

Theoretical Chemistry Colloquium

July 24, 2013 (Wed), 16:00-17:00 RCMS, 2nd floor, Chemistry Gallery

Simulating Ionic Liquid Nanostructure with Quantum Chemistry



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Abstract: Ionic liquids (ILs) are a subset of molten salts, distinguished by having melting points below 100 °C. However, while conventional molecular liquids are structurally homogeneous, ILs are nanostructured. This nanostructure potentially makes ILs excellent solvents for lubrication and heat transfer applications. However, these applications first require a detailed understanding of how and why ILs structure themselves at the molecular level. In this talk I review our recent quantum chemical investigations towards the goal of understanding IL nanostructure in isolated IL clusters and bulk ILs.

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