

Ab Initio Molecular Dynamics Study of the Solvation Structure and EPR Spectrum of Fremys Salt in Water-Methanol Solutions

We propose to simulate the local hydrogen bonding network of a dianion that is solvated in a mixture of water and alcohols by means of Car-Parrinello molecular dynamics simulations. We further aim at directly computing the lineshape of the EPR spectrum of this system, by means of an ensemble of ab-initio calculations of the hyperfine coupling tensors for all protons in the solvent. This will allow an unprecedented insight into the local solvation structure of a complex charged molecule in a binary solvent mixture.