

Abstract Submitted
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Effect of doping and strain on Néel temperature of Cr_2O_3 : An ab initio study SAI MU, ALEKSANDER WYSOCKI, KIRILL BELASHCHENKO, Department of Physics and Astronomy, University of Nebraska-Lincoln — Cr_2O_3 is a promising material for applications involving electrically switchable exchange bias [1]. For practical purposes it is desirable to enhance its Néel temperature (308K). Here we employ first principles calculations to elucidate the effect of substitutional doping and epitaxial strain on electronic structure and magnetism of Cr_2O_3 . We use the supercell method and consider both transition metal (V, Ti, Mn, Fe, Co, Ni) and anion (N, B) impurities. We deduce the effect of doping on Néel temperature (T_N) by calculating the total energy change when the local moment on a transition metal impurity or on the Cr atoms near the anion impurity is flipped. We found that the transition metal impurities and N are detrimental to T_N . On the other hand, B impurities are expected to increase the Neel temperature.

[1] X. He. *et. al.* Nature Matter. **9**, 579 (2010).

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