MIXED CLUSTERS OF H_2 AND H_2O: INSIGHTS FROM THEORY AND SIMULATIONS

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Water-hydrogen clusters are of considerable interest for both fundamental and practical reasons; in particular, a better understanding of their nature has implications in astrophysics and in the field of hydrogen storage. The present research investigates the quantum dynamics of water-hydrogen clusters based on a new interaction potential, exact bound-state calculations, and Feynman Path Integral simulations. We first discuss the development of a reduced-dimension effective potential for the water-hydrogen interaction. The quality of this potential is assessed by comparing the results of exact dimer and trimer bound-state calculations performed using the full-dimension and reduced-dimension surfaces both with each other and with experimental rovibrational spectra. We then perform Path Integral Monte Carlo and Path Integral Molecular Dynamics simulations of larger clusters using this newly developed effective potential, focusing on the quantum delocalization effects of *para*-hydrogen and its superfluidity in the presence of water as the size of the hydrogen clusters grow. Spectroscopic observables will be computed and compared to available experiments. This work is a prelude to an exploration of the possible impact of these quantum effects on the behaviour of nano-scale water clathrates.