Abstract Submitted
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A simple model for the description of correlation effects in molecular conductors[1] MATTHIAS ERNZERHOF, FRANCOIS GOYER, Department of Chemistry, University of Montreal — To model transport through molecular electronic devices (MEDs), we use a non-Hermitian Hamiltonian [1] for the description of open systems that exchange current density with their environment. The infinite contacts are replaced by complex source-sink potentials (SSPs) [1]. Employing a Hubbard interaction term, we include electron-correlation effects in our approach [2]. Electron interaction is considered in the molecule and neglected in the contacts. Among other strongly correlated problems, we discuss the change in conductance upon bond breaking. In the limit where the electron repulsion is strong compared to the binding energy (as it is the case in a stretched bond) a strong suppression of conductance is observed due to the localization of electrons. Other interesting phenomena, which cannot be accounted for with conventional (independent electron) approaches, are discussed as well. [1] F. Goyer, M. Ernzerhof, and M. Zhuang, J. Chem. Phys. 126, 144104 (2007); M. Ernzerhof, J. Chem. Phys. 127, 204709 (2007). [2] A. Goker, F. Goyer, and M. Ernzerhof, J. Chem. Phys. 129, 194901 (2008); M. Ernzerhof, J. Chem. Phys. 125, 124104 (2006).

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