Dynamics of excited states in carbon nano-rings

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The nano-rings of cycle-para-phenylenes (CPPs) and related compounds represent model systems to study the optical properties of carbon nanotubes. Because of their cyclic conjugation, these structures present unique and interesting photophysical properties [1]. In the present work, we investigate the excited-state, non-adiabatic dynamics of a set of nano-rings which are composed by a segment of seven phenylene interconnected units. The rings are closed by an alyphatic chain of variable length [2], which join the extremes of the phenylene segments. We analyze the effect of the curvature of the nano-rings on the photoexcitation dynamics, and on the subsequent relaxation and redistribution of the excess energy among the electronic and the vibrational degrees of freedom. Specifically, we focus our attention on the influence of the curvature on the localization/delocalization of the electronic transition density, the mechanism of the energy transfer (i.e., through bond or through space), the non-adiabatic couplings, and the impact of the thermal fluctuations on the population transfer to the lowest excited state. Since the relaxation process involves many coupled electronic states, we employ standard tools for dynamical calculations of excited states in non-adiabatic systems [3], in order to compute the electronic state energies, their gradients and couplings.

References

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