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First-principles study of Fe impurities in MgO

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Abstract content
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Transition metal doped dilute magnetic semiconductors offer a number of interesting possibilities in the pursuit of spinelectronic materials which exploit career spin and its associated magnetic moment in addition to its charge, for novel solid-state device applications. We performed a first-principles investigation on the electronic and magnetic properties of Fe as an isolated substitutional impurity defect in MgO, considering the effects of charge state, spin state and Fermi level position. The calculations were carried out within density functional theory, using the plane-wave pseudopotential method and the generalized gradient approximation plus the effective Hubbard U approach. Our results indicate that there is a metastable intermediate spin state for the impurity in the doubly positive charge state, in addition to the high and low spin states. Further, we predict that the positively charged impurity orders ferromagnetically in p-type MgO, with a significantly high magnetic stabilization energy of 21 meV and a large magnetic moment desirable for novel spintronic applications.

Primary author: Dr MOLEPO, Mahlaga (University of South Africa)

Co-author: Prof. LOMBARDI, Enrico (UNISA)

Presenter: Dr MOLEPO, Mahlaga (University of South Africa)

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