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First-Principles Investigation on the Structure of Phase III of Hydrogen[1] MARC DVORAK, Colorado School of Mines, XIAOJIA CHEN, Carnegie Institution of Washington, ZHIGANG WU, Colorado School of Mines — First-principles computations based on the density functional theory have been performed to search for the most stable structure of phase-III solid hydrogen. Specifically the phase diagram at zero temperature is predicted by calculating the static total energy and the zero-point motion. Our results suggest that solid hydrogen under pressures in a range of $\sim 150 - 300$ GPa could have lower symmetry than predicted previously. We will discuss the topological considerations on phase transitions from Phase I to II to III, and the available experimental evidences supporting current finding as well.

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