "Liquid Crystal-Assisted Advanced Functional Materials." °Michael Quevillon and **Jonathan K. Whitmer**. Materials **11**, 64 (2018).
Contribution: Lead PI. Designed the project, directed the research, and wrote the paper.

27. "Simulating the Thermodynamics of Charging in Weak Polyelectrolytes: The Debye Hückel Limit," *Invited Article for Emerging Investigators in Materials Science 2017 Collection.* °Vikramjit S. Rathee, $^{+}$Benjamin J. Sikora, ° Hythem Sidky and **Jonathan K. Whitmer**. Materials Research Express, **5**, 014010 (2018).
Contribution: Lead PI. Designed the project, directed the research, and wrote the paper.

26. "The Emergent Nematic Phase in Ionic Chromonic Liquid Crystals." °Hythem Sidky and **Jonathan K. Whitmer**. The Journal of Physical Chemistry B **121**, 6691–6698 (2017).
Contribution: Lead PI. Designed the project, directed the research, and wrote the paper.

25. "An algebraic geometric method for calculating phase equilibria from fundamental equations of state," °Hythem Sidky, °Alan C. Liddell, Jr., Jonathan D. Hauenstein, Dhagash Mehta and **Jonathan K. Whitmer**. Industrial & Engineering Chemistry Research **55**, 11363–11370 (2016).
Contribution: Co-lead PI. Designed the project, directed the research, and wrote the paper.

24. "A coarse-grained thermodynamic model for the predictive engineering of valence-selective membranes," °Vikramjit Rathee, °Siyi Qu, William A. Phillip and **Jonathan K. Whitmer**. Molecular Systems Design & Engineering **1**, 301–312 (2016).
Contribution: Co-lead PI. Designed the simulation project, performed analysis, directed the research, and wrote the paper.

23. "Elastic properties of common Gay–Berne nematogens from density of states (DOS) simulations," *Invited Article.* °Hythem Sidky and **Jonathan K. Whitmer**. Liquid Crystals **43**, 2285–2299 (2016).
Contribution: Lead PI. Designed the project, directed the research, and wrote the paper.

22. "Reliable mixture critical point computation using polynomial homotopy continuation," °Hythem Sidky, Dhagash Mehta and **Jonathan K. Whitmer**. AIChE Journal **62**, 4497–4507 (2016) .
Contribution: Lead PI. Designed the project, directed the research, and wrote the paper.

21. "Elastic response and phase behavior in binary liquid crystal Mixtures," °Hythem Sidky and **Jonathan K. Whitmer**. Soft Matter **12**, 4489–4498 (2016).
Contribution: Lead PI. Designed the project, directed the research, and wrote the paper.

20. "Sculpting bespoke mountains: determining free energies with basis expansions," **Jonathan K. Whitmer**, °A. M. Fluitt, +J. Qin, °L. Antony, °M. McGovern and J. J. de Pablo. The Journal of Chemical Physics **143**, 044101 (2015).
Contribution: Lead Author. Designed, directed, and performed the research and wrote the paper.

Refereed Publications–Pre-Notre Dame

19. "Chirality selected phase behavior in ionic polypeptide complexes," +S. L. Perry, +L. Leon, °K. Q. Hoffmann, +M. J. Kade, +D. Priftis, °K. A. Black, °D. Wong, °R. A. Klein, °C. F. Pierce III, °K. O. Margossian, +**Jonathan K. Whitmer**, +J. Qin, J. J. de Pablo and M. Tirrell. Nature Communications **6**, 6052 (2015).
Contribution: Interpreted data and edited the paper.

18. "Coarse-grained modeling of DNA curvature," °G. S. Freeman, °D. M. Hinckley, °J. Lequieu, +**Jonathan K. Whitmer**, and J. J. de Pablo. The Journal of Chemical Physics **141**, 165103 (2014).
Contribution: Helped direct research, interpreted data and wrote the paper.

17. "Surface adsorption in nonpolarizable atomic models," +**Jonathan K. Whitmer**, °A. A. Joshi, °R. J. Carlton, N. L. Abbott and J. J. de Pablo. Journal of Chemical Theory and Computation **10**, 5616 (2014).
Contribution: Lead author. Designed, directed, and performed the research and wrote the paper.

16. "Basis Function Sampling: A new paradigm for material property computation," +**Jonathan K. Whitmer**, +C.-c. Chiu, °A. A. Joshi, and J. J. de Pablo. Physical Review Letters **113**, 190602 (2014)
Contribution: Lead author. Designed, directed, and performed the research and wrote the paper.

15. "DNA shape dominates sequence affinity in nucleosome formation," °G. S. Freeman, °D. M. Hinckley, °J. Lequieu, +**Jonathan K. Whitmer**, and J. J. de Pablo. Physical Review Letters **113**, 168101 (2014).
Contribution: Helped direct research, interpreted data and wrote the paper.

