MOLECULAR DYNAMICS SIMULATIONS ON VARIOUS WEAKLY BOUND WATER-PARAHYDROGEN SYSTEMS AT ULTRACOLD TEMPERATURE

MATTHEW SCHMIDT, *Department of Chemistry, University of Waterloo, Waterloo, ON, Canada, N2L 3G1*; CHRISTOPHER ING, *Department of Biochemistry, University of Toronto, 27 King's College Circle, Toronto, Ontario, Canada M5S 1A1*; STEPHEN CONSTABLE, TAO ZENG, JING YANG, MICHAEL NYMAN and PIERRE-NICHOLAS ROY, *Department of Chemistry, University of Waterloo, Waterloo, ON, Canada, N2L 3G1*.

We report path integral molecular dynamics (PIMD) studies on the low temperature properties of weakly bound clusters. We use a new version of the molecular modeling toolkit (MMTK) with an implementation of the Path Integral Langevin Equation (PILE) thermostat. We focus on the low temperature dynamics of parahydrogen clusters with a non-rotating water dopant molecule. We also extend our study to the reverse case where hydrogen is doped in a water cluster. The low temperature properties of parahydrogen clusters within water clathrates are explored. These systems are of great interest in the context of hydrogen storage. We compare our PIMD results to those of more traditional path integral Monte Carlo (PIMC) methods. We also report on an extension of the PIMD approach to zero temperature using the so-called Path Integral Ground State (PIGS) approach. The technique is analogous to diffusion Monte Carlo (DMC) but with important differences that will be presented. We discuss the merits of various trial functions and the PIGS results are benchmarked using exact calculations for small clusters.