Abstract Submitted
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First-principles calculations of electronic transport through graphene with realistic metallic leads SALVADOR BARRAZA-LOPEZ, M. Y. CHOU, School of Physics. Georgia Institute of Technology — We present transmission characteristics for electrons through graphene with realistic metallic contacts. The methodology relies on an in-house version of the electronic transport SMEAGOL code [1], in which the memory required to allocate for the matrices of contact leads and the graphene sheet in the Green's function solver is distributed into more than one processor, for a given electron energy. We are able to accommodate for commensurate graphene-metal supercells which have the correct atomic structure (namely, stress caused by contracting/extending the metal contacts to match the periodicity of graphene is avoided). In addition, and despite of the large size of the leads, the electronic properties and transport are computed at the density-functional theory level [2] within a double-zeta plus polarization basis[3], ensuring the accuracy of the atomic forces in the system, as well as on the final transmission characteristics. [1] A. R. Rocha et al, PRB. **73**, 085414 (2006); [2] J. M. Soler et al, J. Phys.: Condens. Matter **14**, 2745-2779 (2002); [3] J. Junquera et al, PRB **64**, 235111 (2001).

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