On the Molecular Dissociation of Dense Hydrogen and the Solid/Liquid Transition in the Atomic Phase via Free-energy Calculations

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In 1935, Wigner and Huntington predicted that sufficient pressure would cause hydrogen to become atomic and metallic. Since then, theoretical predictions have suggested that the atomic phase will exhibit remarkable properties, perhaps most notably possible quantum melting at low- or zero- temperature. Simulations to support these predictions, however, are extremely challenging, as they must consider numerous complex effects that could drive such a transition, including nuclear quantum effects and entropic (de-)stabilization at finite temperature. In this talk, accelerated path-integral molecular dynamics simulations of the solid and liquid atomic phases are performed at pressures near molecular dissociation to the ultrahigh regime. Coupling-constant integrations at finite temperature are performed to estimate the entropies of the two phases at reference points, and thermodynamic integrations are used to determine the Gibbs free-energies over a wide range of pressure and temperature conditions. From these results, we construct the phase diagram of dense hydrogen, from molecular dissociation to ultrahigh pressures.

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