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Study of the resistance induced by metal contacts in graphene by first-principles methods SALVADOR BARRAZA-LOPEZ, Georgia Tech, MEI-YIN CHOU, Georgia Tech — The detailed knowledge of the resistance induced by metals contacting graphene has been the subject of thorough experimental and theoretical efforts, as these studies conform a necessary stage before graphene could become a viable material for electronic applications. Furthermore, it is desirable to determine optimal interfaces to bring this resistance to its minimum possible values. Theoretical modeling of transport through graphene with real metallic leads is in its first stages, and some assumptions made in the models so far presented lack sound justification or validation from first-principles studies. With a combination of density-functional theory and large-scale non-equilibrium Green's function methods, a thorough study of the conductance/resistance induced by aluminum contacts on suspended graphene is presented, as a function of the graphene's width as well as the magnitude of the suspended length. Beyond an electron-hole asymmetry in the conductance features, we have been able to confirm a conduction gap for widths smaller than 10 nm (in accordance with experimental observation), and to observe the evolution of a prominent peak in the conductance that evolves as a function of the length between the metallic contacts. The insight acquired from simulation can be employed to construct a minimal tight-binding model to predict the conductance through graphene attached to metal leads.

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