Ionic Liquids at Electrified Interfaces: From Double Layers to Decomposition

Justin B. Haskins, Handan Yildirim, Charles W. Bauschlicher, and John W. Lawson

Ionic liquids are versatile electrolytes whose properties at electrified interfaces have the potential to enable technologies such as supercapacitors and Li-metal battery anodes. At electrified carbon surfaces, ionic liquids form an electric double layer that stores energy and provides the foundation for supercapacitors. At electrified lithium surfaces, ionic liquids decompose to form a solid electrolyte interphase that has the potential to stabilize Li-metal anodes in rechargable batteries. The behavior of two ionic liquids of technological importance, [pyr14][TFSI] and [EMIM][BF4], are examined at these electrified interfaces through molecular dynamics and *ab initio* techniques.