عنوان مقاله:

Theoretical study of the structure, vibrational spectra and electronic spectra of TCPP-TCPP as co-sensitized solar cells

محل انتشار:

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خلاصه مقاله:

In this study, we present calculations of various properties of the tetrakis(carboxyphenyl)porphyrin (TCPP) and its complex with Cu (CuTCPP) and TCPP-TCPP couple as sensitizers. The Density Functional Theory (DFT) and Time Dependent DFT (TDDFT) study of these sensitizers were performed, investigating on the geometry, electronic structure and optical properties of the dyes both in the gas phase and in chloroform solution. The absorption bands are assigned to π→ π* transitions. Calculations have been performed using the B3LYP exchange correlations functional, as implemented in the Gaussian09 program package. The geometries of were first optimized using density functional 6-311G(d) method. Natural bond orbital (NBO) analysis was also conducted on optimized geometries. From the orbital analysis and the orbital spatial orientation of HOMO and LUMO for sensitizers, the results show that TCPP-TCPP couple seems to provide higher photo-to-electric conversion efficiencies.

کلمات کلیدی:

Porphyrin, Theoretical study, DFT, Optical absorption, DSSCs