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Preferential adsorption positions for an adsorbed Li atom on the layered black phosphorus structures CONGYAN ZHANG, MING YU, University of Louisville — The preferential adsorption positions for an adsorbed Li atom on the layered black phosphorus were determined by mapping out the total energy as a function of its positions on the layered black phosphorus using the density functional theory based method (referred as VASP [Phys. Rev. B 48, 13115 (1993)]). Various possible adsorption positions including the top of the bridge, the valley, and the interstitial positions of the puckered layers have been studied. It is found that the adsorption energy strongly depends on these positions with different environment. In particular, the most preferential adsorption positions for an adsorbed Li atom are found at the valleys and the interstitials of the puckered layers. The analysis of structural and electronic properties of the black phosphorus layer with the adsorbed Li atom will be discussed.

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