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Solvation of the chloride anion in water: ab initio simulations CUI ZHANG, Department of Chemistry, University of California, Davis, DAVIDE DONADIO, Department of Chemistry, University of California, Davis and Max Planck Institute for Polymer Research, 55128 Mainz, Germany, FRANCOIS GYGI, Department of Computer Science, University of California, Davis, GIULIA GALLI, Department of Chemistry, University of California, Davis and Department of Physics, University of California, Davis — We studied the structural, vibrational and electronic properties of the chloride anion in water using ab initio molecular dynamics. Our investigation has three main objectives: understand the range of perturbation exerted by the anion on the water hydrogen bonded network; identify signatures of the anion perturbation in infrared spectra of the solution and study the extent of charge localization on the anion, as predicted by semi-local (PBE) and hybrid functionals (PBE0). In agreement with recent experiments, we find that the presence of the anion substantially affects only the hydrogen bonding in the first solvation shell, due to a decrease of the dipole moment of the first shell water molecules and thus a weakening of the hydrogen bonds. Such a weakening leads to a slightly blue shifted band in the computed IR spectra. While structural and vibrational properties of the solution are similar within PBE and PBE0, the electronic properties exhibit marked differences.

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