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Ab-initio parametrization of a fully polarizable and dissociable force field for water[1] C. PINILLA, A. IRANI, N. SERIANI, S. SCANDOLO, The Abdus Salam International Centre for Theoretical Physics Trieste, 34151, Italy — A novel all-atom, dissociative, and polarizable force field for water is presented. The force field is parameterized based on forces, stresses and energies obtained form ab-initio calculations of liquid water at ambient conditions. The accuracy of the force field is tested by calculating structural and dynamical properties of liquid water and the energetics of small water clusters. The transferability of the force field to dissociated states is studied by considering the solvation a proton and the ionization of water at extreme conditions of pressure and temperature. In the case of the solvated proton the force field properly describes the presence of both Eigen and Zundel configurations. In the case of the pressure-induced ice VIII / ice X transition and the temperature-induced transition to a superionic phase, the force field is found to describe accurately the proton symmetrization and the melting of the proton sublattice,

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