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First-principles studies of n-type and p-type doping in hematite α-Fe_2O_3[1] QIMING ZHANG, CONGXIN XIA, University of Texas at Arlington — Spin-polarized density functional theory calculations are conducted to study the substitutional anionic doping in hematite α-Fe_2O_3 crystal. Selective Group V and VII impurities, as p-type and n-type dopants, respectively, are investigated. The formation energies are lower under Fe-rich environment in general. The impurity levels are discussed both by the transition levels of the formation energies and the single-particle levels. And the local magnetic structure around an impurity is also analyzed.

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