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An *ab initio* study of the giant magnetocaloric effect in MnAs<sup>1</sup> HYEJUNG KIM, YIA-CHUNG CHANG, SAHRAOUI CHAIEB, University of Illinois at Urbana-Champaign — MnAs is one of the materials which show a giant magnetocaloric effect. Electronic and magnetic properties of MnAs in NiAs structure and hypothetical zinc-blende structure are studied using a full potential linear augmented-Slater-type-orbital (LASTO) method within the local spin density approximation. Total energies and magnetic moments as a function of volume as well as band structures are in agreement with previous calculations employing different methods such as full potential linearized augmented plane wave method and a plane-wave pseudopotential implementation. Exchange coupling parameters are determined with a frozen magnon approach. Using the exchange coupling parameters obtained, a mean-field theory is applied to calculate the quantities of interest such as the magnetic entropy and free energy as a function of temperature and the critical temperature, to evaluate the giant magnetocaloric effect in MnAs.

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