

COMPUTING COLLOQUIUM

THURSDAY, OCTOBER 5

10:30 a.m.

City Center Plaza 259

Aurora Clark

Professor of Chemistry

SCI Fellow

University of Utah



The Topology and Geometry of Soft Matter Interfaces

The simulation and analysis of the time and spatial evolution of soft matter presents unique computational challenges. In the context of analysis, much chemically relevant information is contained in the huge ensemble of atomic configurations, the correlations those configurations may have over large length scales, and their time evolution. Our group has a long history of graph theory applications to chemical systems - from spectral GT descriptors of local and global order, to more recent work employing dynamic community detection. At the same time, we also seek to retain higher-dimensional information and so have recently been employing persistent homology both in static and temporal applications to create new frameworks for interpreting the complex organizational patterns of soft matter systems. Ultimately we desire to unify the geometric and temporal evolution of soft matter with the underlying changes to energy of the system, which will be discussed in the context of sublevelset persistent homology.

Professor Clark joined the Department of Chemistry at the University of Utah in 2022, moving from Washington State University. While at WSU she served as the Director for the Center for Institutional Research Computing, the Interim Director of the WSU-PNNL Institute of Nuclear Science and Technology, and the Director of the Materials Science and Engineering PhD program. Her laboratory uses molecular simulations in high performance computing environments to study chemical processes in extreme and complex chemical environments, with an emphasis upon solution chemistry and liquid interfaces. Her group employs graph theory, computational topology and geometry to extract new information about multiscale and high-dimensional correlations, and she is interested in interpretable and explainable dimensionality reduction problems. Dr. Clark has received several awards for scientific achievement and leadership; in 2017 she was elected a Fellow of the American Chemical Society, in 2019 a Fellow of American Association for the Advancement of Science, and in 2021 the American Physical Society.

 computingphd@boisestate.edu

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 www.boisestate.edu/computing/phd/