An electronically coarse grained model describes water's properties from ice to the supercritical regime

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Recently, a new atomistic simulation method has been introduced, the quantum Drude oscillator model (QDO), which coarse-grains the electronic structure of a complex chemical system into a set of distributed quantum oscillators [1-5]. The model thereby contains, within Gaussian Statistics, all long-range force diagrams – many-body polarization and dispersion beyond the dipole approximation as well as cross interactions – leading to high transferability across many different chemical environments. That is all collective fluctuations in the N-body problem giving rise to long-range interactions are included. This responsiveness means the model can be parameterized to single molecule and dimer properties only, permitting the properties of condensed phase systems to naturally emerge as predictions. An efficient linear scale path integral method provides a strong coupling solution, keeping all diagrams and collective fluctuations allows the method to be applied to simulate large scale condensed systems such as water [4-5] with low overhead compared to standard atomistic models while including all long force diagrams.

In this lecture, the QDO model is described and its predictions of water's properties from the super- cooled regime to ice to the gas-liquid coexistence to the super critical regime including an outstanding prediction of critical point and temperature of maximum density, presented [5,6,7]. Given the model's success, the physics underlying the model is then compared in more detail to other descriptions including dipole polarizable models, fixed point charge models, and the classical Drude model, and the reasons for the outstanding predictions of the QDO treatment discussed in a form a suitable for the general audience.

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4. "Electronically coarse-grained model for water," G.J. Martyna et al., *Phys. Rev. Lett.* **110** 227801 (2013).
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6. "Molecular-Scale Remnants of the Liquid-Gas Transition in Supercritical Polar Fluids", G.J. Martyna et al., *Phys. Rev. Lett.* **115**, 117801 (2015).
7. "Predictions of water's properties in the supercooled regime by an electronically coarse grained model", in preparation.