419d First Principles Monte Carlo Simulations of Water and Hydrogen Fluoride

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This presentation will describe recent efforts aimed at developing an efficient Monte Carlo program for first principles (based on density functional theory) simulations in the canonical, isobaric-isothermal, and Gibbs ensembles. To this extent, configurational-bias and aggregation-volume-bias Monte Carlo techniques and pre-sampling using an approximate potential are combined with the Quickstep energy routine of the electronic structure program CP2K. The results of first principles Monte Carlo simulations for the vapor-liquid coexistence curve of water and the aggregation of hydrogen fluoride in its superheated vapor phase will be presented.