

Room temperatures ionic liquids: computational design of new electrolytes for safer, greener and better lithium ion batteries

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Room Temperature Ionic Liquids (RTILs) have attracted much of the attention of the scientific community in the past decade, mostly due to their novel and highly customizable properties. Being liquid composed solely by ionic species, RTILs generally show negligible vapor pressure, high ionic conductivities and highly tunable solvation properties. Applications of RTILs virtually encompass any field that involves a solvent, ranging from synthetic organic chemistry to solar cells and electrochemistry. In particular, a great attention has been devoted to the possible use of RTILs as safer and greener electrolytes in lithium batteries. To elucidate some of the physical aspects behind transport properties of RTILs, extensive computer simulations have been performed. Diffusivities, viscosities and ionic conductivities of a class of RTILs, as obtained from extensive classical molecular dynamics calculations, are presented over a wide range of temperatures. In particular, as a result of lithium addition, a dramatic structural reorganization is predicted for two of the considered systems, involving the formation of extended percolated networks. The effect of this structural reorganization on lithium transport is analyzed and compared to available experimental results.

Host: Marco Fornari

Cookies and coffee @ 3:30pm in Dow 201.