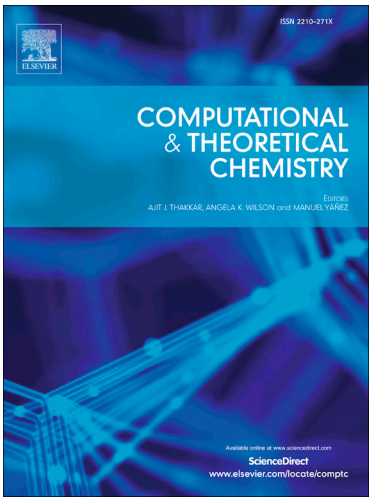

Theoretical Study on Functionalized Anthracene and Tetraceneas Starting Species to Produce Promising Semiconductor Materials

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Theoretical Study on Functionalized Anthracene and Tetraceneas Starting Species to Produce Promising Semiconductor Materials

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Abstract:

In this study, density functional theory calculations were carried through on semiconductor species based on anthracene and tetracene. In particular, the effects of functionalization by electron with-drawing groups(F, Cl, NO_2,CN, and N) on the electronic properties of anthracene and tetracene were studied. According to the calculations, functionalizingby F, Cl, NO_2, and N increases the reorganization energies (λ^+ and λ^-)compared to those of CN-functionalized systems. On the other hand, the functionalization of anthracene and tetracene leads to an enhancement of the adiabatic electron affinities (EA) and the 1^{st} ionization potential (IP) in addition to reducing the HOMO-LUMOenergy gap which implies that the resulting species will have lower kinetic stability and higher carrier mobility compared to unsubstituted anthracene and tetracene.

Keywords: functionalization, anthracene, tetracene, reorganization energy, HOMO-LUMO energy gap.