

Molecular conductance at finite voltage: bias driven evolution of Kohn-Sham-orbitals

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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 TURBOMOLE for a diode molecule, which exhibits a structure of a double quantum dot and has been investigated experimentally ¹. In particular, we investigate 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, et al., Proc. Nat. Acad. Sci. USA, (2005), accepted.