Quantum chemical approach toward rational designing of highly efficient oxadiazole based oligomers used in organic field effect transistors

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Abstract

Density functional theory (DFT) is well suited to explore the properties of the conjugated pi-electron systems. We report the ground-state geometry optimization of newly designed oxadiazole based oligomers using the DFT method with B3LYP functional and 6-31G(auau) basis set. In addition, the relevant absorption spectra at the TD-B3LYP level are also discussed. The LUMO energies of systems 3-system 8 are smaller than the parent molecule (system 1) which revealed that these would be better electron transfer materials than parent molecule. The electrons transported by system 4, system 6, and system 7 would be stabilized against the environment. In addition, it can be seen from their plots of frontier MOs that there exist the conjugated delocalized pi-electron systems in these derivatives and the involvement of electron withdrawing groups will increase their conjugated properties so that the absorption wavelengths are red-shifted. The system 4-system 7 are showing the prominent red-shift of 33, 59, 28 nm, and 11 nm, respectively compared to system 1.

Keywords

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