

Abstract Submitted
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Electronic transport through single-molecule- and monolayer-based molecular junctions¹ LUIS AGAPITO, HAI-PING CHENG, Department of Physics and Quantum Theory Project, University of Florida, Gainesville, Florida 32611 — We report our development for calculating tunneling electronic transport through molecular junctions, which are composed of two contact leads and the active device in between. The surface Green's function of the contact leads is obtained following a non-iterative, exact procedure using ab initio data computed with the same level of theory and localized basis set than those used for the active device*. In a 1-dimensional in-wire setting, we describe the electrical switching performance of a single oligo-phenylene-ethynylene molecule connected to graphene-nanoribbons leads. Moreover, in a more realistic 2-dimensional setting, such as the case of self-assembled molecular monolayers, the method is extended to include intermolecular and packing-density effects. * Agapito, L. A.; Cheng, H. P. *Journal of Physical Chemistry C* **2007**, 111, 14266.

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