Quantum dynamics of photoprocesses in extended molecular systems

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Conjugated polymers and similar extended, photoactive systems are not only characterized by the properties of the single building blocks but also by the intrinsic properties of excitations in delocalized electronic systems involving the formation and dynamic of excitonic states. A variety of site-site interactions involving excitation energy transfer (EET), charge transfer (CT), vibronic couplings and trapping effects determine the dynamical behavior of extended systems. The associated electron-phonon couplings and coherent dynamical effects require a rigorous quantum dynamical treatment.
The coherent, torsion-driven EET in poly-phenylene-vinylene (PPV)[(i)] oligomers is investigated using the multiconfiguration time-dependent Hartree (MCTDH)[(ii)] method as well in its original form as in the modified version using variational multiconfigurational Gaussians (G-MCTDH)[(i)]. The parametrization of the applied Hamiltonian is based on semiempirical and ab-initio calculations.

References

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