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Magnetic and electronic properties of h-BN nanosheets with nonmetal atoms adsorbed: a first-principles study

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Since the discovery of graphene, due to its unique two-dimensional (2D) layered physical structure and the extraordinary electronic properties with a Dirac cone, a wide range of research enthusiasm on 2D materials have been provoked. In a number of recent reports, 2D materials have exhibited better properties than conventional materials, which will be a potential candidate for future electronic, optoelectronic and spintronic devices. Recently, a new graphene-like semiconductor hexagonal BN (h-BN) has been widely studied. The h-BN monolayer is a direct band gap material (4−5 eV), which makes it possible to produce potential applications in electronic and optoelectronic devices. In addition, transition metal (TM) atoms are considered to be the source of magnetism, the magnetic properties of the BN nanosheets with TM dopants have been widely studied. The TM atoms can cause total Hamiltonian perturbation, eventually leading to changes in electronic structures, which makes it a substantial application in magnetic electronic devices. However, there is less research on 2D-BN materials with nonmetal adsorbed, which is highly theoretical and practical significance. Therefore, as shown in Fig. 1a, we study magnetic properties of 2D-BN adsorbed with different nonmetals (C, Cl, F, and O) by first-principles method. According to adsorption energies, different nonmetal atoms prefer different adsorption sites. The ground state of F adsorbed system is nonmagnetic. While C, Cl, and O atoms are adsorbed, a magnetic moment of 1.99, 0.98, and 2.01 μB is induced respectively. Furthermore, we investigate the magnetic coupling between two O adatoms, as shown in Fig. 1b. Based on our calculations, a long-range FM interaction was found in two O atoms adsorbed system, which was well explained by a simple Heisenberg mode, as shown in Fig. 1c. Our results indicate some promising candidates of O-adsorbed 2D-BN materials in future spintronic applications.

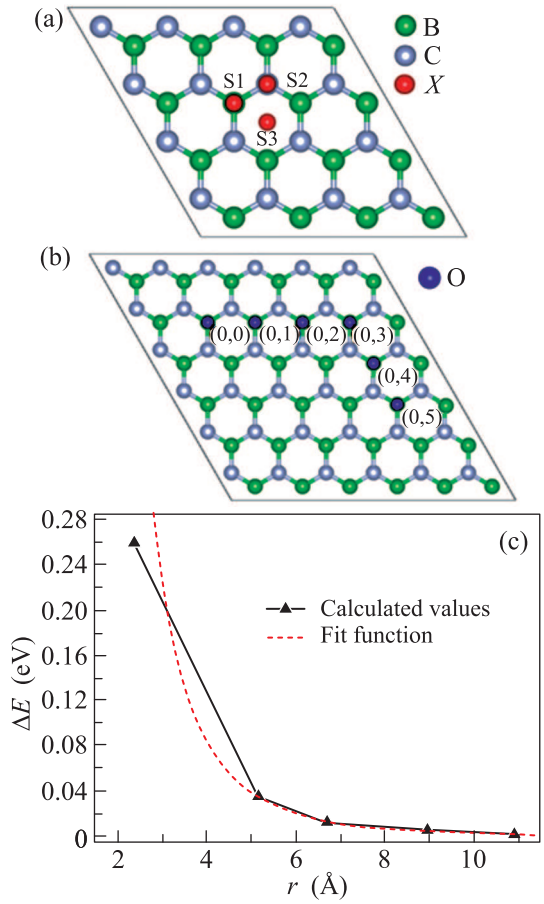

Fig. 1. (Color online) (a) – Top view of three different adsorption sites in the 4×4×1 h-BN monolayer with X atoms adsorbed (X = C, Cl, F, and O) marked S1, S2 and S3. (b) – The configurations in BN monolayer of 4 × 4 × 1 supercell with two O atoms adsorbed. (c) – Total energy difference (ΔE) as a function of the O-O distance (d). The red dashed line is the magnetic correlation function [J(r)] vs the O-O distance (d)

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