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Charge transport in two-terminal graphene junctions with bonding metal contacts BARRAZA-LOPEZ SALVADOR, M. Y. CHOU, School of Physics. Georgia Institute of Technology — One has to attach graphene to metal leads to measure charge transport characteristics. In a number of experiments a thin Ti film is grown on top of graphene and additional metal leads (e.g., Au or Al) are created on top of this film. Ti forms covalent bonds with graphene, destroying the linear dispersion at the Ti/graphene contact. For practical reasons (i.e., the use of Hamiltonians with a linear dispersion) most theoretical approaches either consider only the effects of the inhomogeneities caused by the insulating substrate, or, when two-terminal calculations exist, use assumptions that preclude quantitative modeling. These assumptions include: (i) extremely large bias steps separating the leads and the central region of the device, or (ii) unusually large imaginary contributions to the self-energies representing metal leads. We depart from these models and follow an atomistic approach to compute transmission characteristics of Ti/graphene/Ti junctions. From these calculations we identify the key physical ingredients determining the transport features, and extract parameters to be used in a quantitative effective model that describes accurately the electronic structure and the transmission probabilities of charge carriers. This work complements our previous results in metal/graphene/metal junctions where the metal does not bond covalently to graphene (PRL **104**, 076807 (2010)).

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