

Abstract Submitted  
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**Electron Transport through Polyene Junctions in between Carbon Nanotubes: an Ab Initio Realization**<sup>1</sup> YIING-REI CHEN, KAI-YU CHEN, Department of Physics, National Taiwan Normal University, KUN-PENG DOU, JUNG-SHEN TAI, Research Center for Applied Sciences, Academia Sinica, HSIN-HAN LEE, Department of Physics, National Taiwan Normal University, CHAO-CHENG KAUN, Research Center for Applied Sciences, Academia Sinica — With both *ab initio* and tight-binding model calculations, we study a system of polyene bridged armchair carbon nanotube electrodes, considering one-polyene and two-polyene cases, to address aspects of quantum transport through junctions with multiple conjugated molecules. The *ab initio* results of the two-polyene cases not only show the interference effect in transmission, but also the sensitive dependence of such effect on the combination of relative contact sites, which agrees nicely with the tight-binding model. Moreover, we show that the discrepancy mainly brought by *ab initio* relaxation provides an insight into the influence upon transmission spectra, from the junction's geometry, bonding and effective potential.

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