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Phase-diagram of high-pressure hydrogen by combining quantum Monte Carlo with quantum nuclear effects

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We computed the state-of-the-art theoretical phase-diagram of hydrogen and deuterium at low temperatures and high pressures (P > 300 GPa), correctly accounting for exact electronic correlations, nuclear quantum effects, and anharmonicity. We combined quantum Monte Carlo techniques to compute accurate internal energies with stochastic self-consistent harmonic approximation to include quantum nuclear effects. Our results push the transition to the atomic state to higher pressures than the ones predicted by previous calculations, suggesting that the observation of the superconductive state below 500 GPa is highly unlikely.