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On the Formation of XLi_3N_2 Compounds (X = Sc-Zn)

JAN HERBST, LOUIS HECTOR, JR., GM R&D Center — Ternary lithium nitrides XLi_3N_2 are known to form for the 3d transition elements X = Sc, Fe. We explore the formation of such compounds for other 3d elements by means of density functional theory using the crystal structures of $ScLi_3N_2$ and $FeLi_3N_2$ as templates. Enthalpies of formation including electronic and phonon contributions are calculated for the most stable structures. Thermodynamic stability with respect to known binary and ternary compounds is investigated in order to assess prospects for phase formation. In the case of $FeLi_3N_2$ we find an antiferromagnetic state lower in energy than the ferromagnetic state previously identified.

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