Quantum molecular dynamics study of ground state properties of parahydrogen clusters and their bosonic isotopologues

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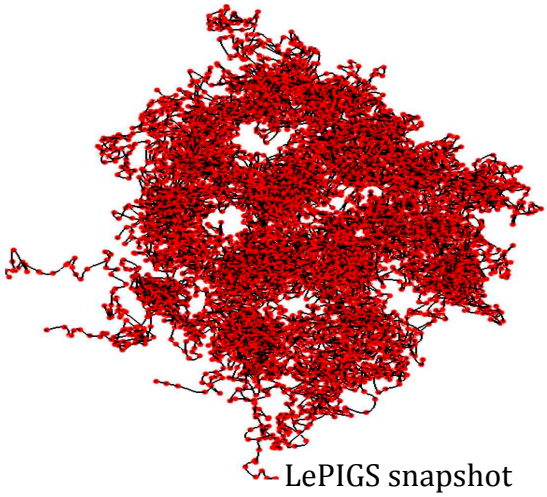
We examine properties of parahydrogen clusters and their bosonic isotopologues (orthodeuterium and paratritium) in the zero temperature limit using a quantum molecular dynamics method known as the Langevin equation Path Integral Ground State (LePIGS) [1,2]. We examine cluster sizes in the range of N=4 - 40. A number of questions of interest include the quantification of the "liquid-like" or "solid-like" nature of parahydrogen clusters and the correct shape of the chemical potential. We compare our results to DMC [3] and PIGS-MC (a Monte Carlo version of PIGS) [4], which give conflicting results.

We also construct an accurate 1D pair potential for each isotopologue in the ground vibrational state using a 6D potential from Hinde [5]. We perform LePIGS simulations and calculate, using perturbation theory [6], the vibrational frequency shift of parahydrogen clusters from N=4-40 and for orthodeuterium and paratritium from N= 4-10 [7]. We compare our results to those calculated using other potential energy surfaces in our simulations and also to experiment. By accurately calculating vibrational frequency shifts, we may be able to assist experimentalists in correct assignment of cluster sizes.



LePIGS snapshot of N=33 paratritium cluster

Future work involves calculating the dissociation energy of the water dimer and extending this work to hydrogen clusters in hydrate clathrates.

References:

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