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Theoretical Study of Substitutional Phosphorus and Nitrogen Pairs in Diamond

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Abstract : Many properties of semiconductor materials (mechanical, electronic, magnetic, and optical) can be significantly modified by introducing a point defect. Diamond offers extraordinary properties as a semiconductor, and doping seems to be a viable method of solving the problem associated with the fabrication of diamond-based electronic devices in order to exploit those properties. The dopants are believed to play a significant role in reducing the energy barrier to conduction and controlling the mobility of the carriers and the resistivity of the film. Although it has been proven that the n-type diamond semiconductor can be obtained with phosphorus doping, the resulting ionisation energy and mobility are still inadequate for practical application. Theoretical studies have revealed that this is partly because the effects of the many phosphorus atoms incorporated in the diamond lattice are compensated by acceptor states. Using spin-polarised hybrid density functional theory and a supercell approach, we explored the effects of bonding one N atom to a P in adjacent substitutional sites in diamond. A range of hybrid functional, including HSE06, B3LYP, PBE0, PBEsol0, and PBE0-13, were used to calculate the formation, binding, and ionisation energies, in order to explore the solubility and stability of the point defect. The equilibrium geometry and the magnetic and electronic structures were analysed and presented in detail. The defect introduces a unique reconstruction in a diamond where one of the C atoms coordinated with the N atom involved in the elongated C-N bond and creates a new bond with the P atom. The simulated infrared spectra of phosphorus-nitrogen defects were investigated with different supercell sizes and found to contain two sharp peaks at the edges of the spectrum, one at a high frequency 1,379 cm^{-1} and the second appearing at the end range, 234 cm^{-1}, as obtained with the largest supercell (216).

Keywords : DFT, HSE06, B3LYP, PBE0, PBEsol0, PBE0-13
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