14. "Interfacial tension of polyelectrolyte complex coacervate phases," +J. Qin, +D. Priftis, °R. Farina, +S. Perry, +**Jonathan K. Whitmer**, °K. Hoffmann, M. Tirrell, and J. J. de Pablo. ACS Macro Letters **3**, 565 (2014).
Contribution: Interpreted data and wrote the paper.

13. "Orientationally glassy crystals of Janus spheres," °S. Jiang, °J. Yan, °**Jonathan K. Whitmer**, °S. A. Anthony, E. Luijten, and S. Granick. Physical Review Letters **112**, 218301 (2014).
Contribution: Designed and performed simulations, wrote the paper.

12. "Measuring liquid crystal elastic constants with free energy perturbations," °A. A. Joshi, +**Jonathan K. Whitmer**, O. Gúzman, and J. J. de Pablo. Soft Matter **10**, 882 (2014).
Contribution: Helped direct research, designed, performed and interpreted simulations, wrote the paper.

11. "Nematic-field-driven positioning of particles in liquid crystal droplets," $^{+}$**Jonathan K. Whitmer**, °X. Wang, $^{+}$F. Mondiot, °D. S. Miller, N. L. Abbott, and J. J. de Pablo. Physical Review Letters **111**, 227801 (2013). *Cover Article. Selected as Editor's Recommendation.*
Contribution: Lead Author. Designed, performed, and interpreted simulations, and wrote the paper.

10. "An experimentally informed coarse-grained 3-site-per-nucleotide model of DNA: structure, thermodynamics, and dynamics of hybridization," °D. M. Hinckley, °G. S. Freeman, $^{+}$**Jonathan K. Whitmer**, and J. J. de Pablo. The Journal of Chemical Physics **139**, 144903 (2013). *Cover Article.*
Contribution: Helped direct research, interpreted data and wrote the paper.

9. "Liquid-crystal mediated nanoparticle interactions and gel formation," $^{+}$**Jonathan K. Whitmer**, °A. A. Joshi, °T. F. Roberts, and J. J. de Pablo. The Journal of Chemical Physics **138**, 194903 (2013); **141**, 029901 (2014).
Contribution: Lead Author. Designed, performed, and interpreted simulations, and wrote the paper.

8. "Modeling the polydomain–monodomain transition of liquid crystal elastomers," $^{+}$**Jonathan K. Whitmer**, °Raj Shekhar, °T. F. Roberts, N. L. Abbott, and J. J. de Pablo. Physical Review E **87**, 020502(R) (2013). *Selected for February 2013 PRE Kaleidoscope Gallery.*
Contribution: Lead Author. Designed, performed, and interpreted simulations, and wrote the paper.

7. "Isotropic–nematic phase transition in the Lebwohl–Lasher model from density of states simulations," °R. Shekhar, $^{+}$**Jonathan K. Whitmer**, °R. Malshe, J. A. Moreno-Razo, °T. F. Roberts, and J. J. de Pablo. The Journal of Chemical Physics **136**, 234503 (2012).
Contribution: Performed simulations, interpreted data and wrote the paper.

6. "Influence of hydrodynamics on cluster formation in colloid–polymer mixtures," *Invited Article.* °**Jonathan K. Whitmer** and E. Luijten. The Journal of Physical Chemistry B **115**, 7294–7300 (2011).
Contribution: Lead Author. Designed, performed, and interpreted simulations and wrote the paper.

5. "Triblock colloidal spheres for directed self-assembly," °Q. Chen, *E. Diesel, °**Jonathan K. Whitmer**, S. C. Bae, E. Luijten, and S. Granick. Journal of the American Chemical Society **133**, 7725–7727 (2011).
Contribution: Helped design the study and wrote the paper.

4. "Supracolloidal reaction kinetics of Janus spheres," °Q. Chen, °**Jonathan K. Whitmer**, °S. Jiang, S. C. Bae, E. Luijten, and S. Granick. Science **331**, 199 (2011).
Contribution: Designed and performed simulations, interpreted simulation and experimental data, and co-wrote the paper.

3. "Sedimentation of aggregating colloids," °**Jonathan K. Whitmer** and E. Luijten. The Journal of Chemical Physics **134**, 034510 (2011).
Contribution: Lead Author. Designed, performed, and analysed simulations and wrote the paper.

2. "Fluid–solid boundary conditions for multiparticle collision dynamics," °**Jonathan K. Whitmer** and E. Luijten. Journal of Physics: Condensed Matter **22**, 104106 (2010).
Contribution: Lead Author. Designed, performed, and analysed simulations and wrote the paper.

