

Abstract Submitted  
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**Effect of monolayer substrates on the electronic structure of single-layer MoS<sub>2</sub>**<sup>1</sup> ALFREDO RAMIREZ TORRES, DUY LE, TALAT S. RAHMAN, Department of Physics, University of Central Florida — We have performed first-principles calculations based on density functional theory (DFT) to study structural and electronic properties of a single layer of MoS<sub>2</sub> deposited on single-layer substrates of hexagonal boron nitride (BN), graphene and silicene. All have a honeycomb structure; hence the formation of heterostructures is expected. Since the lattice mismatch between MoS<sub>2</sub> and these substrates is large, we have considered different periodicities among layers to reduce as far as possible the incommensurability between lattices. Our results show that BN barely affects the electronic structure of isolated single-layer MoS<sub>2</sub>; the DFT gap remains  $\sim 1.8$  eV. Graphene and silicene severely modify the electronic structure introducing additional states within the optical gap. Adsorption on graphene turns the system into a zero band gap semiconductor bringing the conduction bands of MoS<sub>2</sub> down to the Fermi level of graphene. Adsorption on silicene shifts both MoS<sub>2</sub> bands, valence and conduction, towards the silicene Fermi level, in addition to inducing a gap of 55 meV in the silicene itself. We present analysis of possible charge transfer in these systems and discuss the relevance of these hetero structures for practical applications.

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