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First-Principles Calculations of Magnetic Properties of MnBi doped with Co CHANDANI N. NANDADASA, VIVEK DIKSHITH, SUNGHO KIM, SEONG-GON KIM, Mississippi State University, JIHOON PARK, YANG-KI HONG, The University of Alabama — First principles total-energy calculations were performed to investigate the magnetic and electronic properties of MnBi doped with Co. We used Density Functional Theory (DFT) within the generalized gradient approximation (GGA) with Projector Augmented Wave (PAW) potentials. We found that when MnBi was doped with Co,the magnetization increased as the concentration of Co increased. We also calculated magnetic anisotropy energy (MAE) and magnetic anisotropy constant (K_u) of MnBi before and after doping Co.

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