

# CMET Seminar

366 Colburn Lab

Monday, January 14, 2019

2:00 p.m.

*"Observing, understanding and engineering solute diffusion in ionic liquids and ionogels"*



## Alexandra Bayles

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Santa Barbara

Dr. Bayles recently completed her PhD in Chemical Engineering at the University of California Santa Barbara. She earned her BChE from the University of Delaware, where she studied the micromechanics of endoskeletal emulsions under the direction of Professor Eric Furst. While working as a graduate student under the direction of Professors Matt Helgeson and Todd Squires, she developed new microscopy tools to better understand and ultimately engineer improved soft materials. Her key contributions included developing a microfluidic interferometry platform to characterize molecular transport in ionic liquids and ionogels, and in advancing a Fourier-based image analysis technique, differential dynamic microscopy, for high-throughput microrheological characterization. In recognition of this work, Alexandra was named as a US Delegate to the 2017 Lindau Nobel Laureate Meeting on Chemistry, a National Science Foundation Graduate Research Fellow, and a CSP Technologies Teacher-Scholar. In February, Alexandra will begin postdoctoral position with Professor Jan Vermant at ETH Zürich.

Ionic liquids (ILs) are poised to replace conventional industrial fluids in a number of separation and reaction processes. In these applications, ILs offer improved solute selectivity, energy efficient recyclability, higher loading capacity, and reduced environmental toxicity in comparison to traditional organic solvents. However, engineering solute mass transport in ILs has been hindered by a lack of methods to observe it *in operando* that would provide better fundamental insight and rational design guidelines for solute-specific IL formulation. As a result, ILs are often selected from a vast design space of ionic components on the basis of their viscosity vis-à-vis the Stokes-Einstein relation, which assumes that solutes experience the IL as a continuum fluid. To overcome these limitations, we developed a new, label-free method, microfluidic Fabry-Perot interferometry ( $\mu$ FPI), to visualize solute diffusion in soft materials *in situ*. Here, we present several technologically-relevant demonstrations of  $\mu$ FPI to develop mechanistic understanding and quantitative models of transport limitations in ILs. In one case, experiments of water sorption into methylimidazolium ILs and ionogels reveal anomalous concentration-dependent solute diffusivities that violate the Stokes-Einstein relation. Instead, we find that water diffusion is accurately modeled by activated hopping between ion pairs. The magnitude of the activation barrier is quantitatively predicted by the strength of IL-solute hydrogen bonding, providing a direct molecular descriptor with which to engineer the diffusion of polar solutes in ILs. In a second example, studies of reactive CO<sub>2</sub> absorption by amine-functionalized ILs provide detailed reaction-diffusion models for the sorption process, and identify material properties that are critical for determining the loading capacity of the IL. Overall, these examples show how  $\mu$ FPI can be used to develop and improve *a priori* diffusion models in complex liquids, help identify molecular interactions that control diffusion, and ultimately enable rational design of task-specific ILs.

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