

Dynamics of electronically excited cytosine stacks. Utz, Wolfram; Foerner, Wolfgang; Ladik, Janos.

Abstract

The dynamics following localized excitation of a mol. in a chain of stacked ring-shaped arom. mols. was studied. A cytosine stack was chosen as a model system, since the study is based on recent ideas on the mechanism for the creation of double-strand breaks in DNA which require energy transport through DNA. After a π - π^* -excitation a cytosine mol. increases the size of its ring. The excitation and the accompanying geometrical changes are coupled to the electronic system of the chain in a non-linear manner. A tight-binding ansatz with parameters taken from ab initio Hartree-Fock calcns. was used as a math. model for the π -electrons. Initially an excitation is localized on one mol. and these localized excitations move in a random manner through larger parts of the chain. Although this phenomenon most probably is not a solitary wave, the non-linear quasiparticles found in this system transport energy along the chain.