Nanoscale physics

Electrochemical Spiropyran-Merocyanine isomerization

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Nowadays one of the important places in nanotechnologies is assigned to development of nano and molecular electronics. Molecular materials with responsive physical properties are very significant for the design and development of such devices [1]. One of the principle of this devices is photochromism. Another less well-studied principle is electrochromism. One of good example of molecule that satisfies these principles is Spiropyran molecule.

Thus, the aim of this work was to investigate the mechanisms of anionic and cationic spiropyran (SP) – merocyanine (MC) conversion and the field effect on these pathways.

The reaction pathways and intermediate states of anionic and cationic SP-MC conversion are similar with neutral one. But the geometries and the values of energy barriers have been changed noticeably. This is due to the changes in electron density distribution. According to experimental studies the oxidation of SPs takes place in the indole part of the molecule while the reduction takes place in the benzopyran part. Our computational study fully confirms these results.

The neutral and cationic SPs are relatively stable, so they can't be easy changed. In contrary to neutral and cationic isomerizations, anionic SP-MC isomerization has a spontaneous behavior.

Another part of this work is devoted to investigation of field influence on the ring-opening process in the anionic and cationic SP. We've placed a center of Cartesian coordinates is in Cspiro atom. We've observed that the behavior of the system and the geometric structures depends on the direction of applied field. Field that was applied in the direction of benzopyran part favors the ring-opening. Field that was applied in the direction of indole part favors ring closure.

Our results shows the possibility of ring opening and closure control using external inputs.

1. *Singh R., Bohm M., Balasubramanian G.* Energetic and structural properties of different conformations of merocyanine and its protonated forms // Chem. Phys. Let.-2015.**-633.-**P. 287-291.