

Jonathan K. Whitmer

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Education

Ph.D. Physics, University of Illinois, 2011, 3.97 GPA.
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, 4.00 GPA.

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)

Refereed Publications–Notre Dame

22. “Elastic constants of coarse-grained liquid crystal models,” *Invited Article*. Hythem Sidky and **Jonathan K. Whitmer**. *Liquid Crystals*, *in review* (2016).
21. “Elastic response and phase behavior in binary liquid crystal Mixtures,” Hythem Sidky and **Jonathan K. Whitmer**, *Soft Matter* Accepted [DOI 10.1039/C5SM03107A] (2016).
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. *J. Chem. Phys.* **143**, 044101 (2015).

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 Comm.* **6**, 6052 (2015).
18. “Coarse-grained modeling of DNA curvature,” G. S. Freeman, D. M. Hinckley, J. Lequieu, **Jonathan K. Whitmer**, and J. J. de Pablo. *J. Chem. Phys.* **141**, 165103 (2014).
17. “Adsorption of Ions in Nonpolarizable Atomic Models,” **Jonathan K. Whitmer**, A. A. Joshi, and J. J. de Pablo. *J. Chem. Theor. Comput.* **10**, 5616 (2014).
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. *Phys. Rev. Lett.* **113**, 190602 (2014)
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. *Phys. Rev. Lett.* **113**, 168101 (2014).
14. “Interfacial tension of the polyelectrolyte coacervate phases,” J. Qin, D. Priftis, R. Farina, S. Perry, **Jonathan K. Whitmer**, K. Hoffmann, M. Tirrell, and J. J. de Pablo. *ACS Macro Lett.*, **3**, 565 (2014).
13. “Orientationally Glassy Crystals of Janus Spheres,” S. Jiang, J. Yan, **Jonathan K. Whitmer**, S. A. Anthony, E. Luijten, and S. Granick. *Phys. Rev. Lett.*, **112**, 218301 (2014).
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).
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. *Phys. Rev. Lett.*, **111**, 227801 (2013). *Cover Article. Selected as Editor’s Recommendation.*
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. *J. Chem. Phys.* **139**, 144903 (2013). *Cover Article.*
9. “Liquid-Crystal Mediated Nanoparticle Interactions and Gel Formation,” **Jonathan K. Whitmer**, A. A. Joshi, T. F. Roberts, and J. J. de Pablo. *J. Chem. Phys.* **138**, 194903 (2013); **141**, 029901 (2014).
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. *Phys. Rev. E* **87**, 020502(R) (2013). *Selected for February 2013 PRE Kaleidoscope Gallery.*
7. “Isotropic–Nematic Phase Transition in the Lebwohl–Lasher Model,” R. Shekhar, **Jonathan K. Whitmer**, R. Malshe, J. A. Moreno-Razo, T. F. Roberts, and J. J. de Pablo. *J. Chem. Phys.* **136**, 234503 (2012).
6. “Influence of Hydrodynamics on Cluster Formation in Colloid–Polymer Mixtures,” *Invited Article.* **Jonathan K. Whitmer** and E. Luijten. *J. Phys. Chem. B* **115**, 7294–7300 (2011).
5. “Triblock Colloidal Spheres for Directed Self-Assembly,” Q. Chen, E. Diesel, **Jonathan K. Whitmer**, S. C. Bae, E. Luijten, and S. Granick. *J. Am. Chem. Soc.* **133**, 7725–7727 (2011).
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).
3. “Sedimentation of Aggregating Colloids,” **Jonathan K. Whitmer** and E. Luijten. *J. Chem. Phys.* **134**, 034510 (2011).
2. “Fluid–Solid Boundary Conditions for Multiparticle Collision Dynamics,” **Jonathan K. Whitmer** and E. Luijten. *J. Phys.: Cond. Mat.* **22**, 104106 (2010).
1. “Adsorption at the Liquid–Vapor Surface of a Binary Liquid Mixture,” **Jonathan K. Whitmer**, S. B. Kiselev, and B. M. Law. *J. Chem. Phys.* **123**, 204720 (2005).

Other

Contributed Talks and Posters–Notre Dame

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 Phenomena in Binary Liquid Crystal 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. “Helical Conformations of Janus Particles,” APS March Meeting, Boston, MA, March 2012.
13. **Jonathan K. Whitmer**, J. P. Hernández-Ortiz and J. J. de Pablo. “DNA Electrohydrodynamics,” 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. “Hydrodynamics of Janus Particle Clusters,” 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

5. “Soft Materials Design through Free Energy Mapping”, Midwest Thermodynamics and Statistical Mechanics Conference, Miami University (Ohio), May 25, 2016.
4. “Soft Materials Design through 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

Funding

- Department of Energy, Basic Energy Sciences. “Midwest Integrated Center for Computational Materials (MICCoM).” Co-Principal Investigator. 4 years (October 2015–October 2019), \$540,000.

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

- 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

- Aristotle Zervoudakis, 2016–
 - 2016 ND Nano Undergraduate Research Fellow [NURF]

Graduate Students Advised

- Michael Quevillon, 2015–
- Vikramjit Rathee, 2015–
 - One paper in preparation (#25)
 - One contributed talk (#31)
- Hythem Sidky, 2014–
 - NSF Graduate Research Fellowship (2014)
 - One published paper (#21), Two submitted papers (#22, 24), two in preparation (#26, 27)
 - Two contributed talks (#27, 33)

Postdocs Advised

- Benjamin Sikora, 2015–
 - One contributed talk (#32)

Research Staff

- Dhagash Mehta, 2015–
 - One submitted paper (#24), one paper in preparation (#27).

Professional Memberships

- American Society for Engineering Education
- American Institute of Chemical Engineers
- American Physical Society

Service

- College of Engineering Computing Committee, 2015–
- Graduate Student Admissions Committee, Department of Chemical and Biomolecular Engineering, 2015–
- Faculty Recruiting Committee, Soft Materials Area Search, Department of Chemical and Biomolecular Engineering, 2015–

Synergistic Activities

- 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 NDNano collaborative center 2014–.
- Peer Reviewer (Journals Ranked by Google's h5-index):
 - Journal of the American Chemical Society [*h5: 199*], 2015– (1)
 - Physical Review Letters [*h5: 194*], 2015– (3)
 - Langmuir [*h5: 93*], 2016– (1)
 - Soft Matter [*h5: 74*], 2014– (1)
 - Physical Review E *h5: 73*, 2016– (2)
 - The Journal of Chemical Physics [*h5: 71*], 2012– (2)
 - The Journal of Physical Chemistry (A & B) [*h5: 55, 69*], 2014– (2)
 - Biomicrofluidics [*h5: 35*], 2015– (1)
 - RSC Interface Focus [*h5: 27*], 2014– (1)
- Grant Reviewer:
 - American Chemical Society Petroleum Research Fund, 2016– (1)