Tunneling conductance of molecular wires

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Tunneling transport through long, insulating molecular chains is characterized by the exponential decay law $g = g_c e^{-\beta N}$, where N is the number of monomers. In the modern formulation of the tunneling transport, β is determined from the complex band structure of the isolated molecular chain, a procedure that extends far beyond the limitations of simple models that approximate electron tunneling in molecular devices using square potential barriers. However, until recently, an analytic expression for the contact conductance g_c was missing.

In the first part of the talk, I will review a newly formulated theory of tunneling transport in long molecular wires.[1] This theory provides a rigorous way of computing the exponential decay constant and gives g_c as an overlap integral between three well defined and physically relevant quantities: the spectral density of the device at the Fermi level, the potential perturbation of the metallic contacts on the molecular chain, and the evanescent electron waves traversing the molecular chain.

The formalism will be exemplified on molecular devices made of alkyl[2] and phenyl chains linked to gold wires via amine groups. If the time allows, I will present the extension of the theory to the spin dependent transport, in particular to the problem of tunneling magneto-resistance.

[1] E. Prodan and R. Car, DC Conductance of Molecular Wires, Phys. Rev. B **76**, 115102 (2007).
[2] E. Prodan and R. Car, Tunneling conductance of amine linked alkyl chains, Nano Letters (in press)