Abstract Submitted
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Towards a Predictive First-Principles Description of High Pressure Hydrogen with Density Functional Theory[1] MIGUEL A. MORALES, LLNL, JEFFREY M. MCMAHON, UIUC, CARLO PIERLEONI, Univ. of L'Aquila, DAVID M. CEPERLEY, UIUC — We present a study of the influence of the main approximations employed in first-principles descriptions of high pressure hydrogen with Density Functional Theory. We focus on the importance of nuclear quantum effects (NQE) on equilibrium properties of both liquid and solid molecular hydrogen close to dissociation. We find that NQEs strongly influence intramolecular properties, such as bond stability, and are thus an essential part of the dissociation process. In addition, we show how the combination of both thermal and quantum effects make a drastic change to the predicted optical properties of the molecular solid, demonstrating the very limited value of predictions based on classical ions and static crystals. We also focus on the influence of the chosen exchange–correlation density functional on the predicted properties of hydrogen, including the location of the Liquid-Liquid Phase Transition and the pressure dependence of the band gap in the solid.

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