

KINETIC AND ELECTROSTATIC CONTROL OF ELECTROLUMINESCENCE IN MOLECULAR JUNCTIONS

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The Hamiltonian of 1M2-system

$$H = H_e + H_m + H_{\text{int}} + H_f(t)$$

$$H_e = \sum_{r\mathbf{k}\sigma} E_{r\mathbf{k}} a_{r\mathbf{k}\sigma}^+ a_{r\mathbf{k}\sigma} \quad - \text{electrode's Hamiltonian}$$

$$H_m = \sum_{M(N)} E_{M(N)} |M(N)\rangle \langle M(N)| \quad - \text{molecular Hamiltonian}$$

$$H_{\text{int}} = \sum_{r\mathbf{k}\sigma} \sum_{N, MM'} \left[V_{M'(N+1); r\mathbf{k}\sigma M(N)} \times |M'(N+1)\rangle \langle M(N) a_{r\mathbf{k}\sigma} | + h.c. \right]$$

– Hamiltonian of interaction between electrodes and molecule

$$H_f(t) = -\mathbf{E}(t) \sum_{MMN} \mathbf{d}_{MM} |M'(N)\rangle \langle M(N)|$$

– Hamiltonian of interaction with electromagnetic field