1. "Adsorption at the liquid–vapor surface of a binary liquid mixture," *Jonathan K. Whitmer, S. B. Kiselev, and B. M. Law. The Journal of Chemical Physics **123**, 204720 (2005).
Contribution: Lead Author. Performed and interpreted experiments, and wrote the paper.

Other

Software

1. SSAGES: Software Suite for Advanced Generalized Ensemble Simulations. Current version 0.8α (December 23, 2017). https://github.com/MICCoM/SSAGES-public/releases.

Contributed Talks and Posters–Notre Dame

63. "Coarse-Grained Simulations of Weak Polyacid Titration in Explicit Salt," °Vikramjit S. Rathee, °Hythem Sidky, +Benjamin J. Sikora and **Jonathan K. Whitmer**. AIChE Fall Meeting, Pittsburgh, PA, October 2018.

62. "Atomistic Simulation of Ionic Liquid Crystals," °Michael Quevillon and **Jonathan K. Whitmer**. AIChE Fall Meeting, Pittsburgh, PA, October 2018.

61. "TBD," °Vikramjit S. Rathee and **Jonathan K. Whitmer**. Gordon Research Conference on Polymer Physics, Mount Holyoke College, South Hadley, MA, July 2018.

60. "Phase Behavior of Ionic Liquid Crystals for Applications in Anisotropic Battery Electrolytes," °Michael J. Quevillon and **Jonathan K. Whitmer**. FOMMS (Foundations of Molecular Modeling and Simulation), Delavan, WI, July 2018.

59. "Associative charging driven weak polyelectrolyte complexation," °Vikramjit S. Rathee, *Aristotle J. Zervoudakis, °Hythem Sidky, +Benjamin J. Sikora and **Jonathan K. Whitmer**. Midwest Thermodynamics and Statistical Mechanics Meeting, Pittsburgh, PA, June 2018.

58. "Thermodynamic and Phase Behavior of Ionic Liquid Crystals via Fully Atomistic Replica-Exchange Simulations," °Michael Quevillon and **Jonathan K. Whitmer**. Midwest Thermodynamics and Statistical Mechanics Meeting, Pittsburgh, PA, June 2018.

57. +Federico Giberti, °Emre Sevgen, °Hythem Sidky, **Jonathan K. Whitmer**, Giulia Galli, Francois Gygi and Juan J. de Pablo. "First Principle Free Energy Calculations Made Simple: The Example Case of Alanine Dipeptide, from Classical Force-field to Hybrid Functional." APS March Meeting, Los Angeles, CA, March 2018.

56. °Emre Sevgen, °Ashley Guo, °Hythem Sidky, **Jonathan K. Whitmer** and Juan J. de Pablo. "Adaptive Enhanced Sampling with FUNN: Force-biasing Using Neural Networks." APS March Meeting, Los Angeles, CA, March 2018.

55. °Michael Quevillon and **Jonathan K. Whitmer**. "Charge Transport and Phase Behavior of Ionic Liquid Crystals from Fully Atomistic Simulations." APS March Meeting, Los Angeles, CA, March 2018.

54. °Hythem Sidky and **Jonathan K. Whitmer**. "Learning Free Energies from Molecular Simulation using Artificial Neural Networks." APS March Meeting, Los Angeles, CA, March 2018.

53. °Hythem Sidky and **Jonathan K. Whitmer**. "Atomistic Simulations as Bulk Elastic Probes in Liquid Crystalline Systems." APS March Meeting, Los Angeles, CA, March 2018.

52. °Vikramjit S. Rathee, *Aristotle J. Zervoudakis, °Hythem Sidky, +Benjamin J. Sikora and **Jonathan K. Whitmer**. "Charging Behavior of Associating Weak Polyelectrolytes." APS March Meeting, Los Angeles, CA, March 2018.

51. °Hythem Sidky, +Yamil J. Colón, +Benjamin J. Sikora, °Cody Bezik, +Federico Giberti, °Ashley Guo, +Julian Helfferich, Xikai Jiang, °Joshua Lequieu, Jiyuan Li, °Joshua Moller, °Michael Quevillon, +Mohammad Rahimi, +Hadi Ramezani-Dakhel, °Vikramjit Rathee, °Daniel Reid, °Emre Sevgen, +Vikram Thapar, +Michael Webb, Justin Wozniak, Xujun Zhao, Nicola J. Ferrier, Olle G. Heinonen, Giulia Galli, Franois Gygi, Juan de Pablo and **Jonathan K. Whitmer**. "SSAGES: A Comprehensive Platform for Enhanced Sampling Simulations." AIChE Fall Meeting, Minneapolis, MN, October 2017.

50. °Hythem Sidky and **Jonathan K. Whitmer**. "Learning Free Energy Landscapes Using Artificial Neural Networks." AIChE Fall Meeting, Minneapolis, MN, October 2017.

