Abstract

Photovoltaic (PV) cells are one of the most promising alternatives for non-renewable energy resources to facilitate the current energy crises. The future energy scarcity can be dealt with contributions towards cost effective materials for photovoltaic applications. The focus of this research is the synthesis of Schiff bases from phenylene diamine for potential applications in photovoltaics. A novel series (DMBA1-DMBA9) of phenylene diamine analogues with A-π-A and D-π-D type framework is reported in this study. These chromophores are based on phenylene diamine as a π-linker, while the donor moieties in DMBA1, DMBA2, DMBA3, DMBA4, and acceptor moieties in DMBA5, DMBA6, DMBA7, DMBA8, DMBA9 are 1H-indole-4-carbaldehyde, 1H-indole-5-carbaldehyde, 1H-indole-7-carbaldehyde,1H-indazole-5-carbaldehyde,6-chloro-1H-indole-3-carbaldehyde,2-(pyridin-3-yl)benzaldehyde, 6-fluoronicotinaldehyde, 2-chloro-3-fluoroisonicotinaldehyde, and 6-methoxypicolinaldehyde respectively. The structural investigation of the synthesized chromophores has been achieved by 1H-NMR and 13C-NMR, which confirms the formation of Schiff bases. The entire quantum chemical computational study of compounds (DMBA1-DMBA9) was done by utilizing Gaussian 09 program to conduct DFT/TDDFT calculations in association with M06/6-311G(d,p) basis set. The frontier molecular orbitals (FMO) analysis, and global reactivity parameters were also determined. The results of transition density matrix (TDM) analysis performed at DFT level were in accordance with FMO analysis. The electronic charge density was also investigated by DOS with the help of PyMOlyze 2.0 program. The UV/Vis absorption maxima showed that all the synthesized chromophores undergo bathochromic shift in solvent and gas phase. The exciton binding energy Eb calculated for these novel compounds was less than 1.9 eV. Hence, this series of compounds (DMBA1-DMBA9) proved to be potentially stable and promising for photovoltaic applications.