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Characterization of Self-Assembly Processes in Ionic Liquids MICHAEL MCCUTCHEN, SILVINA MATYSIAK, University of Maryland, College Park — Surfactants are commonly used in a large number of industrial applications because of their remarkable ability to influence the properties of surfaces and interfaces. The spontaneous self-assembly of surfactants into micelles in an aqueous environment has been very well characterized. With the emergence of room-temperature ionic liquids (ILs), there is a clear need to revisit the driving forces behind the aggregation of surfactants in IL. This project aims to obtain a mechanistic description of the self-assembly of anionic surfactants ( $SO_4C_6H_{13}$   $SO_4C_8H_{17}$  and  $SO_4C_{12}H_{25}$ ) in an ionic liquid ([EMIM][EtSO4]). We are exploring the evolution of aggregates with time and the stability of micelle-like aggregates using atomistic simulations. The structural phase behavior is also characterized to explore morphological modifications. In addition, structural properties of the ionic liquid close to the aggregates are evaluated to characterize the link between aggregated structure and changes in the solvent structure.

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