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Stability and magnetic interaction of embedded Fe clusters in diamond

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The origin of high Curie temperature ferromagnetism in dilute magnetic semiconductors and oxides has often been attributed to clustering and crystallographic phase separation of magnetic atoms, which has a detrimental impact on the properties of the host material for target applications. To determine the effect of clustering on the magnetic properties of transition metal doped diamond, we present Density Functional Theory calculations on the stability and magnetic interactions of embedded Fe atoms by considering various possible cluster configurations. We find that Fe atoms have a strong tendency to form clusters in diamond, with Fe-C-Fe cluster configurations being energetically more favourable than simple Fe-Fe pair formation. Similarly, the cluster binding energy and ferromagnetic stabilization energy is dependent on the arrangement of Fe atoms within the cluster, with the ferromagnetic state being favoured for smaller clusters containing up to three Fe atoms. Since studies of magnetic interactions of transition metal atoms in semiconductors has mostly focused on single doping assuming homogenous distribution, these results present important implications to the understanding of magnetic ordering of dopants in diamond and other dilute magnetic semiconductors.

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