Photonics of molecular systems

V.Ya. Artyukhov, G.V. Mayer

Tomsk state university, Lenina av., 36, 634050, Tomsk, Russia, artvic@phys.tsu.ru

An intensive development of molecular organic electronics and optical nanomaterials on the basis of organic compounds demands an establishment of interrelations of physical and chemical properties of organic molecular systems (structures) with features of intermolecular interactions and an exciting electromagnetic field.

In the given report influence of intermolecular interactions on electronic states and spectral-luminescent properties of bimolecular system is considered. It is shown, that as the initial stage of quantum-chemical research of this influence the analysis of spatial structure of one-electronic states (molecular orbitals) is necessary.

Using for construction of wave functions of the excited electronic states of single configurations from molecular orbitals the analysis of types of spatial localization of the excited electronic states of bimolecular systems is carried out. At use for calculation bimolecular systems of modern packages of quantum-chemical programs the Hamiltonian system always automatically are included by a member corresponding to intermolecular interaction. Reduction (disappearance) of influence of intermolecular interaction for set-up conformation (a relative spatial arrangement) can be reached only distance increase between system components.

In bimolecular systems intermolecular electronic transitions can be carried out both monomolecular, and. Intermolecular interaction not only defines possibility of intermolecular photoprocesses, but also changes probabilities of monomolecular photoprocesses.

Features of spectral-luminescent properties of multimolecular systems are discussed.

1. V. Ya. Artyukhov and G. V. Mayer. Intermolecular interactions and photoprocesses in molecular systems. Russian Physics Journal, Vol. 55, No. 7, p. 834-842.