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Electronic structural origin of spin-phonon coupling in multiferroic CaMnO_3 HONGWEI WANG, Department of Physics, Temple University, Philadelphia, Pennsylvania 19122, USA, HONG JIANG, State Key Laboratory of Rare Earth Materials Chemistry and Applications, Peking University, Beijing, China, LIXIN HE, Key Laboratory of Quantum Information, University of Science and Technology of China, Hefei, Anhui, 230026, People's Republic of China, XIFAN WU, Department of Physics, Temple University, Philadelphia, Pennsylvania 19122, USA — Spin-phonon coupling is a functionality discovered recently in multiferroics and defined by the shift of polar phonon frequency as a function of varying magnetic ordering. In order to elucidate the electronic structural origin of this effect, in this work, we developed a novel computational method based on Extended Kugel-Khomskii (EKK) model. The maximally localized Wannier functions (MLWFs) are generated from density functional theory (DFT) band structure calculations and used as the basis to calculate the hopping integrals in the EKK model. In addition, the screened Coulomb interactions between MLWFs are computed by the random phase approximation. This method not only reproduces accurately the direct first-principles results but gives us a microscopic explanation. It is found that the large spin-phonon coupling in CaMnO_3 originates from in a large distortion of MLWFs generated by the slater phonon mode, which drastically affects the antiferromagnetic hopping integral in the EKK model. On the other hand, phonon instabilities such as oxygen octahedral rotation will only result in a rigid rotation of MLWFs and the effect of spin-phonon coupling is much weaker.

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