# Quantum effects in the bulk modulus of solid molecular hydrogen


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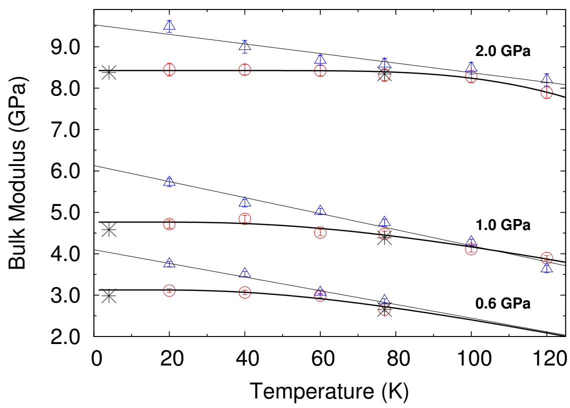
We study the quantum effects on the mechanical and thermodynamic properties of molecular hydrogen solid using path integral Monte Carlo (PIMC) in the isothermal-isobaric ensemble at pressure varying between 0.6 up to 2.0 GPa. The PIMC is quite advantageous than other quantum methods because it is able to provide properties of a quantum system at finite temperature without the need for expertise of the system wave function.

We found that due to anharmonicity the kinetic energy ($K$) is larger than the vibrational potential energy ($U_{vib}$), the ratio $K/U_{vib}$ decreases for rising pressure. The harmonic limit is reached at higher pressures. The root-mean-square displacement ($\Delta r$) as a function of pressure decreases as the pressure is raised. The rate of decreasing is lower for lower temperatures. At T= 20 K the impact of the quantum effects on $\Delta r$ varies from 56% up to 64% in the range of pressure studied. An increases in about four times the temperature decreases the quantum effect contribution in roughly one third. The zero-point lattice vibration increases with increasing of the system pressure. At P= 2.2 GPa the radius of gyration of the paths gives larger contribution for $\Delta r$. The enhancement of the quantum delocalization of the molecules in the solid at high pressures is consistent with the increases of the total quantum vibrational energy.

In the figure we show the bulk modulus of the solid molecular hydrogen for different temperatures at three pressure values. The red circles are PIMC values, the blue triangles are for classical Monte Carlo (MC) values, and the black stars are the experimental values. The lines serve as a guide for the eye only. The agreement between PIMC and experimental values is quite satisfactory. The PIMC and MC get apart from each other due to quantum effects at about T=100 K. As expected, a decrease in temperature leads to an increase in quantum effects whereas a slighlty increasing in pressure causes also slightly increasing in quantum effects of the bulk modulus. As the temperature approaches to zero the slope of the PIMC curves tends to zero in agreement to the requires of the third law of thermodynamic for temperature dependent elastic constants.





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