Dense Hydrogen by First-Principles Path-Integral Molecular Dynamics: Structure of Phase II, Melting Curve, and Beyond

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The role of quantum nuclear zero-point motion in the structural changes of solids H_2 and D_2 under pressure is investigated for the low-temperature phases and around the melting curve by first-principles path-integral molecular dynamics (PIMD) calculations [1].

A radical revision of the current interpretation of the nature of phase II is presented. An isotope difference for the structure of phase II is discovered. Phase II of solid D_2 is identical to the classical counterpart ($C2/c$ space group). Phase II of solid H_2, exhibits large and very asymmetric angular quantum fluctuations. The quantum-mechanically averaged structure (close to $Cmcm$), is different from the most probable one ($Cmc2_1$). That fits the concept of "quantum fluxional solid", which cannot be understood in terms of a single classical structure. The mechanism of the transition into phase III is also obtained. Existing structural data support this microscopic interpretation.

The effect of quantum fluctuations of nuclei on the melting curve and the Plasma Phase Transition is also investigated. We have used the ABINIT code [2], in which we have implemented the path-integral formalism for nuclei. For the sake of numerical efficiency, we have introduced in ABINIT, beyond the already existing levels of parallelization, an additional level of parallelization on the system replicas associated to the discretization of the PI in imaginary time. This level of parallelization has a quasi-linear scalability and, combined to the others, allowed us to perform, by using several thousands of CPU cores, very long DFT-PIMD trajectories of at least 30 000 steps, and up to 100 000 steps in some cases where a high level of statistics was required.

[1] G. Geneste, M. Torrent, F. Bottin, and P. Loubeyre, http://arxiv.org/abs/1205.2290.

[2] X. Gonze *et al.*, Computer Phys. Comm. **180**, 2582 (2009).

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