Investigating the effect of dipole moment on structural and transport properties in liquid water: The NCC(Q) model

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Equilibrium molecular dynamic simulations are carried out to compute structural properties, while within the Green-Kubo formalism single and collective transport coefficients, such as self-diffusion, shear and bulk viscosities, are also determined. In order to investigate the role of the electrostatic contribution and improve previous results from semi-empirical models [1, 2], we employed reparameterized versions of the *ab initio* NCC water potential [3]. We considered dipole moment values previously employed in several commonly used empirical water models, by appropriately modifying the point charges of the H-atom and M-site of the NCC model. A detailed analysis and discussion is presented at various temperatures between 273 and 373 K, along with some guidelines for the proper parametrization of water models in order to predict accurately such properties. We found that the predictions of the NCC(Q), are in much better agreement with the experiment than its predecessor [3]. By analyzing radial distribution functions we show that the repulsive part of the potential needs to be adjusted. Also one can see that the self-diffusion results follow similar trends with the ones for the viscosity (see figure 1), thus we propose the inclusion of the self-diffusion coefficient as a target property in the developing water models.

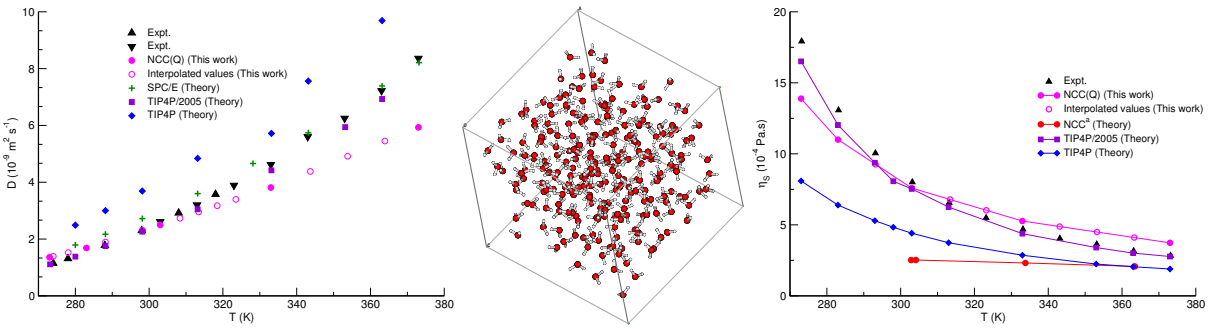

Figure 1: Self-diffusion coefficients and shear viscosity values for the indicated water models.

References

[1] J.S. Medina, *et al.*, Chem. Phys. **388**, 9 (2011)

[2] G.S. Fanourgakis, *et al.*, J. Phys. Chem. A **116**, 2564 (2012)

[3] D.J. Arismendi-Arrieta, *et al.*, http://dx.doi.org/10.1016/j.apradiso.2013.01.020 (2013)