QUANTUM MONTE CARLO STUDIES OF DOPED SOLID PARAHYDROGEN: STRUCTURE AND IR ABSORPTION SPECTRA

R. J. HINDE, *Department of Chemistry, University of Tennessee, Knoxville, TN 37996*.

The infrared absorption spectrum of atom- and molecule-doped solid parahydrogen (p-H_2) exhibits features near 4160 cm^{-1} which are absent from the spectrum of pure solid p-H_2. These absorption features are associated with the $Q_1(0)$ pure vibrational transitions of H_2 molecules located near impurities; the transition moment responsible for this infrared activity arises from weak overlap-induced dopant–H_2 and H_2–H_2 dipoles, and from dopant-induced symmetry breaking of the p-H_2 crystal lattice. Because the transition dipole moment for these infrared features depends sensitively on the structure of the p-H_2 matrix surrounding the dopant, studies of the $Q_1(0)$ absorption feature could provide detailed information about the physics of solvation in highly quantum systems. We present the results of diffusion quantum Monte Carlo (DQMC) simulations of the $Q_1(0)$ absorption lineshape for isolated dopants in solid p-H_2, and briefly discuss the structural and dynamical information provided by our DQMC simulations.