Supporting Information:

Why is MP2-Water “Cooler” and “Denser” than DFT-Water?

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Figure S1: Potential energy curves of a water dimer ($C_s$ symmetry) as a function of the oxygen-oxygen distance calculated by MP2, SCS-MP2, and Cp-MP2 theories with the aug-cc-pVDZ basis set. Cp-MP2 indicates MP2 with a function counterpoise correction for the BSSE.
Figure S2: Distributions of molecular dipole moments in liquid water calculated with MD using forces from modified TTM-3F with three different values of polarizability scale factor \((E)\). The maximum peak of the dipole distribution with \(E = 0.8\), 1.0, and 1.2 is located at 2.52, 2.76, and 2.92 Debye, respectively.

Figure S3: Oxygen-oxygen RDFs of liquid water with \(\rho = 1\) g/cm\(^3\) at \(T = 300\) K calculated with MD using forces from modified TIP4/2005 with three different values of dispersion scale factor \((D)\). The values in parentheses are the average pressure.
Figure S4: Oxygen-oxygen RDFs of liquid water with $\rho = 1 \text{g/cm}^3$ at $T = 300 \text{K}$ calculated with MD using forces from modified Dang-Chang with three different values of dispersion scale factor ($D$). The values in parentheses are the average pressure.

Figure S5: Oxygen-oxygen RDFs of liquid water with $\rho = 1 \text{g/cm}^3$ at $T = 300 \text{K}$ calculated with MD using forces from modified Dang-Chang with three different values of polarizability scale factor ($E$). The values in parentheses are the average pressure.