

Abstract Submitted
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An investigation on work-function enhancement in multilayer graphene ABBAS EBNONNASIR, BRANDEN B. KAPPES, CRISTIAN V. CIOBANU — Using density functional theory calculations, we perform a detailed analysis of the electronic properties of multilayer graphene on a generic substrate. A range of the possible substrate effects is simulated by systematically changing the interlayer distance between the first two graphene layers and leaving the other layers at the nominal graphite spacing. We find that the work function on the graphite-like side varies with the number of layers and with the distance between the first two layers, and we analyze the charge transfer distribution and the surface dipole moment as a function of the distance between the first two graphene layers. We correlate our results with reported experimental observations and provide possible explanations of pronounced work-function variations.

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