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Thermodynamic and Vibrational Properties of $LaTM_5$ (TM = Co, Ni) Hydrides from Density Functional Theory LOUIS HECTOR JR., JAN HERBST, GM Research and Development Center, Warren MI 48090-9055 — Thermodynamic and vibrational properties of $La(TM)_5H_n$ (with TM one of the magnetic transition metals Co or Ni) and their antecedent intermetallics are discussed. Enthalpies of formation, ΔH, are computed with the plane wave density functional method implemented in the Vienna Ab Initio Simulation Package (VASP). All electron projector-augmented wave potentials based upon the generalized gradient approximation are used for the elemental constituents. With suitable supercells, the zero point and finite temperature contributions to ΔH are computed with the direct phonon method using VASP as the computational engine. Phonon dispersion curves and total phonon density of states are examined for soft modes in each compound and important vibrational modes are identified. The computed vibrational spectra for $LaCo_5$ and $LaCo_5H_4$ reveal new information on their crystal structures.

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