

Abstract Submitted
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Computational Aspects of Anisotropy Calculations M. DAENE, D. ABERG, L.X. BENEDICT, Lawrence Livermore National Laboratory, CRITICAL MATERIALS INSTITUTE TEAM — In order to predict magnetic properties from first principles, an accurate and reliable determination of the magneto crystalline anisotropy is needed. We present results using multiple techniques and codes on the Fe₂B-Co₂B system. Furthermore, we investigate the influence of disorder in this system on the anisotropy.

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