49. °Hythem Sidky and **Jonathan K. Whitmer**. "Toward molecular engineering of liquid crystal elasticity: Predicting 5CB Elastic Constants" AIChE Fall Meeting, Minneapolis, MN, October 2017.

48. **Jonathan K. Whitmer**. "Thermodynamics of Charging in Weak Polyelectrolyte Materials" 2nd Notre Dame–Purdue Soft Materials Symposium, West Lafayette, IN, September 2017.

47. **Jonathan K. Whitmer**. "Teaching *with* the Test: Expanded Retrieval Practice for Enhanced Student Outcomes." ASEE Chemical Engineering Summer School, Raleigh, NC, August 2017.

46. °Hythem Sidky and **Jonathan K. Whitmer**. "Learning Free Energy Landscapes Using Artificial Neural Networks." Midwest Thermodynamics and Statistical Mechanics Meeting, University of Notre Dame, Notre Dame, IN, June 2017.

45. °Hythem Sidky and **Jonathan K. Whitmer**. "Toward molecular engineering of liquid crystal elasticity: Predicting 5CB Elastic Constants" Midwest Thermodynamics and Statistical Mechanics Meeting, University of Notre Dame, Notre Dame, IN, June 2017.

44. °Vikramjit Rathee, °Siyi Qu, William A. Phillip and **Jonathan K. Whitmer**. "A coarse-grained thermodynamic model for the predictive engineering of valence-selective membranes." Midwest Thermodynamics and Statistical Mechanics Meeting, University of Notre Dame, Notre Dame, IN, June 2017.

43. °Michael Quevillon and **Jonathan K. Whitmer**. "Phase Behavior of an Ionic Liquid Crystal System." Midwest Thermodynamics and Statistical Mechanics Meeting, University of Notre Dame, Notre Dame, IN, June 2017.

42. *Aristotle J. Zervoudakis and **Jonathan K. Whitmer**. "Modeling Phase Coexistence in Complex Coacervates." Midwest Thermodynamics and Statistical Mechanics Meeting, University of Notre Dame, Notre Dame, IN, June 2017.

41. °Vikramjit Rathee, +Benjamin Sikora and **Jonathan K. Whitmer**. "Weak Polyelectrolytes in Confined Geometries." APS March Meeting, New Orleans, LA, March 2017.

40. °Hythem Sidky and **Jonathan K. Whitmer**. "Toward molecular engineering of liquid crystal elasticity: a predictive study of nCB homologues." APS March Meeting, New Orleans, LA, March 2017.

39. +Benjamin Sikora and **Jonathan K. Whitmer**. "Phase behavior of weak polyelectrolyte materials." AIChE Fall Meeting, San Francisco, CA, November 2016.

38. °Hythem Sidky and **Jonathan K. Whitmer**. "Stacking and elasticity of ionic chromonic liquid crystals." AIChE Fall Meeting, San Francisco, CA, November 2016.

37. °Hythem Sidky, Dhagash Mehta, °Alan Liddell, Jr., Jonathan Hauenstein and **Jonathan K. Whitmer**. "Modeling phase equilibrium using numerical algebraic geometry." AIChE Fall Meeting, San Francisco, CA, November 2016.

36. °Hythem Sidky and **Jonathan K. Whitmer**. "Self-assembly of ionic chromonic liquid crystals." Poster Presentation. 26th International Liquid Crystal Conference, Kent State University, Kent, OH. August 2016.

35. °Hythem Sidky and **Jonathan K. Whitmer**. " Elastic properties of common Gay–Berne nematogens." Midwest Thermodynamics and Statistical Mechanics Conference, Miami University, Oxford, OH, May 2016.

34. °Hythem Sidky, Dhagash Mehta, °Alan Liddell, Jr., Jonathan Hauenstein and **Jonathan K. Whitmer**. "Revisiting nonlinear equations in classical thermodynamic modeling: a numerical algebraic geometry perspective.". Workshop on Software and Applications of Numerical Algebraic Geometry, Notre Dame, IN, May 2016.

33. °Hythem Sidky and **Jonathan K. Whitmer**. "Self-assembly of ionic chromonic liquid crystals", APS March Meeting, Baltimore, MD, March 2016.

32. +Benjamin Sikora and **Jonathan K. Whitmer**. "Explicit-ion effects in the coil–globule transition of weak polyelectrolytes", APS March Meeting, Baltimore, MD, March 2016.

31. °Vikramjit Rathee, °Siyi Qu, *Theodore Dilenschneider, William A. Phillip and **Jonathan K. Whitmer**. "Thermodynamics of ionic transport through functionalized membranes", APS March Meeting, Baltimore, MD, March 2016.

