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Molecular orbital theory of ballistic electron transport through molecules[1] MATTHIAS ERNZERHOF, PHILIPPE ROCHELEAU, FRANCOIS GOYER, Department of Chemistry, University of Montreal — Electron transport through molecules occurs, for instance, in STM imaging and in conductance measurements on molecular electronic devices (MEDs). To model these phenomena, we use a non-Hermitian model Hamiltonian [1] for the description of open systems that exchange current density with their environment. We derive qualitative, molecular-orbital-based rules relating molecular structure and conductance. We show how side groups attached to molecular conductors [2] can completely suppress the conductance. We discuss interference effects in aromatic molecules [3] that can also inhibit electron transport. Rules are developed [1] for the prediction of Fano resonances. All these phenomena are explained with a molecular orbital theory [1,4] for molecules attached to macroscopic reservoirs. [1] F. Goyer, M. Ernzerhof, and M. Zhuang, JCP 126, 144104 (2007); M. Ernzerhof, JCP 127, 204709 (2007). [2] M. Ernzerhof, M. Zhuang, and P. Rocheleau, JCP 123, 134704 (2005); G. C. Solomon, D Q. Andrews, R P. Van Duyne, and M A. Ratner, JACS 130, 7788 (2008). [3] M. Ernzerhof, H. Bahmann, F. Goyer, M. Zhuang, and P. Rocheleau, JCTC 2, 1291 (2006); G. C. Solomon, D. Q. Andrews, R. P. Van Duyne, and M. A. Ratner, JCP 129, 054701 (2008). [4] B.T. Pickup, P.W. Fowler, CPL 459, 198 (2008); P. Rocheleau and M. Ernzerhof, JCP, submitted.

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