Electronic transport through aromatic molecules

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We consider electrical transport through a system of a molecule coupled to two metallic electrodes. We give an overview of some of the issues involved in the problem.[1] We discuss the two regimes of transport, strong molecule-electrode coupling and weak molecule-electrode coupling. In the strong molecule-electrode coupling limit interaction effects beyond the Hartree-Fock (self-consistent field) level can be ignored. The transport can be described by a single particle scattering or Landauer approach. In the weak coupling limit interaction effects on the molecule dominate and the molecule must be treated as a many-body system. The transport can be described by incoherent sequential tunneling of single electrons. We discuss in general terms the relevance of spatial electronic structure, field effects and relaxation on the molecule. Focusing on weak coupling, we discuss in some detail a model for transport through a single benzene molecule. The model is derived by means of electronic structure calculations. The interplay of strong interactions and the spatial structure of the molecular states can lead to various effects in non–linear electrical transport. We demonstrate the appearance of "blocking states", inhibiting transport beyond a certain threshold voltage. This leads to current collapse and strong negative differential conductance for the considered system.[2]

[1] M. H. Hettler, H. Schoeller and W. Wenzel, in *Nano-Physics and Bio-Electronics: A New Odyssey*, eds. T. Chakraborty, F. Peeters and U. Sivan (Elsevier 2002).
[2] M. H. Hettler, H. Schoeller and W. Wenzel, Europhys. Lett. **57**, 571 (2002)