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Research paper

Electronic, optical, and spectroscopic analysis of TBADN organic semiconductor: Experiment and theory

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ABSTRACT

In this study, the electronic, optical and spectroscopic properties of 2-*tert*-Butyl-9,10-di(naphth-2-yl) anthracene (TBADN) semiconductor in different solvents were investigated by experimentally and computationally. Obtained theoretical and experimental UV–VIS spectra of the TBADN were found to be quite in good agreement and can be controlled with various solvents. Refractive index values of the TBADN semiconductor in different solvents were experimentally measured and calculated theoretically. Finally, the FTIR spectra of the TBADN organic semiconductor in different solvents were investigated by theoretical and experimental methods. It was found that the band gap is sensitive to the concentration of the solute.

1. Introduction

Semiconductors (SCs) are generally poor conductors at room temperature and without any external conditions, while their conductivity can be increased with various external conditions. SCs have significant and interesting optoelectronic properties for various technologies such as diodes, photovoltaics, lasers, microelectronics, transistors and detectors. Organic semiconductors (OSCs) have been widely used in energy conversion and medicine [1]. 2-*tert*-butyl-9,10-di(2-naphthyl) anthracene (TBADN) is an OSC. Anthracene derivative, which shows blue emission with high fluorescence quantum yield, have a good film forming property and thermal stability [1] and is usually used as a host.

Furthermore, some researchers made several investigations on energy levels of the highest occupied molecular orbital (HOMO) and the lowest-lying unoccupied molecular orbital (LUMO) of the TBADN organic semiconductor. Chen et al. [2], Khizar-ul-Haq et al. [3], Xu and Khan [4] and Kim et al. [5] reported that the energy separation values among the HOMO and LUMO of the TBADN were found to be 3.1, 2.9, 3.0 and 2.9 eV, respectively. Likewise, on that point are many works on molecular structure, spectroscopy (UV–Visible, FT-IR, FT-Raman), and time-dependent density functional theory (TD-DFT) investigations of several materials in the literature [6–9]. Anitha et al. [6] investigated the spectroscopic properties of the 2,6-Diamino-4-chloropyrimidine for dye sensitized solar cells using DFT. Abosadiya et al. [7] studied on FT-IR, UV/vis, DFT and TD-DFT of the N-(4-chlorobutanoyl)-N′-(2-, 3- and 4-methylphenyl) thiourea derivatives. Issaoui et al. [8] investigated molecular structure, vibrational spectra, HOMO-LUMO, UV properties of the 3-thiophenecarboxylic acid monomer and dimer using Hartree-Fock and DFT methods. Shukla et al. [9] studied on spectroscopic and quantum chemical properties of 1-acetylindole. In a recent work some spectral and sensing parameters of the title molecule were calculated by one of us [10]. In this experimental work, the weighted TBADN molecule was dissolved in 10 ml volume of the related solvents. In the same work the optical band gap values of TBADN molecule in different solvent were also calculated in 10 mL solvent volume.

In this study, the investigation of the optoelectronic properties of the TBADN semiconductor was carried out using quantum mechanical method and experimental methods. In the experimental work the TBADN materials were dissolved homogeneously in 5 mL volume of the related solvents. The UV–VIS spectra and band gap values that obtained in theoretical and experimental work were compared with the recently published experimental work by Erdoğan and Gündüz [10]. Optical properties play a key role in solar collectors, light-emitting diodes, photodetectors, night viewing, lenses, fiber optics, reflectors, optical coatings, antireflection coatings, optical computing, lasers, medical diagnostics,

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flat-panel displays, windows, mirrors, waveguides and optical communication [11].

2. Experimental details

2-*tert*-Butyl-9,10-di(naphth-2-yl)anthracene (TBADN) organic semiconductor molecule and the solvents of tetrahydrofuran (THF), dichloromethane (DCM), chlorobenzene and chloroform solvents were obtained from Sigma-Aldrich. Using these chemicals, the solutions of the TBADN semiconductor for different solvents were prepared. The UV–Vis and Fourier transform infrared (FTIR) spectra of the TBADN semiconductor were recorded. The chemical structure and atomic numbering design of the geometric structures are presented in Fig. 1(a and b), respectively. For the clarity, H atoms were omitted in this design.

2.1. The solutions of the TBADN semiconductor in different solvents

The TBADN semiconductor for THF, DCM, chlorobenzene and chloroform solvents were weighed with an analytical balance (AND-GR-200 Series). The molarities of the THF, DCM, chlorobenzene and chloroform solvents were 51 μM, 46 μM, 40 μM and 43 μM, respectively. The TBADN materials were dissolved homogeneously in 5 ml volume of the related solvents.

2.2. The UV and FTIR measurements for different solvents

Using the solutions of the TBADN semiconductor for THF, DCM, chlorobenzene and chloroform solvents, the UV measurements were recorded with a Spectrophotometer (Shimadzu model UV-1800). The FTIR spectra were collected on a Perkin Elmer Precisely Spectrum One spectrometer in the wavenumber range of 400–4000 cm^{-1} using KBr pellets.

