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An ab initio realization of the transport in molecular junctions with armchair carbon-nanotube leads[1] YIING-REI CHEN, HSIN-HAN LEE, National Taiwan Normal University — We perform an ab initio study for the system of molecular junctions with armchair carbon-nanotube leads. The transport behavior of the different 2-polyene junction cases shows remarkable agreement with the expected interference effect we predict with tight binding model which greatly simplified and omitted realistic parameters. Moreover, the slight disagreements between the ab initio study and the analytic study could be well understood with the parameter tests in the tight binding model.

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