HSEh1PBE- BASED ANALYSIS ON STRUCTURAL AND ELECTRONIC PROPERTIES OF THE NON-STOICHIOMETRIC SILICON CARBIDE FULLERENE (Si$_{24}$C$_{36}$)

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We present the results of first-principles molecular orbitals calculations (HSEh1PBE/6-31g(d) [1]) describing the structural and electronic properties of a new silicon carbide fullerene (SiCF) rich in carbon with a chemical composition of Si$_{24}$C$_{36}$ for the pristine case (in analogy to Boron Nitride fullerene [2]) and doped with nitrogen atoms (Si$_{24}$C$_{36-n}$N$_n$; n=1,5,10,15,20). The results of the simulation indicate that no complex frequencies are obtained; this guarantees the stability of the structure 0D. Also, it presents non-magnetic semiconductor characteristics (HOMO-LUMO gap of 0.89 eV), high polarity, 1.16 D, and low chemical reactivity (?=-5.75 eV), which makes it viable for applications such as drug delivery.

On the other hand, when it is doped with nitrogen atoms shows a transition semiconductor-conductor due to reduction of HOMO-LUMO gap and work function. This behavior indicates their possible usefulness for device design.

**Keywords:** First-Principles Calculations, fullerene, Silicon Carbide

**References:**


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