Physico-chemical nanomaterials science

A Computational Study on the Some Physical Properties of $C_{42}H_6S_6$ Molecule and Its Substructures

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The extraordinary properties and expected potential applications of carbon based materials such as fullerene, graphene and graphyne have motivated substantial research efforts on similar structures [1]. Some graphyne structures were proposed by computationally in 1987 for possible electronic, optical and mechanical properties [2].

We replaced benzene ring by thiophene ring of some graphyne substructures. The new five thio-graphyne substructures have been studied, biggest on $C_{42}H_6S_6$ as in Figure below, computationally. We have studied the structure, energetic, electronic and optical properties of proposed five thio-graphyne substructures. All calculations were performed using density functional theory at the B3LYP/ 6-31+g(d,p) levels.

Figure. $C_{42}H_6S_6$ Structure

1. *Cranford S. W., Buehler M.J.* Mechanical properties of graphyne // Carbon -2011.-P. 4111-4121.
2. *Baughman R. H., Eckhardt H., Kestesz M.* Structure-property predictions for new planar forms of carbons.: Layered phases containing sp^2 and sp atoms // J. Chem Physics-1987.**-87.-**P. 6687-6699.