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First-principles study of Fe-doped MgO

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Abstract content
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We present a theoretical investigation on the structural, thermodynamic and magnetic properties of substitutional iron impurity in rocksalt magnesium oxide, (MgO: Fe_{Mg}) as a candidate dilute magnetic semiconductor for spintronic applications. Ab initio pseudopotential density functional calculations were performed for Fe in MgO at various charge and spin states in order to determine the most stable configurations. The generalized gradient approximation with the on-site Hubbard potential correction was used. We find that the double positively charged (Fe⁺²) with high spin (S=2) state and O_h symmetry center is the most energetically favorable, while the low spin (S=1) state with D_{4h} symmetry center is 0.63 eV higher in energy. The thermodynamic transition levels within the wide MgO bandgap are estimated for the various charge states. Furthermore, we show that Fe introduces spin polarized 3d levels within the bandgap, with magnetic moments and stabilization energies depending on its charge state.

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