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Energetic stability and charge states of 3d transition metals in diamond: Towards a diamond based diluted magnetic semiconductor

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<p>Energetic stability of magnetically ordering dopants in diamond holds the prospect of achieving a diamond based diluted magnetic semiconductor which, in addition to diamond's extreme properties may successfully be considered for spintronic device applications. However, one of the problems to be addressed is that of predicting the most energetically stable lattice configurations or charge states in which such dopants can remain electrically or optically active, and at the same time induce magnetic moments when incorporated into diamond. We report ab initio DFT calculations on the formation energies of isolated 3d transition metal impurities at various lattice sites and charge states in diamond, and show that these impurities introduce deep donor and acceptor levels in the band gap of diamond. We further show that the formation energies as well as the magnetic ordering properties are critically dependent on the position of the Fermi level in the diamond band gap, with formation energies across the 3d series being lower in n-type or p-type diamond compared to intrinsic diamond, suggesting that co-doping with impurities such as boron, nitrogen or phosphorus will considerably enhance their stability in diamond. The majority of the 3d transition metals are found to be energetically most stable at a divacancy site in any charge state, with the formation energy of transition metals in the middle of the 3d series (Cr, Mn, Fe, Ni, Co) being lowest at any lattice site.

Level (Hons, MSc,
   PhD, other)?

PhD

Consider for a student
   award (Yes / No)?

Yes

Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?

Yes

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

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

Presenter: Mr BENECHA, Evans (University of South Africa (UNISA))

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