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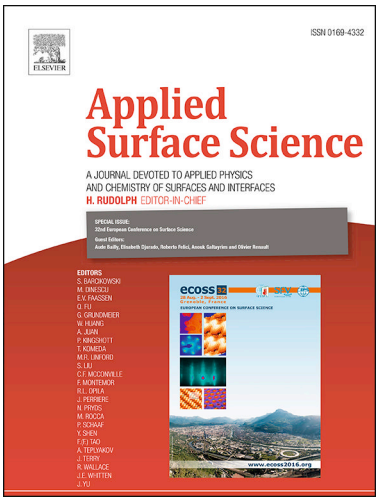

Full Length Article

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Modulating electronic and optical properties of black phosphorous carbide monolayers by molecular doping

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Abstract

First-principles calculations have been performed to study the modulation of the electronic and optical properties of the black phosphorous carbide monolayer (b-PC) by the adsorption of O_2, H_2O, NO_2, and NH_3 molecules. All the molecules are weakly physisorbed on the surface of the b-PC, which act as electron acceptors except NH_3. Especially, O_2 and NO_2 molecules can introduce deep acceptor states in the bandgap of the b-PC. The effects of the external electric field and the in-plane strain were further studied. For the b-PC with the adsorbed O_2, the typical p-type doping can be achieved under an appropriate external electric field. However, the b-PC with the adsorbed NO_2 is the most susceptible to the in-plane strain, as evidenced by the significant changes in the adsorption energy and the charge transfer under the compressive strain. In addition, the optical absorption of the b-PC can be significantly enhanced upon the adsorption of O_2 and NO_2 molecules, which can be further modulated by the external electric field and the in-plane strain. Our calculations predict an effective method to modulate the electronic and optical properties of the b-PC, which may widen its applications in the future electronics and optoelectronics.

Keywords:

First-principle calculation; b-PC; molecular doping; electronic and optical properties

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