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Origin of the spin reorientation transitions in antiferromagnetic MnPt-based alloys PO-HAO CHANG, KIRILL BELASHCHENKO, Department of Physics and Astronomy, University of Nebraska-Lincoln — Antiferromagnetic MnPt exhibits a spin reorientation transition (SRT) as a function of temperature, and off-stoichiometric Mn-Pt alloys also display SRTs as a function of concentration. Here we describe the origin of these SRTs using first-principles calculations based on the coherent potential approximation, treating chemical and thermally-induced spin disorder on equal footing. We find that the experimentally observed SRTs are related to specific features in the band structure, and we perform a detailed analysis of the effects of temperature and concentration on the magnetocrystalline anisotropy.

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