

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Molecular conductance at finite voltage: bias driven evolution of Kohn-Sham-orbitals MAX KOENTOPP, Rutgers University, Department of Chemistry, FERDINAND EVERS, Institute of Nanotechnology, Research Center Karlsruhe, Germany, KIERON BURKE, Rutgers University, Department of Chemistry — Ground state density functional theory calculations yield the exact electron density if the exact exchange-correlation functional is employed. The evolution of the equilibrium density with parametric changes in the Hamiltonian, e.g. realized by a change in the electrostatic potential, can provide crucial information about transport properties, like the Coulomb blockade. To test our ideas, we perform model calculations using the quantum chemistry package TURBOMOLE for a diode molecule, which exhibits the structure of a double quantum dot and has been investigated experimentally [1]. In particular, we explain the origin of the characteristic peak structure in the differential conductance. Our results are consistent with the interpretation that the stepwise increase of the conductance occurs when the number of occupied levels of one of the dots, that have an energy above the lowest unoccupied level of the other dot, increases by one.

[1] M. Elbing, R. Ochs, M. Koentopp, M. Fischer, C. von Hänisch, F. Weigend, F. Evers, H. Weber, M. Mayor, Proc. Nat. Acad. Sci. USA **102**, 8815 (2005).

Max Koentopp
Rutgers University, Department of Chemistry

Date submitted: 01 Dec 2005

Electronic form version 1.4