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High-Pressure Hydrogen from First-Principles[1]

MIGUEL A. MORALES, LLNL

The main approximations typically employed in first-principles simulations of high-pressure hydrogen are the neglect of nuclear quantum effects (NQE) and the approximate treatment of electronic exchange and correlation, typically through a density functional theory (DFT) formulation. In this talk I'll present a detailed analysis of the influence of these approximations on the phase diagram of high-pressure hydrogen, with the goal of identifying the predictive capabilities of current methods and, at the same time, making accurate predictions in this important regime. We use a path integral formulation combined with density functional theory, which allows us to incorporate NQEs in a direct and controllable way. In addition, we use state-of-the-art quantum Monte Carlo calculations to benchmark the accuracy of more approximate mean-field electronic structure calculations based on DFT, and we use GW and hybrid DFT to calculate the optical properties of the solid and liquid phases near metallization. We present accurate predictions of the metal-insulator transition on the solid, including structural and optical properties of the molecular phase.

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