3. Computational procedures

Gaussian 09 software package was used in order to perform theoretical computations [11]. In besides this, DFT calculations with the cc-pVDZ basis set [12–14] and Becke's three parameters hybrid exchange–correlation functional (B3LYP) [15] were used for achieving title molecule's geometry optimizations. The harmonic vibrational frequencies were computed at the same level of theory in the optimized structure, and the obtained frequencies were scaled by 0.970. Vibrational band assignments have been carried out with the help of a molecular visualization program [16].

To get insights into the electronic properties behind the excited state behavior, vertical excitation energies were calculated from the first excited state (S1) at the time-dependent density functional theory (TD-DFT) [17–20] level and the first 128 excited states were computed. Besides, applying the Polarizable Continuum Model (PCM) [21–24] it is calculated in the solutions that have used in experimental one. The optimization calculations of THF, DCM and chloroform solvents provided by the PCM method

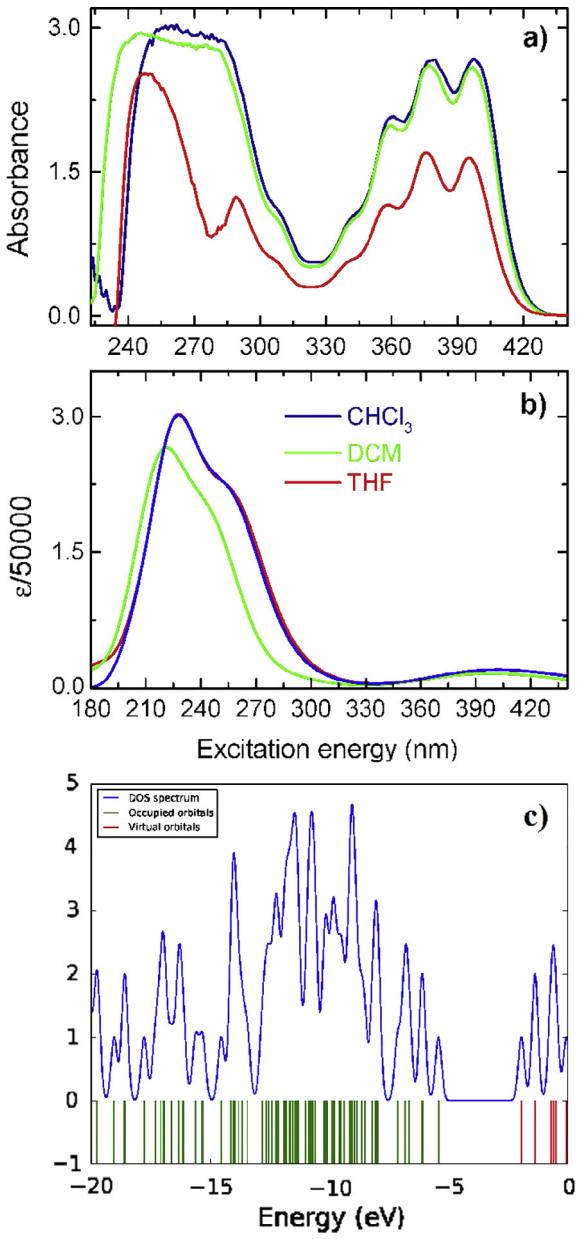

Fig. 2. The absorbance (Abs) or optical density (OD) spectra of the solutions of the TBADN semiconductor for THF, DCM, chlorobenzene and chloroform solvents. (a) Experimental, (b) theoretical and (c) density of states.

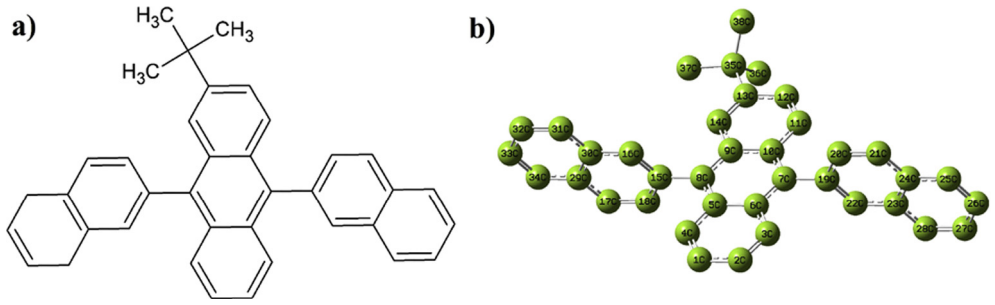

Fig. 1. (a) Molecular structure of TBADN. (b) The theoretical geometric structure of the TBADN. (For the sake of clarity, H atoms not involved in the motifs shown have been omitted.)