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Stability of transition metal nitrogen and boron defect complexes in diamond

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Energetic stability of transition metal ions in diamond holds the prospect of achieving a diamond based dilute magnetic semiconductor, which, in addition to diamond's extreme properties may successfully be considered for spintronic device applications. However, the high formation energy of transition metal ions in diamond leads to low concentration of dopant ions, which has a detrimental impact on the achievable Curie temperature. We investigate the stability of 3d transition metal defect complexes of nitrogen (TM-N) and boron (TM-B) in diamond using ab initio GGA+U Density Functional Theory electronic structure calculations. Specifically we consider the formation energies of these complexes for various charge states and lattice sites, in comparison with that of isolated single transition metal defects. We find that the formation of the TM-N, TM-N complexes is significantly lower by 4-4.5 eV, compared to that of single transition metals in diamond, demonstrating that co-doping with shallow donors or acceptors will considerably enhance the concentration and stability of transition metals in diamond.

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