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Cohesion of Mg_2FeH_6 and Related Complex Hydrides DAVID SINGH, Oak Ridge National Laboratory, SAMED HALILOV, University of Pennsylvania, R. GUPTA, CEA, Saclay, M. GUPTA, Universite Paris-Sud — The stability and bonding of complex K_2PtCl_6 structure hydrides is analyzed using results of density functional calculations. The cohesion is dominated by ionic contributions. The 18-electron rule generally followed in these compounds results from their ionic character combined with crystal field effects. Density functional results for the formation energies are presented and implications for hydrogen storage are discussed.

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