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Structural and electronic properties of solvated benzene and hexafluorobenzene from *ab initio* simulations MARKUS ALLESCH, Department of Theoretical and Computational Physics, Graz University of Technology, Austria, and Lawrence Livermore National Laboratory, Livermore, CA, ERIC SCHWEGLER, Lawrence Livermore National Laboratory, Livermore, CA 94550, GIULIA GALLI, Lawrence Livermore National Laboratory, Livermore, CA 94550 and University of California at Davis, Davis, CA 95616 — We have studied the aqueous solvation of benzene and hexafluorobenzene using extensive first principles molecular dynamics simulations. By employing a rigid water approximation [1], we have been able to efficiently address long time-scale simulations (∼100 ps) within a first-principles context. Our analysis of radial, spatial and tilt angle distribution functions of first shell water molecules reveals structural details in the axial and equatorial regions of the solute. In particular, we have identified strong orientational ordering near the faces of the rings and cage-like spacial structures in the equatorial regions. The structural properties of the first solvation shell lead to subtle changes in the electronic structure of water, e.g. changes in dipole moments. [1] M. Allesch, et al. J. Chem. Phys. 120, 5192 (2004) This work was performed under the auspices of the U.S. Dept. of Energy at the University of California/Lawrence Livermore National Laboratory under contract no. W-7405-Eng-48.

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