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Half-metallic ferromagnetic ordering in Fe-doped diamond

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Abstract content
   (Max 300 words)

Half-metallic semiconductor materials are envisaged to achieve high spin polarisation and electrical injection efficiency desirable for spintronic device development. However, lack of fundamental material properties and low ferromagnetic transition temperatures has hindered practical room temperature applications. We report ab initio pseudopotential DFT calculations on the magnetic ordering properties of Fe-doped diamond and show that half-metallic ferromagnetic ordering can be achieved in diamond – which is well known for its extreme material properties – by incorporating Fe+1 at the substitutional lattice site. We find substitutional Fe+1 to be the most stable form of Fe in p-type diamond for Fermi energies in the range of 0.37 - 0.98 eV above the valence band maximum, which, importantly, corresponds to that of boron doped diamond; this is likely to further increase the spin charge concentration if Fe is co-doped with boron in diamond. At the substitutional site, we find that isolated Fe+1 possesses a magnetic moment of 1.0 μB per Fe+1 ion in a diamond supercell and a large ferromagnetic stabilization energy of 33 meV, with the Fermi level crossing bands for only the spin-up orientation, demonstrating that Fe-doped diamond is likely to form a half-metallic diluted ferromagnetic semiconductor.

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PhD

Main supervisor (name and email)
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