Abstract Submitted
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Electron transport in molecular devices SIMONE PICCININ, Department of Chemistry, Princeton University, Princeton, USA, RALPH GEBAUER, The Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy, ROBERTO CAR, Department of Chemistry and Princeton Institute for the Science and Technology of Materials, Princeton University, Princeton, USA — We apply a novel quantum kinetic approach [1] to study transport in molecular devices. Our scheme is based on a master equation for the reduced electronic density operator and includes dissipation by inelastic scattering with the phonons. A proper choice of the gauge allows us to use periodic boundary conditions. Here we adopt a plane-wave pseudopotential scheme within time-dependent Density Functional theory. We apply the scheme to the well studied case of a benzene-dithiol molecule sandwiched between two gold electrodes. Our results are in general agreement with previous calculations based on open boundary scattering schemes. Our calculated I-V characteristics is also close to recent experimental results. We discuss how transport through the molecular device is affected by dissipative processes in the metallic electrodes. Work partially supported by NSF through Grant DMR-0213706 to the MRSEC PCCM and by DOE through Grant DOE-DE-FG02-01ER45928.

[1] R. Gebauer, R. Car, Phys. Rev. B **70, 125324 (2004)**

Simone Piccinin
Department of Chemistry, Princeton University, Princeton, USA

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