Abstract Submitted
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**Non-Born-Oppenheimer diffusion Monte Carlo calculations of solid molecular and atomic hydrogen**[1] YUBO YANG, University of Illinois Urbana-Champaign, NORM TUBMAN, University of California Berkeley, DAVID CEPERLEY, University of Illinois Urbana-Champaign — We present dynamic-lattice (non-Born-Oppenheimer) diffusion Monte Carlo (DMC) calculations on zero-temperature candidate structures of solid hydrogen at several pressures from 200 GPa to 500 GPa. Four molecular (Cmca-4, Cmca-12, C2/c and P6(1)22) and one atomic (I4(1)/amd) structures are investigated. The candidate structures are roughly separated by 10 mev/proton in enthalpy, making small energy contributions important for the accurate prediction of phase boundaries. In dynamic-lattice DMC, we treat both electrons and protons as quantum particles. This incorporates anharmonic lattice vibrations at the DMC level as well as nonadiabatic coupling between the electron and proton motions. We use an analytic expression for the electron-proton Jastrow to remove the electronic single-particle orbital cusps and allow the electronic wave function to dynamically follow the protons.

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