MAR05-2004-005160

Abstract for an Invited Paper
for the MAR05 Meeting of
the American Physical Society

Structural and dynamical properties of water under ambient and high-pressure conditions

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The structural and dynamical properties of water are investigated with *ab initio* molecular dynamics. A series of density functional theory based simulations is presented where the effect of temperature at ambient density is explored in order to demonstrate the level of accuracy that can be achieved, and the open challenges that remain in describing liquid water [1,2]. In addition to water at ambient density, the effect of high-pressures, in a regime where molecular dissociation plays a dominant role, is explored for both liquid water and the high-pressure phases of ice. In particular, large-scale two phase simulations of water are used to determine the melting temperature of water in the range of 10 to 50 GPa [3]. This work was performed under the auspices of the US Department of Energy by the University of California at the LLNL under contract no W-7405-Eng-48. * In collaboration with Jeffery C. Grossman, François Gygi and Giulia Galli. [1] "Towards an assessment of the accuracy of density functional theory for first principles simulations of water", J. Grossman, E. Schwegler, E. Draeger, F. Gygi and G. Galli, *J. Chem. Phys.* **120**, 300 (2004); and "Towards an assessment of the accuracy of density functional theory for first principles simulations of water II", E. Schwegler, J. Grossman, F. Gygi and G. Galli, *J. Chem. Phys.* **121**, 5400 (2004). [2] "First principles simulations of rigid water", M. Allesch, E. Schwegler, F. Gygi and G.Galli, *J. Chem. Phys.* **120**, 5192 (2004). [3] "Dissociation of water under pressure",E. Schwegler, G. Galli, F. Gygi, and R. Hood, *Phys. Rev. Lett.* **87,** 265501 (2001); and E. Schwegler, F. Gygi and G. Galli (manuscript in preparation).