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Ab Initio Thermochemistry and Elastic Properties of Alkaline Earth Hydrides LOUIS HECTOR, JR., JAN HERBST, GM R&D Center, WALTER WOLF, PAUL SAXE, Materials Design — In addition to comprising a scientifically interesting class of materials, the binary alkaline earth hydrides are important components of hydrogen sorption/desorption reactions. Of critical importance for predicting the thermodynamic stability of hydrides is the enthalpy of hydride formation, ΔH, which links the temperature and pressure of hydrogen sorption via the van't Hoff relation. We compare LDA and GGA predictions of the heats of formation and elastic properties of alkaline earth metals and their binary hydrides BeH_2, MgH_2, CaH_2, SrH_2, and BaH_2 using a plane wave density functional method. Phonon calculations using the direct method enabled prediction of the zero point energies of each material and the 0K and 298K heats of formation. We also computed the 0K and 298K cohesive energies for the alkaline earth metals. Born effective charge tensors were computed via the Berry phase method and enabled prediction of the phonon dispersion curves with LO/TO zone center splittings. It was found that the LO/TO splittings have no effect on the computed zero point energies and heats of formation. The elastic constants were computed with a least squares fitting method using a set of sequentially-applied strains to improve the accuracy of each calculation. Comparison of results from the least squares methodology with prior results using the Hartree-Fock method suggest that the former is substantially more accurate for predicting hydride elastic properties.

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