

## Interactions of 2D-Layered Materials with Ionic Liquids

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Several aspects of nanoscience and nanotechnology involve the use of liquids in contact with nanomaterials, for example as solvents for the dispersion, preparation and chemical modification of nano-objects, as media for transport through nanopores, or as electrolytes in energy-storage devices. In order to understand and control matter at the nanometer level we have to understand the properties of the fluid media, which do not behave as a simple continuum at these scales, and of the interfaces. We must describe in detail the molecular interactions between the fluids and the nanomaterials, an area where important progress can be made. This presentation will focus on ionic liquids as media to dissolve different kinds of nanoscale objects. Ionic liquids interact through Coulomb and van der Waals forces (including hydrogen bonds), and form organized phases that are heterogeneous at the nanometer scale. Among the nanomaterials of interest are 2D-layered solids in which covalently bonded sheets with thickness of one or a few atoms are held together by van der Waals forces. Examples are functionalized graphene, hexagonal boron nitride or molybdenum disulfide. In these materials the inter-layer forces are of a similar nature as those present in liquids. Some of the challenges these systems pose, mainly to the field of molecular simulation, are: i) the heterogeneous structure of the ionic liquids matches the size of the nano-objects leading to solvation effects that are not present in simple molecular liquids; ii) most often different classes of atomistic model are used to represent the liquid phase and the materials, and so the fluid-solid interactions necessary for molecular simulation studies are not sufficiently well known; iii) the functionalization of the materials drastically changes their interactions and affinity for different solvents; iv) dissolution and exfoliation are phenomena that happen on longer time scales than what is possible to simulate at the atomistic level, nonetheless it is important to describe interactions in detail. The final aim of this study is to improve our understanding of the physical chemistry of systems containing liquids and nanomaterials, enabling the rational design of solvent systems.