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The phase diagram of solid hydrogen at high pressure: A challenge for first principles calculations[1] SAM AZADI, MATTHEW FOULKES , Imperial College London — We present comprehensive results for the high-pressure phase diagram of solid hydrogen. We focus on the energetically most favorable molecular and atomic crystal structures. To obtain the ground-state static enthalpy and phase diagram, we use semi-local and hybrid density functional theory (DFT) as well as diffusion quantum Monte Carlo (DMC) methods. The closure of the band gap with increasing pressure is investigated utilizing quasi-particle many-body calculations within the GW approximation. The dynamical phase diagram is calculated by adding proton zero-point energies (ZPE) to static enthalpies. Density functional perturbation theory is employed to calculate the proton ZPE and the infra-red and Raman spectra. Our results clearly demonstrate the failure of DFT-based methods to provide an accurate static phase diagram, especially when comparing insulating and metallic phases. Our dynamical phase diagram obtained using fully many-body DMC calculations shows that the molecular-to-atomic phase transition happens at the experimentally accessible pressure of 374 GPa. We claim that going beyond mean-field schemes to obtain derivatives of the total energy and optimize crystal structures at the many-body level is crucial.

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