QUANTUM SOLVATION: PATH INTEGRAL MONTE CARLO CALCULATIONS OF THE H_2-HF AND D_2-HF BINARY COMPLEXES IN LIQUID HELIUM DROPLETS

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Path Integral Monte Carlo (PIMC) simulations were performed for the H_2-HF complex in helium droplets. These simulations are based on the quantum-classical isomorphism[a,b] and correctly incorporate quantum effects at the temperature of the droplets (0.37K). For comparison, simulations of the D_2-HF complex in helium droplets were also performed in order to compare the effects of the quantum helium solvent on the heavier D_2 molecule. Interpretations of the experimental results (from the preceeding talk) based on these simulations will be discussed.

[a] D. M. Ceperley, *Rev. Mod. Phys.* **67**, 279 [1995]
[b] D. Chandler, P. G. Wolynes, *J. Chem. Phys.* **74**, 4078 [1981]