TAILORING THE FERMI LEVEL OF THE LEADS IN MOLECULAR-ELECTRONIC DEVICES

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The dependence of the transport properties on the specific location of the Fermi level in molecular electronics devices is studied by using electrodes of different materials. The zero-bias transport properties, which are obtained by using a combination of density functional theory and non-equilibrium Green's functions [1], are shown to depend dramatically on the elemental composition of the electrodes, even though the shape of the transmission coefficients is very similar. By using alkaline materials, an idea well known in the organic LEDs community [2], it is possible to move the Fermi level from the HOMO-LUMO gap to the LUMO resonance and change dramatically the length dependence of the conductance of molecular wires, which opens the possibility of using molecules with different lengths and very similar conductances in nanoscale circuits. This method shows how to dramatically increase the conductance of molecular devices and alter qualitatively and quantitatively their electronic and transport properties.

References:

[1] A. R. Rocha, V. M. García-Suárez, S. Bailey, C. Lambert, J. Ferrer, and S. Sanvito, Phys. Rev. B **73** (2006), 085414.

[2] T. Wakimoto, Y. Fukuda, K. Nagayama, A. Yokoi, H. Nakada, and M. Tsuchida, IEEE Transactions on Electron devices **44** (1997), 1245.

Figures: Real space projection of the density of states on an interval of 0.2 eV around the Fermi level of a molecule between (a) gold leads and (b) sodium leads.