МІНІСТЕРСТВО ОСВІТИ І НАУКИ УКРАЇНИ
СУМСЬКИЙ ДЕРЖАВНИЙ УНІВЕРСИТЕТ

ФІЗИКА, ЕЛЕКТРОНІКА, ЕЛЕКТРОТЕХНІКА

ФЕЕ :: 2017

МАТЕРІАЛИ
та програма

НАУКОВО-ТЕХНІЧНОЇ КОНФЕРЕНЦІЇ

(Суми, 17–21 квітня 2017 року)

Суми
Сумський державний університет
2017

Possible route of the merocyanine-spiropyran transition

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Modern nanotechnological revolution is based on the use of bistable molecules and molecular ensembles as basic elements of high-tech devices.

In this work quantum-mechanical investigations of the potential surface merocyanine-spiropyran transformation were carried out. Under dark conditions, such transition will be possible when potential barrier with height ~ 0.7 eV is overcomed. Rotating the phenyl moiety relative to the plane of the molecule by 90 ° without simultaneously changing all other parameters of the molecule (optimization of the molecular structure) increases the molecule's energy by 1.376 eV.

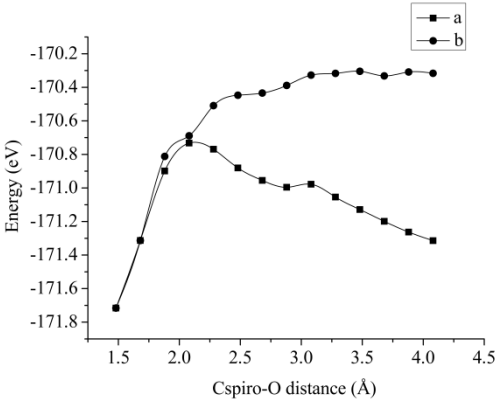

Figure 1 − The dependence of the electron system's energy of the molecule from the Cspiro-O distance in a case of an ordinary MC → SP transition (a) and MC →SP transition with fixed 90º angle between indoline and phenyl (b).

The excitation of the merocyanine molecule to the S1-state makes the rotation of the phenyl moiety by 90° energetically beneficial. At the same time, the energy distance ΔE (S0 → S1) decreases to 0.58 eV. This ensures a rapid nonradiative relaxation of the excitation of the molecule.

The reversible transformation from spiropyran to merocyanine molecule under the light influence can serve as a conductivity switch of a cell. Such cell will be based on a single spiropyran molecule.