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First-principles evidence of Mn moment canting in hole-doped $Ba_{1-2x}K_{2x}Mn_2As_2$[1] JAMES GLASBRENNER, National Research Council/Naval Research Laboratory, IGOR MAZIN, Naval Research Laboratory — The compound $BaFe_2As_2$ is the proptotypical example of the 122 family of high-T_c Fe-based superconductors that crystallize in the $ThCr_2Si_2$ structure. Isostructural compounds can be formed by replacing Fe with another transition metal; using Mn produces the material $BaMn_2As_2$. Despite its lack of superconductivity, the material is interesting in its own right. Recent experimental studies have shown that hole-doping the compound by substituting K for Ba leads to metallic behavior and a spontaneous, weak, in-plane magnetization, which was attributed to the holes fully polarizing independent of the Mn moments, producing half-metallic behavior. However the observed in-plane magnetization can also be understood as a small canting of the Mn moments. Using density functional theory, we demonstrate that a Mn moment canting occurs upon hole-doping the compound. We argue that this is due to the competition between the super- and double exchange interactions, which we support using a simple tight-binding model of the superexchange-double exchange interaction and the Andersen Force Theorem. Our calculations also rule out an in-plane polarization of As holes as an explanation for the in-plane magnetization. [1]J. K. Glasbrenner and I. I. Mazin, arXiv:1311.1537

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