30. **Jonathan K. Whitmer** and °Hythem Sidky. "Elastic behavior of liquid crystal mixtures", AIChE Fall Meeting, Salt Lake City, UT, November 2015.
29. **Jonathan K. Whitmer**. "Soft materials design through free energy mapping", ND*nano* Soft Materials Symposium, Notre Dame IN, November 2015.
28. **Jonathan K. Whitmer**. "Calculating free energies with basis expansions," Midwest Thermodynamics and Statistical Mechanics Conference, Ames, IA, May 2015.
27. °Hythem Sidky and **Jonathan K. Whitmer**. "Phase behavior of binary liquid crystal mixtures: a density-of-states based approach", Midwest Thermodynamics and Statistical Mechanics Conference, Ames, IA, May 2015.
26. **Jonathan K. Whitmer**. "Mesoscale simulations of soft materials", ND*nano* Meeting, Notre Dame, IN, March 18, 2015.
25. **Jonathan K. Whitmer**. "Elastic response of liquid crystalline mixtures," APS March Meeting, San Antonio, TX, March 2015.
24. **Jonathan K. Whitmer**. "Enhanced sampling for simulation of soft materials", ND*nano* Soft Materials Symposium, Notre Dame IN, November 2014.
23. **Jonathan K. Whitmer**, +Chi-cheng Chiu, °Abhijeet A. Joshi and Juan J. de Pablo. "Basis function sampling: a new paradigm for material property computations," AIChE Fall Meeting, Atlanta, GA, November 2014.

Contributed Talks and Posters–Pre-Notre Dame

22. +**Jonathan K. Whitmer**, +Chi-cheng Chiu, °Abhijeet A. Joshi and Juan J. de Pablo. "Basis function sampling for material property computations," APS March Meeting, Denver, CO, March 2014.
21. °Kyle Q. Hoffmann, **Jonathan K. Whitmer**, +Jian Qin, +Dimitris Priftis, +Sarah L. Perry, +Lorraine Leon, +Matthew Kade, Matthew Tirrell and Juan J. de Pablo "Multiscale simulation of complex coacervates," APS March Meeting, Denver, CO, March 2014.
20. Matthew Tirrell, +Sarah L. Perry, +Lorraine Leon, +Matthew Kade, +Dimitris Priftis, °Katie Black, °Kyle Q. Hoffmann, +**Jonathan K. Whitmer**, +Jian Qin and Juan J. de Pablo. "Stereoregularity drives precipitation in polyelectrolyte complex formation," APS March Meeting, Denver, CO, March 2014.
19. +Jian Qin, +Dimitrios Priftis, °Robert Farina, +Sarah L. Perry+, Lorraine Leon, +**Jonathan K. Whitmer**, °Kyle Q. Hoffmann, Matthew Tirrell and Juan J. de Pablo. "Surface tension of polyelectrolyte coacervates," APS March Meeting, Denver, CO, March 2014.
18. +**Jonathan K. Whitmer** and Juan J. de Pablo. "Molecular simulation of liquid crystal phases and assembly," IME Seminar, Chicago, IL, September 19, 2013.
17. +**Jonathan K. Whitmer**, +Julio C. Armas-Perez, °Abhijeet A. Joshi, °Tyler F. Roberts, and Juan J. de Pablo. "Nanoparticle solubility in liquid crystalline defects,", APS March Meeting, Baltimore, MD, March 2013.
16. °Ming Han, +**Jonathan K. Whitmer** and Erik Luijten. "Clustering of attractive colloids in flow," APS March Meeting, Baltimore, MD, March 2013.
15. +**Jonathan K. Whitmer**, °Daniel M. Hinckley, °Gordon S. Freeman, Juan P. Hernández-Ortiz, D. C. Schwartz and Juan J. de Pablo. "Multiscale computational modeling of DNA," Poster Presentation, Biology of Genomes Meeting, Cold Spring Harbor Laboratory, May 2012.
14. *C. Eck, +**Jonathan K. Whitmer**, °Q. Chen, S. Granick and E. Luijten. "Stability of helical Janus clusters," APS March Meeting, Boston, MA, March 2012.
13. +**Jonathan K. Whitmer**, J. P. Hernández-Ortiz and J. J. de Pablo. "Electrohydrodynamics of DNA in confinement," APS March Meeting, Boston, MA, March 2012.

