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DFT high-throughput screening of transition metal dopant in MnBi for better magnetic properties[1] LIN-LIN WANG, NIKOLAI A. ZARKEVICH, Ames Laboratory, ICHIRO TAKEUCHI, University of Maryland, College Park, YIYING YE, VLADIMIR ANTROPOV, MATTHEW J. KRAMER, DUANE D. JOHNSON, Ames Laboratory — To improve the magnetic properties of MnBi, especially magnetic energy product, we use density functional theory (DFT) calculations to study alloying effects on MnBi properties with transition metals (TMs), both as dopant and soft phase in an exchange-spring magnet composite. We have considered various defects in the NiAs-type structure with interstitial and substitutional sites. Via high-throughput screening for dopants from groups 3-16, we have DFT trends in impurity formation energy, magnetization, structural parameters, magnetoanisotropy, etc. Early and late TMs prefer to occupy the Mn sites, while mid-TMs are not stable. Early and late TMs are antiferromagnetically coupled, while mid-TMs are ferromagnetically coupled to MnBi. For $3d$ mid-TMs, there is no increase in magnetization. However, energetically favorable mid-late-TM substitutes at Mn sites can improve the magnetic anisotropy. To investigate improving the magnetic energy product of a composite alloy system, we also detail the coupling between MnBi thin films with soft magnetic materials having a high magnetization.

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