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Magnetic interactions in 3d transition metal-doped diamond

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Abstract content
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Ferromagnetic ordering of dopants in semiconductors offers a possible route towards the development of hybrid devices capable of incorporating the conventionally separate functionalities of semiconductor structures and magnetism in one material system for applications in the emerging field of spintronics. However, achieving high ferromagnetic stabilization energies in these materials has posed the main challenge for development of devices capable of operating at room temperature.

We present density functional theory calculations on the magnetic interactions of 3d transition metal-doped diamond and show that ferromagnetic ordering can be achieved in diamond with significant ferromagnetic stabilization energies than has been achieved in the archetypal dilute magnetic semiconductor Mn doped GaAs up to now.

In p-type diamond, we find that ferromagnetic ordering is likely to be achieved for Cr⁺² at the divacancy and Fe⁺¹ at substitutional lattice sites, with magnetic stabilization energies of 16.9 meV and 33.3 meV, respectively. In n-type diamond, we find that V⁻² and Cu⁻² exhibit ground state ferromagnetic ordering when occupying the divacancy lattice site, with ferromagnetic stabilization energies of 21.6 meV and 27.5 meV, respectively, while ferromagnetic ordering occurs in intrinsic diamond only in divacancy Co⁰, with a magnetic stabilization energy of 13.8 meV.

These results indicate that semiconductor diamond may sustain ferromagnetic ordering with both n-type and p-type carriers in the same material host, which is crucial in realizing bi-polar spin-polarised transport.

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Primary author: Dr BENECHA, Evans (University of South Africa)

Co-author: Prof. LOMBARDI, Enrico (University of South Africa)

Presenter: Dr BENECHA, Evans (University of South Africa)

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