Signal Transmission through Molecular Quantum-Dot Cellular Automata: A Theoretical Study on Creutz-Taube Complexes for Molecular Computing
(Electronic Supplementary Information)

Ken Tokunaga*

Research and Development Center for Higher Education,
Kyushu University, Ropponmatsu 4-2-1, Fukuoka 810-8560, Japan

(Dated: December 7, 2008)

---

*E-mail:`tokunaga@rche.kyushu-u.ac.jp`

I. ELECTRONIC STRUCTURE

Molecular orbitals (MOs) of **py** complex calculated by HF method (Fig. S1) show the same tendency with those by DFT method. It is easy to see that a set of 112β, 113β, and 114β of HF method corresponds to a set of 112β, 113β, and 114β of DFT method. Similar to 112β and 113β of Fig. 4, 113β and 114β of Fig. S1 are mainly constructed from two $4d_{yz}$ orbitals, and have bonding and anti-bonding characters, respectively.

MOs of **bpy** complex in Fig. S2 are quite different from those by DFT method due to its C_1 geometrical symmetry. At both q=+0.5 and q=−0.5, all MOs are localized on the particular part of the molecule. Electronic structure of **bpy** complex is little influenced by the switch of the input. Namely, electric field originated from injected one-electron is not enough to move electron from one side to the other side of the **bpy** complex.

II. REVERSE SWITCHING

In the *normal* switch of the article, q^{i} and q^{f} have mainly positive sign and negative sign, respectively. Fig. S3 shows time evolution of Mulliken charge by the *reverse* switch in which q^{i} and q^{f} have mainly negative sign and positive sign, respectively. Different from the normal switch, at the initial condition, Q_1 has larger positive charge than Q_2. (q^{i}, q^{f}) dependence of T, A, and t_{st} of reverse switch are very similar to that of *normal* switch.

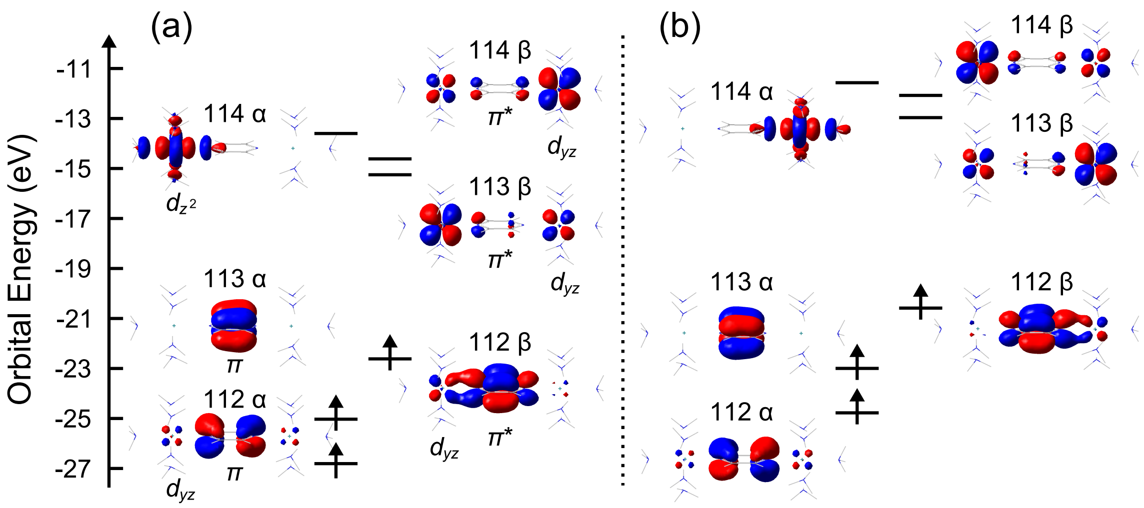

FIG. S 1: Frontier molecular orbitals and orbital energies of **py** complex calculated by HF method with (a) q^{i}=+0.5 and (b) q^{f}=−0.5. $r_{q-\mathrm{Ru}}$=5Å

