MAR07-2006-001528

Abstract for an Invited Paper
for the MAR07 Meeting of
the American Physical Society

Excess Electrons in Water: Clusters, Interfaces, and the Bulk

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The presence of charged species at interfaces plays a central role in a wide range of physical processes. Heterogeneous electron transfer is among the most notable examples with implications in electrochemistry, atmospheric chemistry, heterogeneous catalysis, or from a more general viewpoint, in biological through-space electron transfer reactions. An excess electron in an aqueous environment may be considered as a useful model for studying key energetic, structural and dynamic aspects of these complex phenomena. Excess electrons are known to stabilize in bulk water, as hydrated electrons. Hydrated electron systems with reduced dimensionality, such as negatively charged, finite size water clusters, and excess electrons at aqueous interfaces of infinite size, have also been studied for a while. In the present work we will overview the results of a series of mixed quantum-classical molecular dynamics simulations aimed to examine the physical properties of various aqueous excess electron systems. The investigated systems include finite size water cluster anions, infinite ambient water/air, supercooled water/air, Ih ice/air, amorphous ice/air interfaces, and the fully hydrated electron. The discussion will focus on the critical issue whether the excess electron localizes in interior-bound states completely surrounded by water molecules, or on the water surface (interface) with significant electronic amplitude appearing outside the molecular frame (surface-bound states). Correlations of the excess electron state with the size, internal energy, and the local molecular structure of the environment will be illustrated. We will also demonstrate the dramatic influence of the excess electron state on the observable physical properties. The possible interconnections of the finite size cluster anions, the electrons at the infinite size water/air interfaces, and the three-dimensional, fully hydrated electron are also explored in comparison with available experimental data.