Path-integral simulation of solid hydrogen under high pressure

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Solid hydrogen, an important constituent of some planets, has been attracting not only geophysicists but also physicists working on condensed matter physics for more than six decades. Recent high-pressure studies revealed three relevant phases of solid molecular hydrogen: phase I (high-temperature, low-pressure phase), phase II (low-temperature phase), and phase III (high-pressure phase). Spectroscopic data suggest that symmetry breakings occur on passage into phases II and III, which may be related to orientational orderings of the molecules. The phase boundaries dividing the three phases exhibit strong isotope effect, indicating that quantum effect of hydrogen nuclei is important.[1)]

Here we repoprt on quantum distributions of protons in the three phases obtained by the first-principles path integral molecular dynamics (FP-PIMD) method, in which interatomic forces are calculated precisely based on the density functionaly theory.[2)] The distributions have entirely different symmetries from those predicted by conventional simulation which treat protons classically.[3)]

References

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