

Abstract Submitted
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A new class of half-metallic ferromagnets based on the pnictide superconductors from first principles.¹ SINEAD GRIFFIN, JEFFREY NEATON, Lawrence Berkeley Natl Lab/UC Berkeley — Most theoretical and experimental efforts in the Fe-pnictide class of superconductors aim to optimize the superconducting T_c . Significant substitution with other transition-metal ions is detrimental to superconductivity, however recent experiments on doped BaMn_2As_2 point to its potential as a half-metallic ferromagnet. Using ab initio calculations we investigate Mn-based structures as a new family of half-metallic ferromagnets, and discuss tuning the chemical composition and physical parameters for optimal device performance.

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