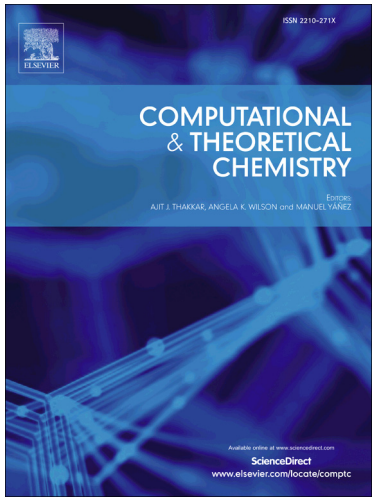

A DFT Study on reactivity, aromaticity and absorption spectra of Perylo[1,12-b,c,d] thiophene tetraester doped with B, N, O, Se and BN

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Abstract:

Reactivity, aromaticity and absorption spectra of Perylo[1,12-b,c,d] thiophene tetraester doped with B, N, O Se and BN have been discussed in the light of Density Functional Theory (DFT) and Time Dependent Density Functional Theory (TDDFT). Doping with electron rich and electron deficient centres affects the reactivity and aromaticity of the thiophene tetraesters. A significant shift in the absorption spectra is observed in case of B and BN doped species. Aromaticity of the species is gauged by nucleus independent chemical shift (NICS). Results show that the doped species vary in their reactivity and aromaticity. N, O or Se doped species exhibit almost comparable excitation energies and absorption peaks.

Keywords: Reactivity, absorption spectra, thiophene tetraester, excitation energy, aromaticity, NICS.