COMPUTATIONAL DFT MODELLING OF OPTICAL PROPERTIES OF NEW NEUTRAL HEXACOORDINATED SI(DPP)2 COMPLEX

Bimukhanov A.N., Aldongarov A.A., Irgibaeva I.S.
L. N. Gumilyov Eurasian National University, Republic of Kazakhstan

In recent years, there has been a significant increase in a structural diversity of stable hexacoordinate silicon complexes, especially ones containing pincer ligands. Also they are attractive candidates for organic electronic applications including OLED, OPV, and OFETs since they are thermally robust, redox-active, non-polar, and electronically tunable through synthetic modification [1-3].

In our work we consider optical properties, based on the density functional theory, of new neutral hexacoordinated $Si(DPP)_2$ complex, containing the 2,6-diphenyl pyridine ligand. Recently we were able to synthesize and explore $Si(DPP)_2$ compound as a potential electron transport layer and electroluminescent layer in organic electronic devices [4]. Computational modelling helps to make a comparative analysis of theoretical and recent experimental data for studying the optical properties. In previous studies, we were able to show that experimentally observed properties are reasonably matched with predicted theoretical calculations [5].

All quantum-chemical calculations of the $Si(DPP)_2$ complex have been carried out using density functional method, implemented in the Gaussian09 software package [6]. Nowadays, this method includes a wide range of different functionals. Properties of the object have been calculated using B3LYP functional.

Analysis of the obtained data using computational modeling additionally helps to investigate the electronic structure and gives a better understanding the balanced bipolar nature of $Si(DPP)_2$ structure. For example calculations of highest occupied molecular orbital (HOMO) helped to observe unusual delocalized σ-orbital symmetry around the SiC_4 plane, in case of lowest unoccupied molecular orbital (LUMO) by contrast is a more conventional delocalized pi-orbital spread out over the entire molecule.

On the ground of comparison of theoretical and experimental structural and optical data it was shown that the theoretical method we have used describes $Si(DPP)_2$ complex reasonably well.

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