

James McCarty

Assistant Professor

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Professional Appointments

Aug 2019 - Present Assistant Professor of Computational Biochemistry
Department of Chemistry and Biochemistry
Western Washington University, Bellingham, WA, U.S.A.

March 2017 - July 2019 Postdoctoral Fellow
Department of Chemistry and Biochemistry
University of California Santa Barbara, Santa Barbara, CA, U.S.A.
Advisors: Profs. Joan-Emma Shea and Glenn H. Fredrickson

Feb 2014 - Feb 2017 Postdoctoral Fellow
Department of Chemistry and Applied Biosciences
ETH Zürich, Switzerland
Advisor: Prof. Michele Parrinello

Education

Ph.D., Chemistry, December 2013

University of Oregon, Eugene, OR

Advisor: Prof. Marina Guenza

Doctoral Thesis: *"Multiscale modeling and thermodynamic consistency between soft-particle representations of macromolecular liquids"*

B.S., Biochemistry, March 2007

California Polytechnic State University, San Luis Obispo, CA

Magna cum laude

Research Interests

Molecular dynamics simulation in life and materials science
Statistical mechanics and enhanced sampling of rare events
Protein dynamics, biophysics, soft condensed matter
Computational simulations of polymer field theories
Coarse-graining and liquid state theory

Publications

- S. P. O. Danielsen, J. McCarty, J.-E. Shea, K. T. Delaney, and G. H. Fredrickson, "Small ion effects on self-coacervation phenomena in block polyampholytes," *J. Chem. Phys.*, 151, 000000 (2019); doi: 10.1063/1.5109045
- S. P. O. Danielsen, J. McCarty, J.-E. Shea, K. T. Delaney, and G. H. Fredrickson, "Molecular design of self-coacervation phenomena in block polyampholytes," *Proc. Natl. Acad. Sci. USA*, 116, 8224-8232 (2019)
- J. McCarty, K. T. Delaney, S. P. O. Danielsen, G. H. Fredrickson, and J.-E. Shea, "Complete phase diagram for liquid-liquid phase separation of intrinsically disordered proteins" *J. Phys. Chem. Lett.*, 10, 1644-1652 (2019)
- Y. Lin, J. McCarty, J. N. Rauch, K. T. Delaney, K. S. Kosik, G. H. Fredrickson, J.-E. Shea, and S. Han, "Phase diagram reveals a narrow equilibrium window for the complex coacervation of tau and RNA under cellular conditions," *eLife*, 8:e42571 (2019) [co-first author]
- A. Arsiccio, J. McCarty, R. Pisano, and J.-E. Shea, "The effect of surfactants on surface-induced denaturation of proteins: evidence of an orientation-dependent mechanism," *J. Phys. Chem. B*, 122, 11390 (2018)
- M. G. Guenza, M. Dinpajooh, J. McCarty, and I. Y. Lyubimov, "On the accuracy, transferability, and efficiency of coarse-grained models of molecular liquids," *J. Phys. Chem. B*, 122, 10257 (2018) [selected for ACS Editors' Choice]
- D. Mendels, J. McCarty, P. Piaggi, and M. Parrinello, "Searching for entropically stabilized phases: the case of silver iodide," *J. Phys. Chem. C*, 122, 1786 (2018)
- J. McCarty and M. Parrinello, "A variational conformational dynamics approach to the selection of collective variables in metadynamics," *J. Chem. Phys.*, 147, 204109 (2017).
- G. Piccini, J. McCarty, O. Valsson, and M. Parrinello, "Variational Flooding Study of a S_N2 Reaction," *J. Phys. Chem. Lett.*, 8, 580 (2017).
- J. McCarty, O. Valsson, and M. Parrinello, "Bespoke bias for obtaining free energy differences within variationally enhanced sampling," *J. Chem. Theory Comput.*, 12, 2162 (2016).
- J. McCarty, O. Valsson, P. Tiwary, and M. Parrinello, "Variationally optimized free energy flooding for rate calculation," *Phys. Rev. Lett.*, 115, 070601 (2015).
- D. Ozog, J. McCarty, G. Gossett, A. Malony, and M. Guenza, "Fast equilibration of coarse-grained polymer liquids," *J. Comput. Sci.*, 9, 33 (2015).
- J. McCarty, A. J. Clark, J. Copperman, and M. G. Guenza, "An analytical coarse-graining method which preserves the free energy, structural correlations, and thermodynamic state of polymer melts from the atomistic to the mesoscale," *J. Chem. Phys.*, 140, 204913 (2014).
- A. J. Clark, J. McCarty, and M. G. Guenza, "Effective potentials for representing polymers in melts as chains of interacting soft particles," *J. Chem. Phys.*, 139, 124906 (2013). [co-first author]
- J. McCarty, A. J. Clark, I. Y. Lyubimov, and M. G. Guenza, "Thermodynamic consistency between analytic integral equation theory and coarse-grained molecular dynamics simulations of homopolymer melts," *Macromol.*, 45, 8482 (2012).
- A. J. Clark, J. McCarty, I. Y. Lyubimov, and M. G. Guenza, "Thermodynamic consistency in variable-level coarse-graining of polymeric liquids," *Phys. Rev. Lett.*, 109, 168301 (2012).
- J. McCarty and M. G. Guenza, "Multiscale modeling of binary polymer mixtures: scale bridging in the athermal and thermal regime," *J. Chem. Phys.*, 133, 094904 (2010).

