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On the Formation of $LaFe_5H_n$ JAN HERBST, LOUIS HECTOR, JR., GM R&D Center — Formation of a $LaFe_5H_n$ hydride is explored by means of density functional theory. Enthalpies of formation ΔH with respect to the elemental metals and H_2 are calculated for various hydrogen configurations in four prototype crystal structures. We find $\Delta H < 0$ in many cases, suggesting the existence of $LaFe_5H_n$, as does Miedema's semi-empirical model. ΔH is a minimum for the $LaFe_5H_n$ stoichiometry with hydrogen occupying the 4e, 8g, and 16m sites in the orthorhombic Cccm structure. Phonon dispersion relations and elastic constants computed for that structure exhibit no anomalies, demonstrating vibrational stability. Similar results for $LaFe_5$ indicate that compound may form under pressure.

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