Simulating Phase Equilibria of Water from First Principles

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A series of first-principles Monte Carlo simulations in the Gibbs ensemble were carried out to examine the vapor-liquid coexistence properties of water. Studies were performed using the Becke-Lee-Yang-Parr (BLYP) and Perdew-Burke-Ernzerhof (PBE) exchange/correlation density functionals. The results show boiling and critical temperatures that are lower than experiment for the BLYP functional and higher than experiment for the PBE functional. The temperature dependence of the hydrogen bonded networks and dipole moment distributions are also examined.