

«The calculation of the fluorescence quantum yield of conjugated compounds with density functional theory»

Nuraliev M.K.

For electronic devices like light-emitting transistors or light-emitting diodes, internal fluorescence quantum yield is the key value to characterize the light efficiency. For organic conjugated compounds, the internal fluorescence quantum yield can be estimated as the ratio of the radiative relaxation constant to the sum of radiative and non-radiative relaxations constants. Non-radiative transitions include internal conversion and intersystem crossing. In this work, it is supposed that the main channel of non-radiative relaxation is the intersystem crossing. Spin-orbit interaction during the transition of molecule from the singlet state to triplet state is the reason of intersystem crossing. To calculate the rate of intersystem crossing, it is necessary to estimate the matrix element of the spin-orbit interaction. We propose a simple model where the matrix element of the spin-orbit interaction was estimated with the electron density at all atoms. All calculations in the current work were performed using the Density Functional Theory (DFT).

The simple model is applied for oligothiophene-phenylenes and oligoacenes. For oligothiophene-phenylene compounds, the results show a good correlation with experimental values in solution from the literature obtained. Also it was shown that the presence of a phenyl in the center of the molecule increases the fluorescence quantum yield. In oligoacenes, the fluorescence quantum yield is estimated as unity. That values are not observed in experimental data for solutions. The first reason of this discrepancy is the intersystem crossing to the excited triplet state. The second reason is there is no accounting for internal conversion within this model.