Physico-chemical nanomaterials science

DFT calculations on the Structure, Electronic and Optical Properties of hBN-$C_{66}H_{17}$ Molecules

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The hybridization flexibility (sp, sp^2 and sp^3) of carbon atom leads to bonding ability to other carbon atoms gives a variety of carbon allotropes such as diamond, graphite, fullerene and carbon nanotubes. After the experimental isolation of graphene in 2004, all 2D carbon allotropes have subjected a great attention. One of them is 2D graphyne structure and its sub/derived structures [1,2]. Some graphyne and gaphyne-like 2D structures were proposed by computationally with possible applications in science and industry [1,2]. One of the proposed graphyne-like structure is $C_{66}H_{17}$ molecule as in Figure below. We replaced selected benzene ring(s) by borazine ring(s) of $C_{66}H_{17}$ graphyne substructure. We have studied the structure, highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energies, polarizability, anisotropic polarizability and first static hyperpolarizability properties of proposed hBN-graphyne substructures. All calculations were performed using density functional theory at the B3LYP/6-31g(d,p) level.

Figure. $C_{66}H_{17}$ Structure

1. *Cranford S. W., Buehler M.J.* Mechanical properties of graphyne // Carbon -2011.-P. 4111-4121.
2. *Kim B.G, Choi J. H.* Graphyne: Hexagonal network of carbon with versatile Dirac cones // Phys. Rev. B-2012.-**86.**-P. 115435-115440.