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Mg and MgN_3 Cluster in Diamond: Quantum Mechanical Studies

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Abstract : The geometrical, electronic and magnetic properties of the neutral Mg center and MgN_3 cluster in diamond have been studied theoretically in detail by means of an HSE06 Hamiltonian that includes a fraction of the exact exchange term; this is important for a satisfactory picture of the electronic states of open-shell systems. Another batch of the calculations by GGA functionals have also been included for comparison, and these support the results from HSE06. The local perturbations in the lattice by introduced Mg defect are restricted in the first and second shell of atoms before eliminated. The formation energy calculated with HSE06 and GGA of single Mg agrees with the previous result. We found the triplet state with C_{3v} is the ground state of Mg center with energy lower than the singlet with C_{2v} by ~ 0.1 eV. The recent experimental ZPL (557.4 nm) of Mg center in diamond has been discussed in the view of present work. The analysis of the band-structure of the MgN_3 cluster confirms that the MgN_3 defect introduces a shallow donor level in the gap lying within the conduction band edge. This observation is supported by the EMM that produces n-type levels shallower than the P donor level. The formation energy of MgN_2 calculated from a 2NV defect (~ 3.6 eV) is a promising value from which to engineer MgN_3 defects inside the diamond. Ion-implantation followed by heating to about 1200-1600°C might induce migration of N related defects to the localized Mg center. Temperature control is needed for this process to restore the damage and ensure the mobilities of V and N, which demands a more precise experimental study.

Keywords : empirical marker method, generalised gradient approximation, Heyd–Scuseria–Ernzerhof screened hybrid functional, zero phono line
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