Abstract Submitted
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MnBi: a better magnet via computational design NIKOLAI A. ZARKEVICH, LIN-LIN WANG, Ames Laboratory, ICHIRO TAKEUCHI, University of Maryland, College Park, MATTHEW J. KRAMER , DUANE D. JOHNSON, Ames Laboratory — Using DFT-based methods, we study the magnetic properties of MnBi in the technologically important low-temperature phase. We identify the origin and behavior of the magnetoanisotropy and magnetism versus structure and doping. We perform high-throughput screening for dopants that improve magnetoanisotropy (larger, c-axis only – no reorientations) and magnetization, and chemical and structural stability. We also assess the best-in-class materials for exchange-spring coupled magnet, without the use of rare-earth elements. Experimental assessment of the predictions is also provided. Work was supported by the U.S. Department of Energy, ARPA-E under REACT (0472-1526), using methods develop under support by the Office of Basic Energy Science, Division of Materials Science and Engineering (DE-FG02-03ER46026 and DE-AC02-07CH11358). Ames Laboratory is operated for the U.S. DOE by Iowa State University under contract DE-AC02-07CH11358.

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