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Connexions between density and dielectric properties of water¹ LUANA PEDROZA, DANIEL ELTON, MARIVI FERNANDEZ-SERRA, Stony Brook University — As it is well known, water has a high dielectric constant, which is connected both to the molecular dipole moment and to the intermolecular bonding through hydrogen bonds. Although some classical force fields can reproduce this dielectric constant, they do not take into account the environment-dependent perturbations of the individual dipoles and their relation to the local structure and network of the liquid. In this work, we investigate in detail the distribution of molecular dipoles for different densities of liquid water, obtained with ab initio molecular dynamics simulations and compare them to those obtained using a classical, polarizable, empirical force field. We calculate the dipole moment for different choices of exchange-correlation functionals, including van der Waals correction. In addition, we analyze the correlation between the dipolar coupling and the vibrational spectrum of water. In this way, we can get a better understanding on how local electronic effects play a role in the determination of global properties of water, such as its dielectric constant and density

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Luana Pedroza Stony Brook University

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