A polarizable coarse-grained water model for dissipative particle dynamics

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ABSTRACT

In this talk we present a polarizable water model for the Dissipative Particle Dynamics (DPD) method. Our model is based on long-range electrostatics and Drude oscillators, and we calibrate the model using the compressibility and the dielectric constant of water. We then show the validation process by sampling the dielectric properties of solutions of sodium chloride at various concentrations. Additionally, we present the applicability of our model in equilibrium and electroporation simulations of a pure DPPC bilayer, a pure cholesterol domain and a mixed DPPC-cholesterol membrane in polarisable water. Finally, we present the simulation of transport of a short DNA segment through a DPPC bilayer driven by an external electric field. We conclude that our new water model is suitable for the DPD simulations of systems where polarization effects play an essential role.

REFERENCES

[1] E. K. Peter, I. V. Pivkin, *A polarizable coarse-grained water model for dissipative particle dynamics* J. Chem. Phys., Vol.141, 164506, (2014).