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Effect of stacking on the transport properties of few-layer graphene: NEGF-DFT investigation MATHEUS LIMA, JOSÉ EDUARDO PADILHA, RENATO PONTES, ANTÔNIO J. R. DA SILVA, ADALBERTO FAZZIO, University of São Paulo (IFUSP) — We study the effect of the stacking order on the electronic transport properties of few-layer graphene (FLG) by performing ab initio calculations based on the formalism that combines non-equilibrium green's functions and density functional theory. The stacking of the layers - Bernal (ABA), Rhombohedral (ABC) or even a combination between them - have to be considered as an extra degree of freedom and consequently the FLG properties are highly sensitive to the stacking configuration. In particular, the band structures and the transport properties of FLG present a behavior markedly distinct from that for single layer. We consider FLG from trilayer to dodecalayer in both stacks. We show that for FLG, in the Rhombohedral stacking, a simple counting of bands cannot be used to predict the amount of conducting channels. We also show that for FLG, in the Rhombohedral stacking, the outermost layers dominate the contribution to the transmittance whereas for the Bernal stacking the innermost layers also present a significant contribution to the transmittance. Moreover, we investigate the effect of bias voltage and the temperature in the transport properties of FLG. We acknowledge the INCT/CNPq, CAPES and FAPESP for the financial support.

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