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Electron transport in molecular devices SIMONE PICCININ, Princeton University - Department of Chemistry, RALPH GEBAUER, ICTP - Trieste (Italy), ROBERTO CAR, Princeton University - Department of Chemistry — We present an application of a recently proposed quantum-kinetic scheme for non equilibrium transport properties in nanoscale systems, based on a Liouville-master equation for the reduced density operator and combined with a Density Functional Theory description of the electronic structure [1,2]. The systems studied are the well known benzene-dithiol sandwiched between two gold electrodes and the gold quantum point contact. The results we obtain are in general agreement with previous theoretical works and with recent experimental measurements. We analyze the spatial distribution of the current density and the effect of geometrical distortions on the transport properties.

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