Abstract Submitted for the MAR17 Meeting of The American Physical Society

Transport through Polyene Junctions in between Angled-cut Armchair Carbon Nanotubes¹ YIING-REI CHEN, MING-KUAN LIN, National Taiwan Normal University — Single-polyene and two-polyene molecular junctions bridging carbon nanotube (CNT) leads are further studied in this work. We calculate and investigate the Greens function of the CNT leads from the edge into the bulk tube, to show the oscillation in the layer-by-layer DOS of the cross-cut armchair CNTs, and the edge states of the cross-cut zigzag CNTs. Also exhibiting a zigzag rim at the cut, an angled-cut armchair CNT gives a layer-by-layer DOS that shows not only evanescent edge states, but also an oscillation into the bulk tube. We study the polyene junction transport with these angled-cut armchair CNT leads, to find the interference between transport channels. The contributions from the bulk states and edge states are differentiated, by understanding the difference in the Greens functions obtained from direct integration method and iterative method, separately.

¹This work is supported by the Ministry of Science and Technology of the Republic of China under Grant No.105-2112-M-003-015-

Yiing-Rei Chen National Taiwan Normal University

Date submitted: 12 Dec 2016

Electronic form version 1.4