Effet of edge fluorination and chlorination on structures, stability, electronic and charge transport properties of benzo[o]bistriphenylene[2,1,12,11-efghi:2',1',12',11'-uvabc]ovalene molecule : DFT study.

Marius Ousmanou Bouba

University of Maroua: Universite de Maroua

Fridolin Tchangnwa Nya (✉ nyafridolin@yahoo.fr)

University of Maroua: Universite de Maroua <https://orcid.org/0000-0002-8882-6987>

Christine Yvette Ngui

University of Maroua: Universite de Maroua

Jean Marie Ndjaka

University of Maroua: Universite de Maroua

Research Article

Keywords: DFT, Charge transport, n-type material, Optoelectronic, Nanographene

Posted Date: February 22nd, 2021

DOI: <https://doi.org/10.21203/rs.3.rs-213420/v1>

License: This work is licensed under a Creative Commons Attribution 4.0 International License.

[Read Full License](#)

Abstract

We have investigated the structures, electronic properties, hole and electron mobilities of fluorinated and chlorinated nanographene of benzo[*o*]bistriphenyleno[2,1,12,11-efghi:2',1',12',11'-uvabc]ovalene (TCHG) molecules, using the density functional theory (DFT) and Marcus-Hush charge transfer theory. The calculated geometric parameters and the IR spectrum for chlorinated TCHG are in good agreement with the experimental data. Our theoretical investigations have shown that fluorination and chlorination significantly reduce the bandgap energy of TCHG. The obtained adiabatic electron affinities (AEAs) values are 2.76 and 2.93 eV respectively, indicating the air-stable materials. The calculation of charge carriers mobilities in chlorinated dimer shows that the mobility of the electrons is ten times that of the holes, suggesting an n-type behavior. We have shown that the fluorination and chlorination of TCHG are promising pathways for the design of new materials useful in optoelectronics

Full Text

Due to technical limitations, full-text HTML conversion of this manuscript could not be completed. However, the latest manuscript can be downloaded and [accessed as a PDF](#).

Figures

Figure 1

Monomeric structures of (a) TCHG, (b) TCFG and (c) TCCG. As optimized at the B3LYP-D3/6-31+G(d,p) level of theory.

(a)

(b)

(c)

Figure 2

B3LYP-D3/6-31+G(d,p)-calculated bond-length change (in Å) upon reduction and oxidation in (a) TCHG, (b) TCFG and (c) TCCG molecules.

Figure 3

Vibrational IR spectra of (a) TCHG, (b) TCFG and (c) TCCG at the B3LYP/6-31+G(d,p) level.

(a)

(b)

(c)

Figure 4

Total, partial and overlap density-of-states of (a) TCHG, (b) TCFG and (c) TCCG. H and L designate HOMO and LUMO levels, respectively

Figure 5

Optimized dimeric structures of (a) TCHG, (b) TCFG and (c) TCCG. As optimized at the ω B97XD/ 6-31g(d) level of theory.

Figure 6

Top-view and side-view plots of schematic diagrams of isosurfaces (a-c) for dimeric TCHG , TCFG and TCCG, respectively. Isovalues of 0.02 e/Å.