

## SIMULATION STUDIES OF THE VIBRATIONAL DYNAMICS OF *para*-HYDROGEN CLUSTERS

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This paper discusses the construction and application of reduced-dimensional potential energy surfaces for use in performing simulation of para-hydrogen clusters. Simple spherical averaging and ‘adiabatic-hindered-rotor’ averaging<sup>a</sup> treatments of the angular degrees of freedom are considered and compared. The resulting one-dimensional surface is used in quantum Monte Carlo simulations of para-hydrogen clusters of varying sizes. Energetic, and structural properties are computed and compared to previously published results, and vibrational frequency shifts are predicted and compared to available experimental measurements.

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<sup>a</sup> H. Li, P.N. Roy and R.J. Le Roy, *J. Chem. Phys.* **133**, 104305 (2010).