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A Molecular Understanding of the Toxic Interactions of Ionic Liquids Towards a Lipid Biomembrane[1] BRIAN YOO, EDWARD MAGINN, YINGXI ZHU, Univ of Notre Dame — There is a growing urgency to understand the toxicity of ionic liquids (ILs) due to their potential leakage into aquatic environment via aqueous waste streams in many large-scale commercial applications. Better understanding in the molecular interactions of ILs, primarily those in the popular imidazolium-class, with biological systems can serve as a physical foundation for their future design into ecologically benign ones. Here we investigate the toxic interaction of IL aqueous solutions with a supported lipid bilayer as a model cell membrane, using a combined experimental (fluorescence microscopic measurements) and multiscale simulation-based analysis. Both experimental and computer simulation studies have shown that the interactions of ILs with a supported lipid bilayer can lead to the insertion of ILs into the lipid bilayer, causing biomembrane morphological changes into multilayers, fibers, and/or vesicles with a strong dependence on the alkyl side chain length of IL cations. Using atomistic and coarse grained simulations, we have examined the potential of mean force of IL upon approaching a lipid bilayer and resulting changes in the mechanical compliance of lipid bilayer induced by IL interactions. We find that the resulting IL-lipid bilayer complexes can be strongly dependent on the ILs' ability to form cationic micelles.

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