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 preceding talk) based on these simulations will be discussed.

$^a$D. M. Ceperley, Rev. Mod. Phys. 67, 279 [1995]