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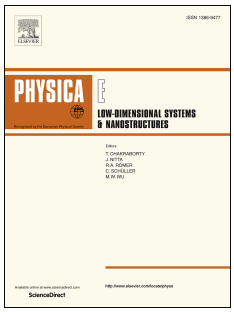

Electronic and vibrational properties of TMDs heterogeneous bilayers, nontwisted bilayers silicene/TMDs heterostructures and photovoltaic heterojunctions of fullerenes with TMDs monolayers

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Electronic and vibrational properties of TMDs heterogeneous bilayers, nontwisted bilayers silicene/TMDs heterostructures and photovoltaic heterojunctions of fullerenes with TMDs monolayers

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Abstract

In the recent years, many studies have been showed that bilayer and heterobilayer transition metal dichalcogenides might offer properties superior to those of monolayer. Nevertheless, only very few have been synthesized. Using first-principles calculations, we study the structural, electronic and vibrational properties of new transition metal dichalcogenides heterogenous bilayers (i.e, $MX_2/M'X'_2$ with M, M′ = Pd, Pt, W; X, X′ = S, Se). Also, we investigate the structural, vibrational and electronic properties of silicene/TMDs and C_{60}/TMDs. Our results show that the predicted geometry can well reproduce the structural parameters, where very well agreement was obtained between the calculated and previous studies for the monolayers. Our calculations show that all the heterobilayers are indirect band-gap semiconductors with the exception of the $WS_2/PdSe_2$ and $WSe_2/PdSe_2$ heterobilayers, which are metallic systems. In the case of the heterostructures bilayers (silicene/MX_2), the band-gap is decreased when Pd is changed to Pt, and when the atomic number of X increases, the band-gap increases. Also, by analyzing the electronic band structures and the electron density, it appeared that C_{60}/MX_2 is a promising system for photovoltaic applications.

Keywords: TMDs heterogeneous bilayers, nontwisted bilayers silicene/TMDs, photovoltaic heterojunctions, first-principles calculations

1. Introduction

In the last seven years, graphene [1] has received very great attention due to its unique physical properties and potentials application [2]. However, for certain applications in electronic and optoelectronic graphene is

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