12. $^{+}$**Jonathan K. Whitmer** and J. J. de Pablo. "DNA Electrohydrodynamics," University of Wisconsin GSTP Seminar, Madison, WI, January 2012.
11. °**Jonathan K. Whitmer**, °Q. Chen, °S. Jiang, S. C. Bae, S. Granick and E. Luijten. "Helical assembly of Janus particles," APS March Meeting, Dallas, TX, March 2011.
10. °M. Bloom, °**Jonathan K. Whitmer** and E. Luijten. "Polymer transport near rough surfaces," APS March Meeting, Dallas, TX, March 2011.
9. °J. Yan, °S. Jiang, °**Jonathan K. Whitmer**, °S. Anthony, E. Luijten and S. Granick. "Glassy dynamics in the rotator phase of two-dimensional Janus crystals," APS March Meeting, Dallas, TX, March 2011.
8. °**Jonathan K. Whitmer** and Erik Luijten. "Orientation dependence of Janus particles in Stokes flow sedimentation," Poster Presentation, CECAM Workshop on Mesoscale Hydrodynamic Methods, Lausanne, Switzerland, July 2010.
7. °**Jonathan K. Whitmer** and Erik Luijten. "Self-assembly of amphiphilic Janus colloids," Soft Materials Seminar, University of Illinois, April 2010.
6. °**Jonathan K. Whitmer** and Erik Luijten. "Clusters of Janus particles in stokes flow," APS March Meeting, Portland, OR, March 2010.
5. °**Jonathan K. Whitmer** and Erik Luijten. "Dynamics of Janus Particles," Poster Presentation, Boulder School for Condensed Matter and Materials Physics, Boulder, CO, July 2009.
4. °**Jonathan K. Whitmer** and Erik Luijten. "Colloids with arbitrary slip boundary conditions," APS March Meeting, Pittsburgh, PA, March 2009.
3. °**Jonathan K. Whitmer** and Erik Luijten. "Sedimentation of aggregating colloidal suspensions," Soft Materials Seminar, University of Illinois, October 2008.
2. °**Jonathan K. Whitmer** and Erik Luijten. "Simulating collective dynamics of confined colloids," APS March Meeting, New Orleans, LA, March 2008.
1. °**Jonathan K. Whitmer** and Erik Luijten. "Hydrodynamic interactions in colloidal matter," Soft Materials Seminar, University of Illinois, February 2008.

Invited Talks

Invited Talks–Notre Dame

12. "Conformations of Weak Polyelectrolytes in Confined Geometries," 2018 AIChE Fall Meeting. Pittsburgh, Pennsylvania, October 2018.
11. "TBD," 30$^{\text{th}}$ International Conference on Science and Technology of Complex Fluids, Universidad Autónoma de San Luis Potosí (Mexico), June 18, 2018.
10. "Modeling the Structure and Properties of Soft Materials," Liquid Crystal Institute, Kent State University, November 8, 2017.
9. "Modeling the Structure and Properties of Soft Materials," Department of Chemical and Biomolecular Engineering, University of Pennsylvania, October 4, 2017.
8. "Thermodynamics of Charging in Weak Polyelectrolyte Materials," 2017 AIChE Fall Meeting. Minneapolis, Minnesota, October 2017.
7. "Toward Molecular Engineering of Liquid Crystal Elasticity," Reunión Anual de la Red Temática de Materia Condensada Blanda. Universidad de Guanajuato (Mexico), August 4, 2017.
6. "Toward Molecular Engineering of Liquid Crystal Elasticity," Gordon Research Conference on Liquid Crystals—Rational Design of Multi-Scale Materials and Their Emerging Applications. University of New England, June 21, 2017.
5. "Designing soft materials with free energy mapping," Midwest Thermodynamics and Statistical Mechanics Conference, Miami University (Ohio), May 25, 2016.

4. "Designing soft materials with free energy mapping," Statistical Physics Seminar, Department of Physics, Universidad Autónoma de San Luis Potosí (Mexico), May 20, 2016.

Invited Talks–Pre-Notre Dame

3. "Probing instability and self-assembly through free-energy mapping," Departments of Materials Science and Chemical Engineering, University of Delaware, February 24, 2014.
2. "Probing instability and self-assembly through free-energy Mapping," Department of Chemical Engineering, University of Illinois at Urbana–Champaign, February 19, 2014.
1. "Probing instability and self-assembly through free-energy Mapping," Department of Chemical and Biological Engineering, University of Notre Dame, February 4, 2014.

Honors and Awards–Notre Dame

- Emerging Investigator in Materials Science, Materials Research Express, 2018.

Funding

Dollar amounts reflect the amount directed to Professor Whitmer's research.

Pending Applications

6. Department of Energy, Basic Energy Sciences. "Molecular Simulations of Interfacial Reactions Informed by Neural-Network Model Chemistries." Co-lead PI. 4 years (January 2019–January 2023), $500,000.
5. Department of Energy, Basic Energy Sciences. "ECRP: Modeling Phase Behavior and Transport in Ionic Liquid Crystals." Principal Investigator. 5 years (August 2018–July 2023), $750,000.

Current Awards

4. National Science Foundation, Division of Materials Research. "CAREER: Targeting Assembly in Colloidal Materials by Tilting the Free Energy Surface" Principal Investigator. 5 years (March 2018–March 2023), $563,176.
3. Notre Dame International. "PODEMOS: Promotion of Discourse through Engineering Materials Opportunities for Students." Principal Investigator. 1 year (July 2017–June 2018), $20,000.
2. Department of Energy, Basic Energy Sciences. "Midwest Integrated Center for Computational Materials (MICCoM)." Co-Principal Investigator. 4 years (October 2015–October 2019), $540,000.