I. Y. Lyubimov, J. McCarty, A. Clark, and M. G. Guenza "Analytical rescaling of polymer dynamics from mesoscale simulations," *J. Chem. Phys.*, 132, 224903 (2010).

J. McCarty, I. Y. Lyubimov, and M. G. Guenza. "Effective soft-core potentials and mesoscopic simulations of binary polymer mixtures," *Macromol.*, 43, 3964-3979 (2010).

J. McCarty, I. Y. Lyubimov, and M. G. Guenza. "Multiscale modeling of coarse-grained macromolecular liquids," *J. Phys. Chem. B.*, 113, 11876-11886 (2009).

Awards

UCSB ScienceLine award in physics/chemistry/engineering for outstanding contribution to promoting science education in K-12 schools, University of California Santa Barbara, 2018

Dow Materials Institute and the Materials Research Laboratory travel award to attend APS national meeting in Los Angeles, CA, March 2018

University of Oregon Travel Award to attend ACS national meeting in Indianapolis, IN, September 2013

NSF Graduate STEM Fellow in K-12 Education (GK-12), University of Oregon, 2012 - 2013

Graduate Science Literacy Program Fellow, University of Oregon, 2012

University of Oregon Travel Award to attend APS national meeting in Boston, MA, March 2012

Fellowship to attend workshop on Multiscale Theory and Simulation at the University of Chicago, Chicago, IL, June 2012

MCC Travel Award to attend First Les Houches School in Computational Physics: Soft Matter, Les Houches School in Computational Physics, France, June 2011

The College of Arts and Sciences Henry V. Howe Scholarship Award, University of Oregon, 2010

Biochemistry student of the year, California Polytechnic State University, 2007

Selected Talks

"Conditions for complex coacervation of the microtubule-associated tau protein predicted from field theoretic simulations," American Physical Society, March Meeting, March 7, 2019, Boston, MA.

"Application of fully-fluctuating field theoretic simulations to study liquid-liquid phase separation in biology," Complex Fluids Design Consortium Annual Meeting, January 29, 2019, Santa Barbara, CA.

"Field-theoretic simulations of discrete Gaussian chain polyelectrolytes as a model for coacervation in intrinsically disordered peptides," American Physical Society, March Meeting, March 5, 2018, Los Angeles, CA.

"Recent Applications of the Variationally Enhanced Sampling Method," MARVEL Junior Retreat, July 19, 2016, Les Diablerets, Switzerland.

"Lessons from Analytical Coarse-graining: Representability, Thermodynamic Consistency, and Long Range Correlations," American Chemical Society National Meeting, September 9, 2013, Indianapolis, IN.

"How Reliable Are Soft Potentials? Ensuring Thermodynamic Consistency Between Hierarchical Models of Polymer Melts," American Physical Society, March Meeting, March 1, 2012, Boston, MA.

"Thermodynamic Consistency in Highly Coarse-Grained Models of Polymer Melts," American Physical Society, Northwest Section Meeting, Saturday, October 22, 2011, Corvallis, OR.

“Effective Pair Potentials and Mesoscale Simulations of Binary Polymer Blends,” American Physical Society, March Meeting, March 15, 2010, Portland, OR.

“A Multiscale Modeling Procedure for Simulations of Polymer Melts,” American Physical Society, Northwest Section Meeting, Friday, May 15, 2009, Vancouver, BC, Canada.

Teaching Experience

Co-Organizer and Instructor - MARVEL School on Variationally Enhanced Sampling, Università della Svizzera italiana (USI), Lugano, Switzerland, February 2017

Teaching Assistant, Computational Chemistry, University of Oregon, Fall 2013

Teaching Assistant, General Chemistry, University of Oregon, Summer 2013

Science Literacy Program Fellow, University of Oregon 2012

- Co-Instructor: Information, Quantum Mechanics, and DNA
For non-science majors, introduction to the physical and chemical principles governing how information is stored and transmitted through DNA. Duties include preparing and presenting lectures, in-class inquiry based activities, holding regular office hours, and assisting in course development.
Program website: <http://scilit.uoregon.edu>

Teaching Assistant, General Chemistry Laboratory, University of Oregon, 2011-2012

Research Mentor for visiting undergraduate student, Crystal Valdez, through the research experience for undergraduates (REU) program, University of Oregon, 6/09-8/09

Research Mentor for undergraduate student, Ha H. Truong, University of Oregon, 2010-2011

Teaching Assistant, Advanced General Chemistry Laboratory, University of Oregon, 2007-2008

Outreach

ScienceLine Scientist, University of California Santa Barbara 2017-2018

- Program that fosters the interest of K-12 students in science education. Students and teachers send science questions to ScienceLine and receive answers from scientists.

Participant in JSU-UCSB Workshop on Gas Phase Spectroscopy and Theoretical Approaches, University of California Santa Barbara, 2018

- Part of an NSF funded JSU-UCSB Partnership For Research and Education in Materials Science grant to foster research collaborations between UCSB and Jackson State University and to establish infrastructure for the education, training and mentoring of minority students

National Science Foundation GK-12 Program Fellow, University of Oregon 2012-2013

- NSF funded program to assist classroom teachers in rural Oregon with science curriculum and inquiry-based learning. Fellowship duties included designing and teaching daily science lessons to K-8 students over a six week sabbatical in rural Oregon.
Additional information: <http://stemcore.uoregon.edu/stem-programs/uo-programs/gk-12-fellows/>