
**Transport through a
molecular tunnel junction:
some insights from a
multiconfigurational
point of view**

Martin Verot

ENS Lyon,
Laboratoire de Chimie
69364 Lyon CEDEX 07, France
martin.verot@ens-lyon.fr

We demonstrate how a few key parameters, extracted from wavefunction-based methods (post Hartree-Fock) control the electron transport through a simple molecular system. The transport of molecules ranging from lowly correlated systems (H_2 -like) to highly correlated ones (O_2 -like) is investigated.

For magnetic systems where several spin states are involved, we will show that both the energy spectrum and the wavefunction structure have an impact on the conductance observed. With this toy model, further properties (“spin-valve” behavior, Zeeman effect) can also be investigated to see the importance of the multiconfigurational description of such molecular filters.