Supplementary Material

Enhancing electron transport in molecular wires by insertion of a ferrocene center

Yan-Yan Sun,[a] Zheng-Lian Peng,[a] Rong Hou,[b] Jing-Hong Liang,[c] Ju-Fang Zheng,[a] Xiao-Yi Zhou,[a] Xiao-Shun Zhou,*[a] Shan Jin,*[b] Zhen-Jiang Niu[a], Bing-Wei Mao[c]

[a]Zhejiang Key Laboratory for Reactive Chemistry on Solid Surfaces, Institute of Physical Chemistry, Zhejiang Normal University, Jinhua, Zhejiang 321004, P. R. China.
E-mail: xszhou@zjnu.edu.cn
[b]Key Laboratory of Pesticide & Chemical Biology of the Ministry of Education, College of Chemistry, Central China Normal University, Wuhan 430079, P. R. China.
E-mail: jinshan@mail.ccnu.edu.cn
[c]State Key Laboratory for Physical Chemistry of Solid Surfaces and Chemistry Department, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen, Fujian 361005, P. R. China

Figure S1

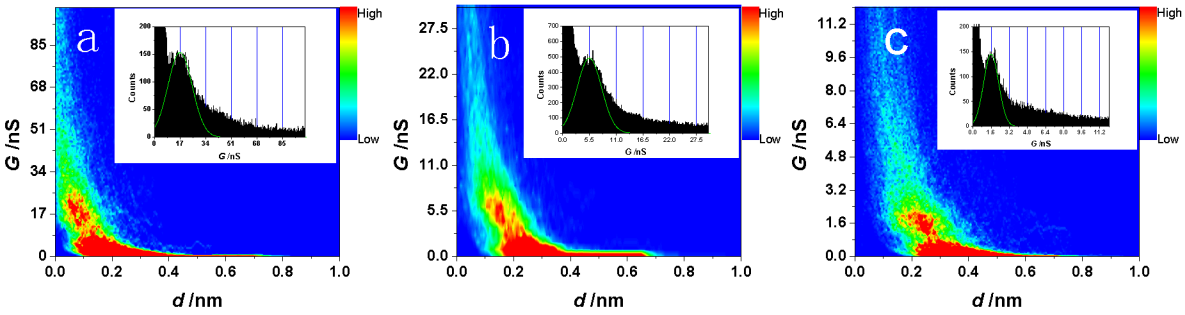


Figure S1 Two-dimensional histograms of (a) HC, (b) MC and (c) LC value of 1,4-Phenylenedipropionic acid. Insets are the corresponding conductance histograms.

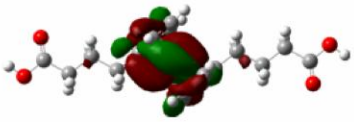
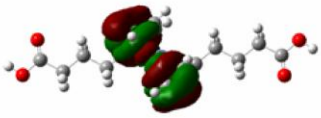
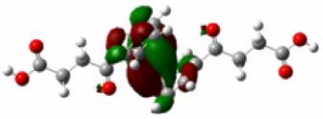
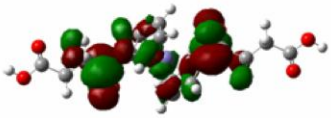
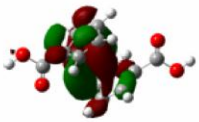
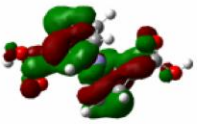
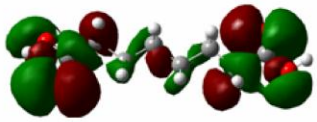
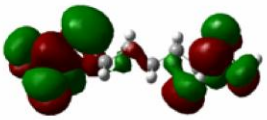
Table S1

Table S1 The HOMO and LUMO levels of molecules calculated by the DFT code SIESTA.

Molecules	**HOMO (eV)**	**LUMO (eV)**	**HOMO-LUMO Gap (eV)**
Fc-1	-4.22	-1.48	2.74
Fc-2	-4.55	-2.10	2.45
Fc-3	-4.54	-1.84	2.70
1,6-hexanedicarboxylic acid	-6.39	-1.12	5.27
terephthalic acid	-6.67	-3.18	3.49

Table S2

Table S2 The frontier molecular orbitals of Fc-1, Fc-2, Fc-3, 1,6-hexanedicarboxylic acid and terephthalic acid.

Molecules	HOMO	LUMO
Fc-1		
Fc-2		
Fc-3		
1,6-hexanedicarboxylic acid		
terephthalic acid