INTERACTIONS OF IONIC LIQUIDS WITH METALS: FRICTION AT SURFACES AND SOLVATION OF NANOPARTICLES

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Abstract:

In this communication we report a study of the interactions between metals and room-temperature ionic liquids. A molecular interaction model was developed to describe as accurately as passible the interactions between the ionic liquid and metallic materials, enabling the molecular simulation of nanoparticles in ionic liquids and also of ionic liquids at surfaces. The intermolecular energy between fragments of the ions and a cluster of metal atoms was calculated using a density functional suitable for non-covalent interaction, and a classical site-site potential function was adjusted to these results. Polarization of the metallic atoms was also included in order to represent the interactions of charged species with a conducting material.

Ionic liquids display a high degree of self-organization and some are suitable as media for generation and stabilization of metallic nanoparticles (NPs). A ruthenium NP solvated in $[C_1C_nIm][NTf_2]$ was simulated using molecular dynamics in order to obtain energetic and structural information. It was demonstrated that the size and the shape of NPs are modulated by the nature of the ILs. However, the stabilization of NPs is a complex issue and the question of precisely how ILs stabilize transition metal NPs remains under debate. Calorimetric and simulation results contribute to an understanding at the molecular level of the stabilization mechanism of RuNPs in 1-alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ionic liquids.

The second objective of this work, within the European Marie Curie Network MINILUBES, is the calculation of thermophysical and tribological properties of new ionic lubricants. By confining the ionic liquid between two metallic surfaces, the ordering and interactions of the lubricant with the surfaces is also investigated. Finally, by introducing shear, friction forces at the solid-liquid interface are calculated. The structure property relation established by these methods help to guide the development of high-performance tribological systems.