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Original Research

The Role of Insertion of Li atom in C_{60}-Porphyrin-Metalloporphyrin, M = (V, Cr, Ni, Cu) as dyes in the DSSC by Using the Theoretical Outlook

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ABSTRACT

In the present investigation, density functional theory with Grimme correction and time-dependent semi-empirical ZINDO/S approaches have been employed to scrutinized supra-molecular triad system as a dye sensitizer and also effect of insertion of Li atom into the C60 cavity. The impacts of the kind of transition metal in the Porphyrin ring and insertion of Li atom in the C60 fullerene on the energies of frontier molecular orbital (FMO) and UV–Vis spectra have been considered. Structural optimizations of supra-molecular triad and quantum molecular descriptor (QMD) have been carried out through the SIESTA package. We have analyzed charge transfer between two interacting species trough well-known Mulliken, Hirshfeld and Voronoi charges analysis. In addition light-harvesting efficiency (LHE), electronic transitions, chemical hardness (η), electrophilicity index (ω), electron accepting power (ω+) have been obtained with using the Orca package. We can learn that supra-molecular triad complexes Li@C_{60}–Porphyrin–Metalloporphyrine (M = V, Cr, Ni and Cu) with low energy gap, highest light-harvesting efficiency (LHE) are outstanding efficient as Dye-sensitized solar cell (DSSC) industry.

Keywords: Dye-sensitized solar cell; encapsulation; LHE; DFT; TD-semiempirical

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