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Vibrational effects to unidirectional π -electron rotation in an aromatic ring molecule with low-symmetry

Recently we proposed a new lasers-control scheme for unidirectional π -electron rotation in an aromatic ring molecule with low-symmetry having no degenerate electronic states [1]. In this control scheme we assumed a fixed nuclei condition, and two relevant excited states subject to dynamical Stark shift using two linearly polarized UV lasers. Each laser is set to selectively interact with one of the two electronic states, the lower and higher excited states are shifted up and down with the same detuning, respectively, and two excited states become degenerate at their midpoint.

In this presentation for more realistic numerical simulation of unidirectional pi-electron rotation, we take into account the nuclear vibrational effect in a molecular system. The total wave function is separated into electronic and nuclear parts under the B.O approximation. The vibrational states in each excited state follow the Franck-Condon principle. It is also interesting to investigate the interactions between the relevant two electronic states through the vibronic (non-adiabatic) couplings, and the vibronic couplings through the breakdown of the B.O approximation can be estimated at the equilibrium nuclear distance. We show a result of numerical simulation and discuss how the nuclear vibrations affect the unidirectional pi-electron rotation.

Reference

[1] H. Mineo, M. Yamaki, G.S. Kim, Y. Teranishi, and Y. Fujimura, Phys. Chem. Chem. Phys. 18, 26786 (2016).

Author: Mr LA, kiet (Master student, Ho Chi Minh City University of Education)