Tuning the conductance of a molecular switch

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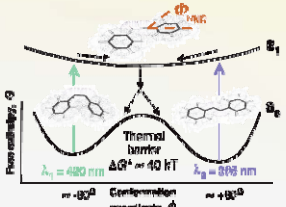
motivation

molecular electronics: realize at the molecular scale electronic functions from conventional semiconductor-based technologies

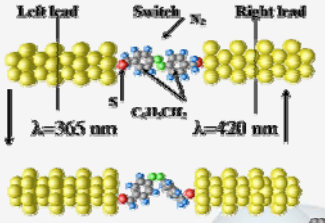
azobenzene (two phenyl rings joined by a double N-bridge): promising molecular switch candidate as:

it's **bistable**

it's **photosensitive**



Hugel *et. al.*, *Science* 296 (2002)

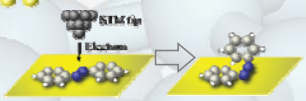


electrical switch:

with **Au-electrodes**

Choi *et al.*, *PRL* **96**, 156106 (2006) --exp.--
Zhang *et al. PRL* **92**, 158301 (2004) --theor.--
Zhang *et al. PRB* **73**, 125445 (2006) --theor.--

Result: *trans* ≠ *cis* ? YES



But... gold is
NOT flexible enough ☹
NOT **nanoscopic** ☹

→ **CARBON NANOTUBES as nanoscopic electrodes** **?!**

methodology

DFT-based tight-binding combined with Keldysh Green function techniques ⟷ **Minimal model Hamiltonians**

Siesta[1], sc-**DFTB**[2] + **Green function techniques**[3] within Landauer formalism using the extended molecule concept

Physical observables:

linear conductance G

electrical current $I(V)$

$$G = 2\,(e^2/h)\,t(E_F) \qquad t(E)\text{=QM transmission}$$

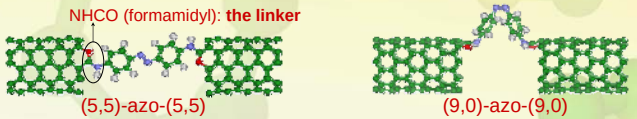
$$I = \frac{2e}{h}\int \mathrm{Tr}\left[\Sigma^{<}(E)G^{>}(E) - \Sigma^{>}(E)G^{<}(E)\right] dE$$

[1] http://www.uam.es/departamentos/ciencias/fismateriac/siesta/

[2] M. Elstner, D. Porezag, G. Jungnickel, J. Elsner, M. Haugk, Th. Frauenheim, S. Suhai, and G. Seifert, *PRB* **58**, 7260 (1998)

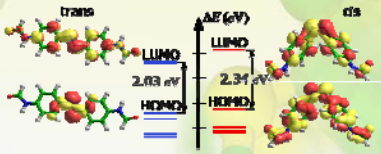
[3] H. Haug, A.-P. Jauho, *Quantum Kinetics in Transport and Optics of Semiconductors*, Springer (1998)

results: an azobenzene molecular switch

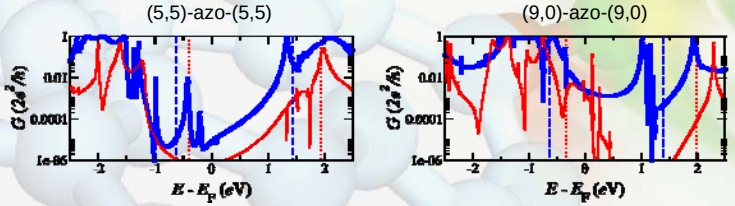


Some crucial issues:

- switching: ***cis*** vs. ***trans***
- role of **chirality?**
- role of **interface topology/chemistry?**



Conductance through the junctions:



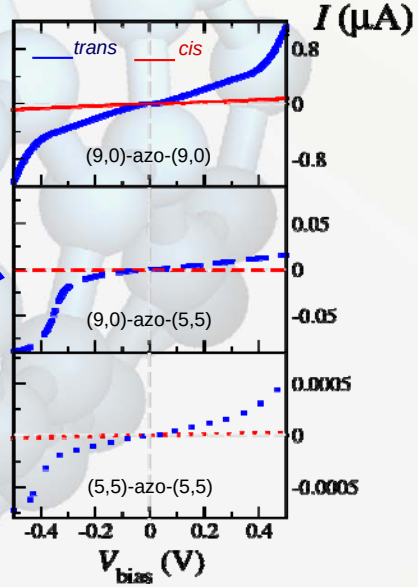
Conclusions out of the I(V) characteristics:

- Dramatic difference betw. *trans* and *cis* azobenzene

→ **molecular switch possible**

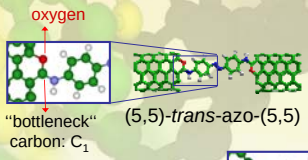
- chirality-dependent rectifying behavior
- *armchair* CNTs act detrimentally on junction conductance

→ CNT chiralities crucial, fine tuning of charge injection efficiency via interface chemistry (**local chemical gating**)

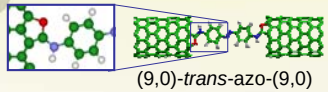


CNT-molecule interface: a minimal model

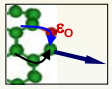
Interface with armchair CNTs



Interface with zigzag CNTs

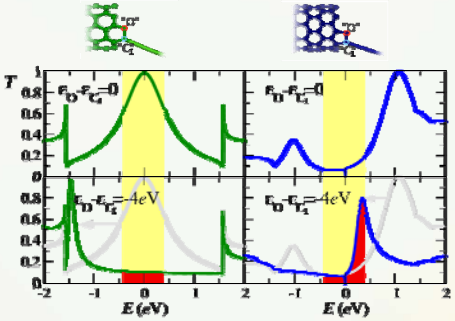


Role of oxygen: π-orbital model



$$t(E) = 4\Gamma_R\left\{\Gamma_L^{11}\left[\left|G_{C_1C_1}(E)\right|^2 + \left|G_{C_1O}(E)\right|^2\right] + 2\Gamma_L^{12}\,\mathrm{Re}\left(G_{C_1C_1}G^{*}_{C_1O}\right)\right\} \approx 4\Gamma_R\Gamma_L^{11}\left|G_{C_1O}(E)\right|^2$$

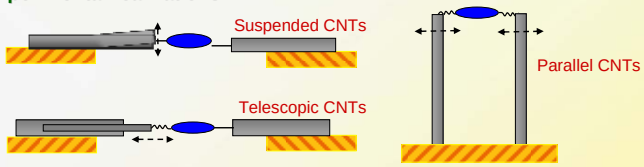
AC-dimer-WBL **ZZ-dimer-WBL**



Conclusions out of our minimal model:

CNT-azobenzene interface plays a crucial role in determining transport:
Oxygen charge state controls DOS on "bottleneck" C-atom (**chemical gating**)
Edge-state of zigzag CNTs shows a dominant effect

Experimental realizations?



Main reference:
M. del Valle, R. Gutiérrez, C. Tejedor, and G. Cuniberti, Nature Nanotechnology, to appear (2007)