Past Awards

1. National Science Foundation, Division of Chemical, Bioengineering, Environmental and Transport Systems (CBET). "2017 Midwest Thermodynamics and Statistical Mechanics Conference (MTSM)." 1 year (April 2017–March 2018), $12,000.

Honors and Awards

- Postdoctoral
  - DOE INCITE Grant, "Molecular Engineering Through Free Energy Mapping." Argonne Leadership Computing Facility, 60 Million CPU hours, 2014
  - Genomic Sciences Training Program, University of Wisconsin, 2011–2013
- Graduate (University of Illinois)
  - List of Teachers Ranked as Excellent by their Students, 2005–2006, 2011
  - Materials Computation Center Travel Award, 2010
  - Boulder School for Condensed Matter and Materials Physics, 2009
- Undergraduate (Kansas State University)
  - Meritorious Participant, Mathematical Contest in Modeling, 2004–2005
  - Ronald D. Parks Memorial Scholarship in Physics, 2004
  - Barry M. Goldwater Scholarship in Science and Engineering, 2003
  - John P. Giese Scholarship in Physics, 2003
  - Robert C. Byrd Honors Scholarship, 2000–2004
  - Kansas State University Putnam Scholar, 2000-2004
  - Elks National Foundation Scholarship, 2000–2004
  - Dane G. Hansen Foundation Scholarship, 2000–2001

Teaching Experience–Notre Dame

- Fall 2018: CBE 60542, Mathematical Methods in Chemical Engineering (Graduate)
- Spring 2018: CBE 20260, Chemical Engineering Thermodynamics I (Undergraduate)
- Spring 2018: CBE 22260, Chemical Engineering Thermodynamics I Tutorials (Undergraduate)
- Spring 2017: CBE 20260, Chemical Engineering Thermodynamics I (Undergraduate)
- Spring 2017: CBE 22260, Chemical Engineering Thermodynamics I Tutorials (Undergraduate)
- Fall 2016: CBE 60542, Mathematical Methods in Chemical Engineering (Graduate)
- Spring 2016: CBE 20260, Chemical Engineering Thermodynamics I (Undergraduate)
- Spring 2016: CBE 22260, Chemical Engineering Thermodynamics I Tutorials (Undergraduate)
- Fall 2015: CBE 60542, Mathematical Methods in Chemical Engineering (Graduate)
- Spring 2015: CBE 20260, Chemical Engineering Thermodynamics I (Undergraduate)
- Spring 2015: CBE 22260, Chemical Engineering Thermodynamics I Tutorials (Undergraduate)
- Fall 2014: CBE 60542, Mathematical Methods in Chemical Engineering (Graduate)

Teaching Experience–University of Illinois

- Spring 2011: PHYS 213, Thermal Physics (Undergraduate)
- Spring 2011: PHYS 214, Quantum Physics (Undergraduate)
- Spring 2006: PHYS 213, Thermal Physics (Undergraduate)
- Spring 2006: PHYS 214, Quantum Physics (Undergraduate)
- Fall 2005: PHYS 211, Mechanics (Undergraduate)

Undergraduate Students Advised

- Arsenii Panteleev, 2018–
  - 2018 ND Energy Slatt Undergraduate Fellow
- Joseph Sabat, 2017–2018
  - Independent Study Research on Biomolecular Simulations.
- Soren Kyhl, Summer 2017
  - Summer Research on Colloidal and Atomic Clusters
- Nishi Kashyap, Summer 2017
  - 2017 ND*nano* Undergraduate Research Fellow [NURF] from IIT–Delhi.
- Alisha Agrawal, Summer 2017
  - 2017 ND*nano* Undergraduate Research Fellow [NURF] from IIT–Delhi.
- Catherine Drummond, Fall 2016
  - Independent Study Research on Biomolecular Simulations
- Jiahong Shen, Summer 2016
  - 2016 International Summer Undergraduate Research Experience (iSURE) student from Fudan University (Shanghai, China).
- Aristotle Zervoudakis, 2016–2018
  - 2016 ND*nano* Undergraduate Research Fellow [NURF]
  - 2017 ND Energy Slatt Undergraduate Fellow
  - One contributed poster (#42) and contributed to two conference presentations (#52, 59)
  - One published paper (#32)

