Effect of external field on the I-V characteristics through the molecular nano-junction

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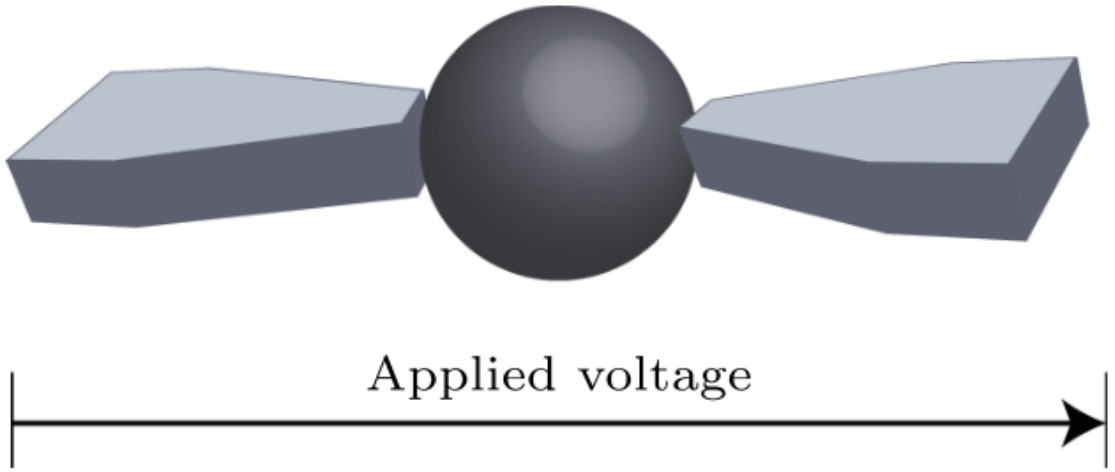
Overview

Background

As the basic functional unit of molecular electronics, the structure of single molecular nano-junction sandwiched between Nano-electrodes has been attracted many interests in molecular science. The charge transmission dynamics problems received increasing attention and have been subsequently studied extensively, in particular, its current voltage (IV) characteristics induced by an external field.



Method Section

In the system of molecular nano-junction which composed by a molecule between a pair of leads, with the method of extended General Master Equation, the characteristic curves of stationary and transient current have been computed and explained theoretically. It is found that the current can be evidently controlled via some factors adjustments, such as external field, the relaxation of molecules, intra-molecular vibration energy redistribution, and others.

Theoretical Model Description

The introduced electron-vibrational states, are used for an expansion of the overall molecular junction Hamiltonian:

$$H = H_{mol} + H_{lead} + H_{mol-lead} + H_{mol-field} \tag{1}$$

The Hamiltonian of the molecular part:

$$H_{mol} = \sum_{\alpha} \hbar\varepsilon_{\alpha} |\psi_{\alpha}\rangle \langle\psi_{\alpha}| + \sum_{\alpha\beta} W_{\alpha\beta} |\psi_{\alpha}\rangle \langle\psi_{\beta}| \tag{2}$$

The quadratic quantized form of the Hamiltonian of leads:

$$H_{lead} = \sum_{X=L,R} H^{X}_{lead} = \sum_{X=L,R} \sum_{k,s} \hbar\omega_{Xks} \alpha^{\dagger}_{Xks} \alpha_{Xks} \tag{3}$$

Theoretical Model Description: Hamiltonian

The Hamiltonian of the interaction between the leads and the molecule:

$$\begin{aligned} H_{mol-lead} = & \sum_{X=L,R} \sum_{k,s} T_X(N+1a, Nb, ks) \times \alpha_{Xks} \left|\varphi_{N+1a}\right\rangle \left\langle\varphi_{Nb}\right| \\ & + \sum_{X=L,R} \sum_{k,s} T_X(Na, N+1b, ks) \times \alpha_{Xks} \left|\varphi_{Na}\right\rangle \left\langle\varphi_{N+1b}\right| \end{aligned} \tag{4}$$

Theoretical Model Description

The coupling to the external optical field:

$$H_{mol-field}(t) = -\sum_{\alpha,\beta} |\alpha\rangle \langle\beta| \, \vec{d}_{\alpha\beta} \cdot \vec{E}(t) \tag{5}$$

The filed form:

$$\vec{E}(t) = \vec{n} \cdot E(t) e^{-i\omega t} + c.c. \tag{6}$$

The general form of rate equation:

$$\frac{\partial}{\partial t} P_\alpha(t) = -\sum_{\beta} [P_\alpha(t) K_{\alpha\to\beta}(t) - P_\beta(t) K_{\beta\to\alpha}(t)] \tag{7}$$

Numerical Simulation

Result Analysis

Thank You