Quantum Interference in Molecular Conductance through Alternant and Non-Alternant Hydrocarbons

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Exploring charge transport properties through single molecules is an active theoretical and experimental area not only in molecular electronics but also in molecular sensing. One of the most striking quantum effects in molecular conductance is destructive quantum interference (QI), where conductivity is significantly suppressed. Recently, growing attention has been devoted to QI because it has the potential to open doors to many new applications, such as thermoelectric devices, molecular switches, and spin filters. Predicting QI in both alternant and non-alternant hydrocarbons is a goal of theoretical work in molecular electronics.

A significant challenge to be addressed in molecular electronics is to further develop chemical intuition to understand and predict QI features. In this study, an orbital rule is markedly ameliorated so that it can capture the manifestation of QI not only in alternant hydrocarbons but also in non-alternant ones. The orbital-based prediction about the occurrence of QI in a non-alternant hydrocarbon shows good agreement with experimental results. A simple perturbation theoretic line of reasoning suggests that frontier orbital phase and splitting play a pivotal role in QI phenomena (see Figure 1).[1]

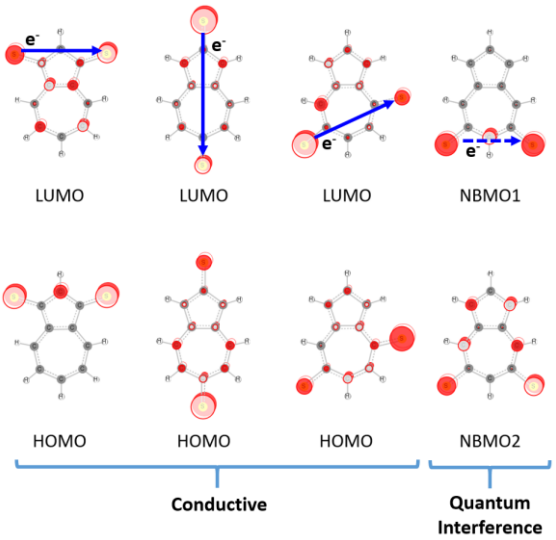

Figure 1. Orbital-based prediction of the occurrence of QI in a nonalternant, azulene.

1) Tsuji, Y.; Yoshizawa, K. *J. Phys. Chem. C* **2017**, *121*, 9621-9626.

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