New First Principles Based Water Model Predicts Liquid Water Anomalies in the Supercooled Regime in Good Agreement with Experiments

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A revised version of the Water potential from Adaptive force matching for Ice and Liquid (WAIL) was developed with improved description of dispersion based on Symmetry Adapted Perturbation Theory (SAPT). The model has no adjustable parameters and relies solely on fitting first principles information. The new model, named revised WAIL (rWAIL), shows improved predictions of the properties of water when compared to the previously published WAIL model. The rWAIL model is used to study the properties of supercooled water. The rWAIL model shows evidence of a liquid-liquid phase transition (LLPT) in the supercooled regimes with the liquid-liquid critical point (LLCP) at 203 K and 90 MPa. This estimate is in good agreement with a recent polynomial fit to the experimental density of water. Also, the fit to the surface tension of supercooled water based on the rWAIL model shows excellent agreement with the corresponding fit to experimental data. The fit to the surface tension reveals an exponential growth in the supercooled regime that is likely a result of the emergence of a low-density liquid form of water. The simulation thus unites two separate experimental fits with one first-principle based model lending strong evidence of a LLPT in real water.