Graduate Students Advised

- Jiale Shi, 2017–
- Anne Leonhard, 2017–
  - 2017 Notebaert Fellow.
- Michael Quevillon, 2015–
  - Two papers published (#28, 29)
  - Three conference presentations (#55, 58, 62) and two posters (#43, 60)
  - Contributor and tester for SSAGES open-source software project (2015–2017), Team leader and core developer for SSAGES (2018–current).
- Vikramjit Rathee, 2015–
  - Four published papers (#24, 27, 29, 32)
  - Three conference presentations (#31, 52, 63)
  - Three conference posters (#44, 59, 61)
  - Validation tester for SSAGES open-source software project.
  - Contributed to LAMMPS/SAPHRON oepn-source MD/MC interface.
- Hythem Sidky, 2014–
  - CBE Department Best Candidacy Award (2017)

- NSF Graduate Research Fellowship (2016)
- Twelve published papers (#21–23, 25–27, 29–34)
- Delivered or contributed to nineteen conference presentations (#27, 33–35, 37, 38, 40, 46, 48–54, 56, 57, 59, 63)
- Two conference posters (#36, 45)
- Core developer for SAPHRON and SSAGES open-source software projects, team leader for SSAGES project (2016–2017).

Postdocs Advised

- Benjamin Sikora, 2015–2016
  - Two conference presentations (#32, 39)
  - Two published papers (#27, 29), one paper submitted (#32) and one in preparation (#37)
  - Team leader and core developer for the SSAGES open-source software project (2015–2016).

Research Staff

- Dhagash Mehta, 2015–2016
  - Two published papers (#22, 25)
  - Two conference presentations (#34, 37)

Professional Memberships

- American Institute of Chemical Engineers (AIChE)
- American Physical Society (APS)
- International Liquid Crystal Society (ILCS)

Service

- College of Engineering College Council, 2017–
- College of Engineering Computing Committee, 2015–
- Graduate Student Admissions Comittee, Department of Chemical and Biomolecular Engineering, 2015–
- Faculty Recruiting Comittee, "Soft Materials" and "Computation and Theory" Area Searches, Department of Chemical and Biomolecular Engineering, 2015–

Synergistic Activities

- Organizer for PODEMOS collaboration and undergraduate exchange initiative sponsored by Notre Dame International through the Mexico City Global Center, 2017–
- Organized Sessions for APS March Meeting
  1. Free Energy Mapping in Biology and Materials Science (DCOMP/GSOFT, 2017)
- Organized Sessions for the AIChE Annual Meeting
  1. Atomistic and Molecular Modeling and Simulation of Polymers (8A/1A/ComSEF, 2017)
  2. Nanoscale Phenomena in Macromolecular Systems (8A, 2017)
  3. Multiscale and Coarse-Grained Modeling of Polymers (8A/1A/ComSEF, 2016)
- Organized and/or taught short courses in molecular simulation methods:
  1. 2017 MICCoM Summer School

2. 2017 APS GSOFT Short Course
3. 2016 Heidelberg@ND

- Host and Organizer for 2017 Midwest Thermodynamics and Statistical Mechanics Conference.
- Session Chair for AIChE Fall Meeting, 2016–
- Session Chair for APS March Meeting, 2016–
- Everyday Chemistry of Cooking outreach at South Bend Clay High School [Chemistry classes of J. Kindelan and Y. Wolter], 2016–
- Presenter at Science Alive! at the South Bend central Library, 2016–.
- Member of NDEnergy collaborative center 2016–.
- Judge for the Northern Indiana Regional Science and Engineering Fair (NIRSEF), Senior Division, 2015–.
- Judge for AIChE Undergraduate Poster Awards, 2014–
- Organizing committee for Notre Dame Soft Polymer Materials Symposium, 2014–.
- Member of ND*nano* collaborative center 2014–.
- Peer Reviewer (Journals ranked by impact factor [IF]):
  - Nature Communications *[IF: 12.001]*, 2017– (1)
  - Journal of the American Chemical Society *[IF: 13.038]*, 2015– (2)
  - Physical Review Letters *[IF: 7.645]*, 2015– (8)
  - Journal of Chemical Theory and Computation *[IF: 5.301]*, 2016– (1)
  - Langmuir *[IF: 3.993]*, 2016– (1)
  - Soft Matter *[IF: 3.798]*, 2014– (5)
  - The Journal of Physical Chemistry (A, B, & C) *[IF: 2.883, 3.187, 4.509]*, 2014– (6)
  - The Journal of Chemical Physics *[IF: 2.894]*, 2012– (7)
  - Biomicrofluidics *[IF: 2.708]*, 2015– (1)
  - RSC Interface Focus *[IF: 2.590]*, 2014– (1)
  - Physical Review E *[IF: 2.252]*, 2016– (4)
  - Physical Review Materials *[IF: n/a]*, 2017– (2)
  - Molecular Simulation *[IF: 1.254]*, 2017– (1)
  - Journal of Visualized Experiments *[IF: 1.232]*, 2017– (1)
  - European Physical Journal E, 2018– (1)
- Grant Reviewer for ACS PRF, National Science Foundation, Department of Energy.