A NEW EQUATION OF STATE FOR SOLID para-HYDROGEN

LECHENG WANG, ROBERT J. LE ROY, PIERRE-NICHOLAS ROY, Centre for Graduate Work in Chemistry and Biochemistry, University of Waterloo, Waterloo, Ontario, Canada.

Solid para-H$_2$ is a popular accommodating host for impurity spectroscopy due to its unique softness and the spherical symmetry of para-H$_2$ in its J=0 rotational level.$^{a,b}$ To simulate the properties of impurity-doped solid para-H$_2$, a reliable model for the ‘soft’ pure solid para-H$_2$ at different pressures is highly desirable. While a couple of experimental$^c$ and theoretical$^d$ studies aimed at elucidating the equation of state (EOS) of solid para-H$_2$ have been reported, the calculated EOS was shown to be heavily dependent on the potential energy surface (PES) between two para-H$_2$ that was used in the simulations.$^e$ The current study also demonstrates that different choices of the parameters governing the Quantum Monte Carlo simulation could produce different EOS curves.

To obtain a reliable model for pure solid para-H$_2$, we used a new 1-D para-H$_2$ PES reported by Faruk et al.$^f$ that was obtained by averaging over Hinde’s highly accurate 6-D H$_2$–H$_2$ PES.$^g$ The EOS of pure solid para-H$_2$ was calculated using the PIMC algorithm with periodic boundary conditions (PBC). To precisely determine the equilibrium density of solid para-H$_2$, both the value of the PIMC time step $\tau$ and the number of particles in the PBC cell were extrapolated to convergence. The resulting EOS agreed well with experimental observations, and the hcp structured solid para-H$_2$ was found to be more stable than the fcc one at 4.2K, in agreement with experiment. The vibrational frequency shift of para-H$_2$ as a function of the density of the pure solid was also calculated, and the value of the shift at the equilibrium density is found to agree well with experiment.

$^c$ I. F. Silvera, Rev. Mod. Phys. 52, 393(1980).