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The torsional potential energy surfaces of conducting polymer in the class of carbazole derivatives were carried out by *ab initio* (HF and MP2) and density functional theory (B3LYP and BH&HLYP) calculations with several basis sets. The torsional potentials were fitted to a six-term truncated Fourier expansion for validity the methods and basis sets. The results show that the exchange-correlation (B3LYP and BH&HLYP) effects of density functional theory tend to systematically decrease the relative torsional energies. The ground state geometries from BH&HLYP calculations can provide relatively accurate predictions of vertical excitation energies better than that of obtained from B3LYP geometries. This can suggest that the Fourier least-squares-fitted method is appropriate for method validation. The vertical excitation energies were calculated by the time-dependent density functional theory using BLYP, BP86, BH&HLYP, PBE1PBE and B3LYP functional with the 6-311++G(2d,2p) basis set based on B3LYP/6-311G(d,p) optimized geometries. From the results, TD-PBE1PBE and TD-B3LYP methods predict the excitation energies for Cz-dimer, Cz-co-Fl and Cz-co-Th (3.84, 3.83 and 3.89 eV, respectively) in good agreement with experimental data (3.85, 3.83 and 3.84 eV, respectively). An analysis of the vertical singlet-singlet transition was also performed and the results indicated that for Cz-dimer, Cz-co-Fl and Cz-co-F, S_1 transition plays an important role, whereas the S_2 is important for Cz-co-P and Cz-co-Th. Excitation to the S_1 and S_2 states corresponds almost exclusively to the promotion of an electron from the HOMO to LUMO. In Cz-co-F, this transition is unstable due to low oscillator strength. The structural geometries of ground and excited state were performed by the B3LYP and TD-B3LYP, respectively, using several density functional theories with the SVP and TZVP basis sets. The geometry of excited state was found to be more planar than ground state. Absorption and emission energies from the relaxed excited states were obtained from TDDFT calculations performed on the S_1 optimized geometries and excellent agree well with experimental data.

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