First-principles computation of electronic transport through single molecules and molecular monolayers

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We present our development for calculating electron tunneling probabilities through molecular devices at the equilibrium level. A molecular device is defined to be composed of two contact leads, modeled as semi-infinite crystalline materials, and an active device, in the form of a single molecule or a monolayer of those molecules. The surface Green's function of the contact leads is obtained following a non-iterative, exact procedure that post-processes the ab initio data computed at the same level of theory and localized basis set than those used for the active device[1]. We describe the electrical switching performance of a single oligo-phenylene-ethynylene molecule connected to graphene-nanoribbons leads to exemplify a 1-dimensional in-wire setting. For the more realistic 2-dimensional setting, which is the case of self-assembled molecular monolayers, the method is extended to account for intermolecular and packing-density effects.

(1) Agapito, L. A.; Cheng, H. P. *Journal of Physical Chemistry C* **2007**, *111*, 14266.