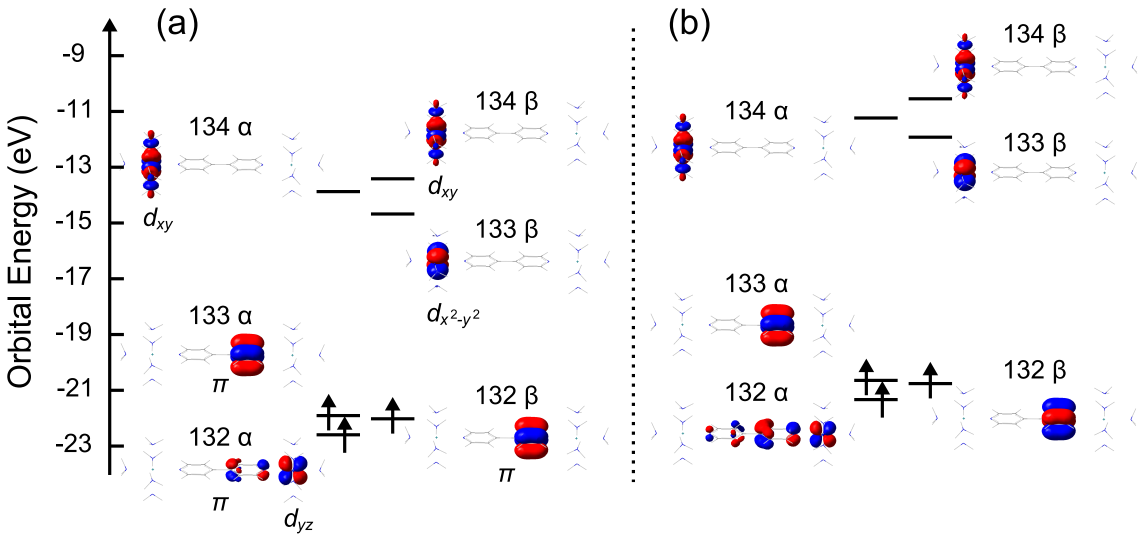

FIG. S 2: Frontier molecular orbitals and orbital energies of **bpy** complex calculated by HF method with (a) q^{i}=+0.5 and (b) q^{f}=−0.5. $r_{q-\mathrm{Ru}}$=5Å

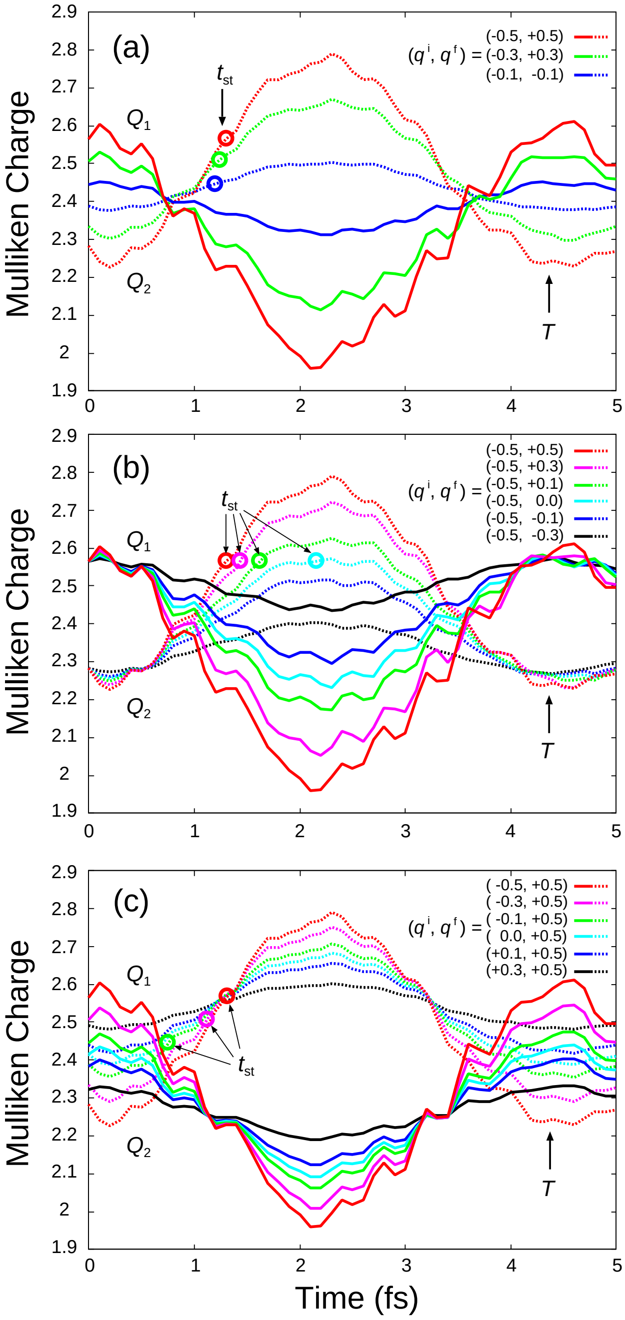

FIG. S 3: Time evolution of Mulliken charge of **py** complex calculated by DFT method upon reverse switch. (a) Both initial charge q^{i} and final charge q^{f} vary, but $|q^{\mathrm{i}}| = |q^{\mathrm{f}}|$: ($q^{\mathrm{i}}$, q^{f}) = (−0.5, +0.5), (−0.3, +0.3), (−0.1, +0.1). (b) Only final charge q^{f} varies: (q^{i}, q^{f}) = (−0.5, −0.3 ∼ +0.5). (c) Only initial charge q^{i} varies: (q^{i}, q^{f}) = (−0.5 ∼ +0.3, +0.5).