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Abstract

Based on first-principles total-energy calculation, we investigate the electronic structures of bilayer graphene, one of which layers possesses atomic or topological defects, to explore the possibility of band gap engineering of graphene by means of physisorption of defective graphene. Our calculations show that the pristine graphene layer possesses a finite energy gap between bonding and antibonding π states because of the potential undulation caused by the other graphene layer with defects. We also found that the gap values strongly depend on the defect species and their mutual arrangement with respect to the pristine layer.

Keywords: Bilayer graphene, Band gap, Electronic structure, Interlayer hybridization

1. Introduction

Following the synthesis of graphene from bulk graphite [1, 2, 3, 4], graphene is attracting much attention in the field of low-dimensional science and nanotechnology [5, 6]. Graphene is the ultimate version of atomic layered materials, consisting of hexagonally bonded sp^2 C atoms. This geometric structure endows graphene with unique physical and chemical properties, which allow us to observe the unusual quantum Hall effect and remarkable carrier mobility [7, 8]. From a technological view, because of their sheet structure with

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