Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Conductance and Activation Energy for Electron Transport in Series and Parallel Intramolecular Circuits

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Supporting information

Fig. S1 and Fig. S2 show the activation energy of the six types of intramolecular circuits plotted versus N repeated units with the correlation time $\tau_c^{-1} = 0.0744$ eV. The cases (i)–(iii) and (iv)–(vi) correspond to series and parallel circuits, respectively. Fig. S1 exhibits several similar characteristics to Fig. 5. First, the conduction mechanism can be divided into three regimes. Second, the activation energies are almost zero in the tunneling regime while they are nearly the same non-zero values in the thermally activated hopping regime. Third, the activation energies of the cases (i)–(iii) are insensitive to the correlation time. Fourth, the cases (i) and (iii) have almost the same activation energy. That is, the activation energies are dominated by molecular units with larger on-site energy. For the parallel circuits, Fig. S2 also exhibits several similar characteristics to Fig. 8, but in contrast the activation energies of cases (vi) are dominated by units with smaller on-site energy. Therefore, we can conclude that the phenomenon– the activation energies of series circuits correspond to $E_{\mathrm{act},a}$ in series while the ones of parallel circuits correspond to $E_{\mathrm{act},b}$ in parallel– are insensitive to the

correlation time.

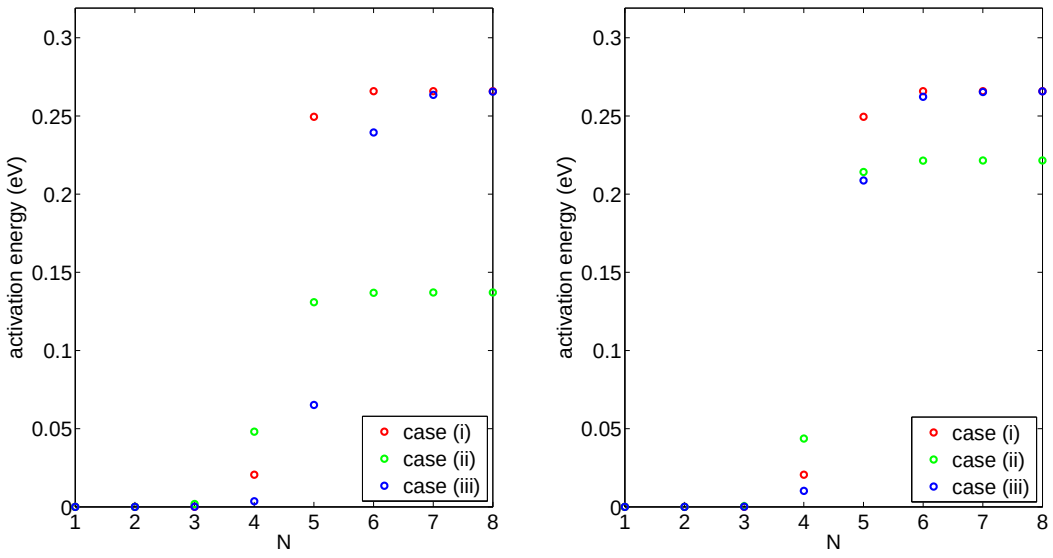

Figure S1: Activation energy of the three types of series circuits plotted against N repeated units with the correlation time $\tau_c^{-1} = 0.0744$ eV for (a) $E_b = 0.30$ eV and (b) $E_b = 0.40$ eV. The other parameters are the same as those in Figure 3(b).

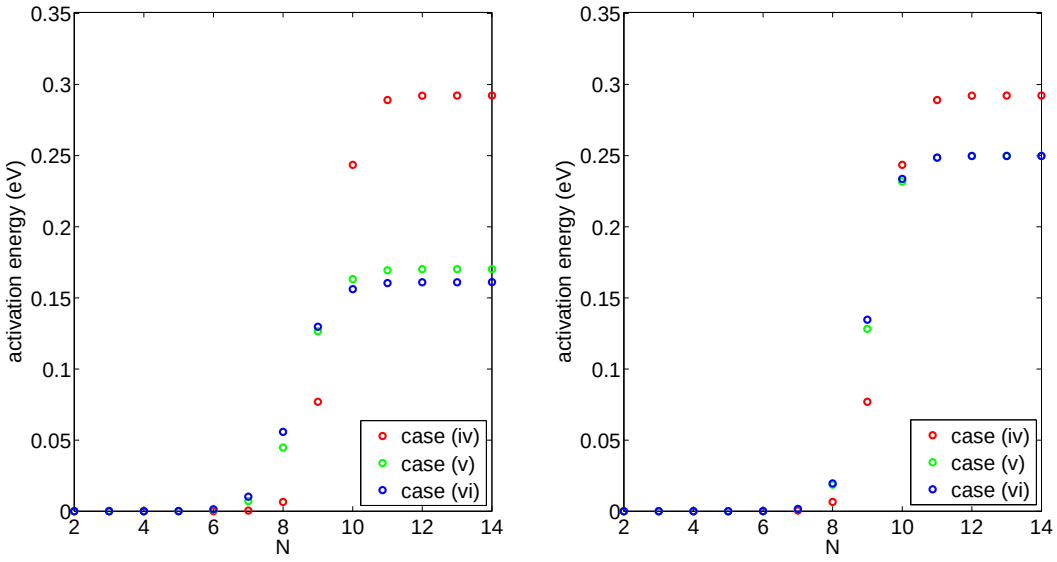

Figure S2: Activation energy of the three types of parallel circuits plotted against N repeated units with the correlation time $\tau_c^{-1} = 0.0744$ eV for (a) $E_b = 0.30$ eV and (b) $E_b = 0.40$ eV. The other parameters are the same as those in Figure 3(b).