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The Stability and Electronic Structure of Magnesium Hydride and Magnesium Deuteride Under High Pressure

The metal polyhydrides have attracted considerable attention because they can evolve into a superconductor with a high value of critical temperature (Tc) under pressure. In this research, we have investigated structures of MgH2, MgH3, and structures that substitution of deuterium instead of hydrogen under pressure 0-300 GPa to determine the stability of structure under high pressure so that it can be used as a fundamental model for future critical temperature calculations. The calculations are performed by using density functional theory (DFT) based code Quantum Espresso in this work. Generalized gradient approximations (GGA) of Perdew-Burke- Ernzerhof (PBE) have been adopted for exchange-correlation potential. The plane-wave energy cutoff is 80 Ry and the set of K points mesh is 12x12x12 for all structures. The band structures reveal the metallic character of the compound. The calculation of energy band structures for MgH2 and MgD2 are not different as the same as MgH3 and MgD3. We found that the convex hull of Mg and H have thermodynamically stable at some pressure and the results of phonon calculations confirm that the structure is dynamically stable.

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