World Academy of Science, Engineering and Technology
International Journal of Chemical and Molecular Engineering
Vol:11, No:11, 2017

Designing Dibenzosilole and Methyl Carbazole Based Donor Materials with Favourable Photovoltaic Parameters for Bulk Heterojunction Organic Solar Cells

Authors : J. Iqbal, Z. Zara

Abstract : Five new Acceptor-Donor-Acceptor (A-D-A) type small donor molecules (M1-M5) namely; dimethyl cyanoacetate terthiophene di(methylthiophene) dibenzosilole (DMCAO3TBS) (M1), dimelononitrile terthiophene di(methylthiophene) dibenzosilole (DMCNTBS) (M2), dimethyl rhodanine terthiophene di(methylthiophene) dibenzosilole (DMRTBS) (M3), dimelanonitrile terthiophene di(methylthiophene) methyl fluorene (DMCNTF) (M4) and dimethyl rhodanine terthiophene di(methylthiophene) methyl fluorine (DMRTF) (M5) were designed and theoretically explored their electronic, photophysical and geometrical properties via DFT best functional MPW1PW91/6-311G (d,p) level of theory with respect to reference molecules dioctyl cyanoacetate terthiophene di(octylthiophene) dioctylfluorene (DCAO3TF) (Ra) and dioctyl cyanoacetate terthiophene di(octylthiophene) octylcarbazole (DCAO3TCz) (Rb). Among the designed donor molecules (M1-M5), M2 and M4 represented lowest band gap value (2.480 eV and 2.47 eV) with distinctive broad absorption peak at 598 and 601 nm in chloroform due to the presence of stronger electron withdrawing acceptor molecule which pulls the λmax value towards red shift. Theoretically estimated reorganization energies of these molecules recommended excellent property of charge mobility. The designed donor molecules M1-M5, demonstrated lower λe value with reference to their λh, showing that these molecules could be ideal candidates for the transfer of electron with and M2, M4 are best among these as champion molecules with having lowest λe (0.006 D and 0.005 D respectively). Additionally, the Voc of M2 and M4 are 2.01 eV and 1.85 eV respectively with reference respect to PCBM. Thus, our present investigation suggested that our designed donor molecules (M1-M5) are suitable candidates for the solar cell and proposed for high and better performance for the small molecule based solar cell devices.

Keywords : dibenzisilol, donor materials, hole mobility, organic solar cells
Conference Title : ICCCC 2017 : International Conference on Chemistry and Chemical Compounds
Conference Location : Havana, Cuba
Conference Dates : November 23-24, 2017