Supplementary Information for ***Acta Phys. -Chim. Sin.*** **2014**, *30* (1), 53-58
doi: 10.3866/PKU.WHXB201311081

碱金属原子掺杂 BDC60 分子中整流特性第一性原理研究

吴秋华 [1]　　赵　朋 [1,*]　　刘德胜 [2]

([1] 济南大学物理科学与技术学院，济南 250022; [2] 山东大学物理学院，晶体材料国家重点实验室，济南 250100)

First-Principles Study of the Rectifying Properties of the Alkali-Metal-Atom-Doped BDC60 Molecule

WU Qiu-Hua[1]　　ZHAO Peng[1,*]　　LIU De-Sheng[2]

([1]*School of Physics and Technology, University of Jinan, Jinan 250022, P. R. China*;
[2]*State Key Laboratory of Crystal Materials, School of Physics, Shandong University, Jinan 250100, P. R. China*)

∗Corresponding author.　Email: zhaopeng_sdu@sohu.com; Tel: +86-531-82769008.

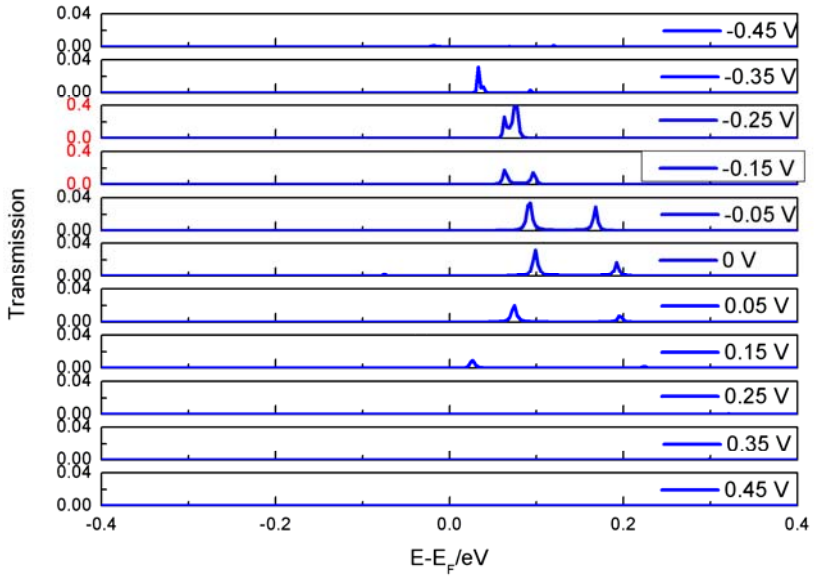

图 S1　K@BDC60 分子结在偏压为 0，± 0.05，± 0.15，± 0.25，± 0.35 以及± 0.45 V 时的透射率谱

Fig.S1　The bias-dependent transmission spectra of K@BDC60 molecular junction at biases 0, ± 0.05, ± 0.15, ± 0.25, ± 0.35 and ± 0.45 V, respectively

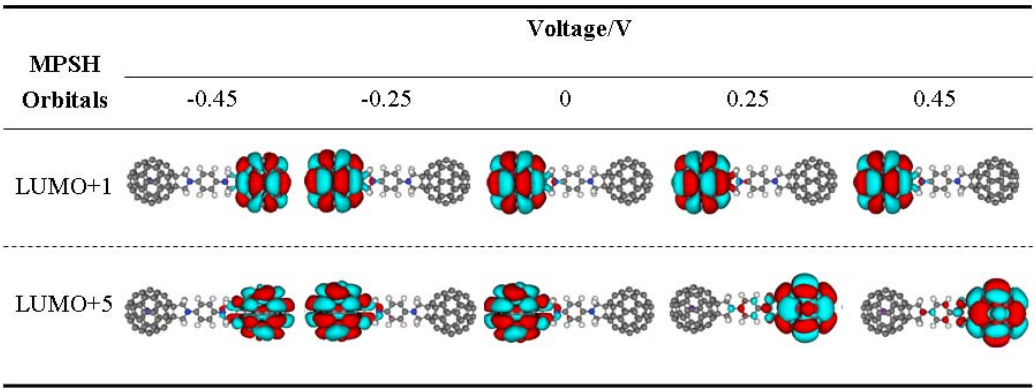

图 S2　K@BDC60 分子结的 LUMO+1 及 LUMO+5 两条分子轨道空间分布随外加偏压的变化

Fig.S2　The spatial distribution of LUMO+1 and LUMO+5 frontier molecular orbitals under different applied biases of K@BDC60 molecular junction