

# TUNNEL MAGNETORESISTANCE OF AN ORGANIC MOLECULE JUNCTION

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Coherent spin-dependent electronic transport is investigated in a molecular junction made of organic molecule (linear chain of benzene rings) attached to two the semi-infinite ferromagnetic (FM) electrodes with finite cross sections (Fig. 1). The work is based on the tight-binding Hamiltonian model and within the framework of a non-equilibrium Green's function (NEGF) technique. It is shown that tunnel magnetoresistance (TMR) of molecular junction can be large (over 60 %) by adjusting the related parameters, and depends on: (i) the applied voltages and (ii) the number of benzene rings.



**Fig. 1.** A schematic representation of the FM/organic molecule/FM molecular junction in two configurations Parallel (P) and Anti-Parallel (AP) magnetization.

Hamiltonian for the system of two ferromagnetic electrodes joined by an organic molecule is proposed in the following form:

$$H = \sum_{i_{\alpha}, \sigma \in L, R} (\epsilon_i - \sigma h_{\alpha}) c_{i_{\alpha}, \sigma}^{\dagger} c_{i_{\alpha}, \sigma} - \sum_{(i_{\alpha}, j_{\alpha}), \sigma} t_{i_{\alpha}, j_{\alpha}} c_{i_{\alpha}, \sigma}^{\dagger} c_{j_{\alpha}, \sigma} + \sum_{\substack{i_{\alpha}, \sigma \in L, R \\ m, \sigma \in M}} (t_{i_{\alpha}, m, \sigma} c_{i_{\alpha}, \sigma}^{\dagger} c_{m, \sigma} + h.c.) + H_M,$$

Hamiltonian for the molecular ( $H_M$ ) is:

$$H_M = \sum_{m, \sigma \in M} \epsilon_{m, \sigma} c_{m, \sigma}^{\dagger} c_{m, \sigma} + \sum_{m, \sigma \in M} (t_{m, m+1} c_{m, \sigma}^{\dagger} c_{m+1, \sigma} + h.c.),$$

The spin dependent Green's function is given as:

$$G_{\sigma}(\epsilon, V) = \lim_{\zeta \rightarrow \infty} [(\epsilon + i\zeta)I - H_M - \sum_{L, \sigma} (\epsilon - eV/2) - \sum_{R, \sigma} (\epsilon + eV/2)]^{-1},$$

where the self-energy matrices contain the information of the electronic structure of the FM electrodes and their coupling to the organic molecule<sup>1</sup>.

## References

- [1] A. Yoshihiro and F. Hidetoshi, Phys. Rev. B 72 (2005) 085431.