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OPTICAL PROPERTIES OF FILMS BASED ON MEROCYANINE DYES

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Merocyanine dyes are donor-acceptor polimethine molecules with unique spectroscopic properties used for design of advanced photonic materials, solar cells ets. Merocyanines, with their wide absorption bands, are suitable applicants for this goal. Optical characteristics of such compounds are very sensitive to a type of solvent, molecular concentration due to that methods and conditions of films preparation should influence their spectra.
Quantum-chemical calculations of optimized molecular geometry for single molecules and their aggregates were performed using ab initio density functional theory method DFT/CAM-B3LYP//6-31G(d, p), transition characteristics were calculated using semi-empirical ZINDO method in Gaussian 09 program package.
Absorbance of films of merocyanine dyes prepared by spin coating on the films comparing to the spectra in solution undergoes to shift of absorption maximums towards red region and new wide maxima appear; absorption intensity of the main peak decreases.
The first one is caused by interaction of the considered molecules due to alternation of atomic charges on the molecular chromophores. As a result of that J- and T-type aggregates are formed, which is confirmed by quantum-chemical calculations. According to the obtained data T-aggregation prevails. Therefore, merocyanine dyes in films absorb more wide spectral region, that is useful for harvesting of solar energy in order to transform it into electricity power in solar elements of organic electronics.

Topics

Session D. Biomedical optics and sensors technology

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