

Abstract Submitted  
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**Understanding the electronic states of one-atom-thick materials on metal substrates**<sup>1</sup> CHANGWON PARK<sup>2</sup>, University of Tennessee, MINA YOON, Oak Ridge National Laboratory — Using density functional theory calculations, we investigated how a coating of one-atom-thick materials modifies the metallic states in space and energy. The most prominent modification is governed by the Pauli exclusion principle, and the accompanying spatial modification of the metallic states causes them to follow the orbital shape of the coating material. The energy level of the metallic surface states also changes through the subtle interplay between dipole layer formation and strong substrate interaction. We chose two-dimensional boron nitride on Cu substrate (2D BN on Cu) as an example system for demonstrating the role of one-atom-thick materials on the substrates metallic states. Specifically, we revealed the nature of some counterintuitive features of STM images of 2D BN on Cu. Implications on the workfunction change and STM interpretation of molecular assemblies are also presented.

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