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A quantum-chemical study of conformational and electronic properties of ter-anthrylene-ethynylene derivatives in neutral and ionized states

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ABSTRACT

The density functional theory (DFT) calculations are applied to the series of 9,10-ter-anthrylene-ethynylene derivatives being in neutral, cationic and anionic charge states to gain insight into their conformational properties, frontier orbitals, ionization potentials (IP), electron affinity (EA) and reorganizations energies. The evolution of intramolecular transfer integrals are investigated within the energy-splitting in dimer (ESD) model using the intermediate neglect of differential overlap (INDO) semi-empirical method, the oscillating behavior is observed both for electrons and holes charge carriers. The computed results are reasonably consistent with data of available experimental and theoretical studies.

KEYWORDS

anthracene derivatives; reorganization energy; π-stacking; transfer integrals

1. Introduction

Over the last few decades organic semiconductors based on the aromatic systems have attracted much attention owing to their application in many fields [1–6], such as organic light-emitting diodes, solar cells, sensors, field-effect transistors etc. Nowadays, the focused efforts are still directed to extend our understanding on the structure–property relations in promising materials for organic electronics. Anthracene derivatives form a wide class of highly efficient, environmentally stable, blue-light emitting candidates playing an important role in the development and practical application of optoelectronic materials. Due to the flat shape and large π-surface area the anthracene ($C_{14}H_{10}$) molecule demonstrates a well-known proclivity to establish ordered aromatic (non-bonded) interactions both in the solution and in the solid state improving stability and charge mobility of the compounds. Recently, several novel anthracene-based compounds with different functionalizations have been synthesized and their devices showed promising light-emitting characteristics and thin film mobility [7, 8]. The optimization of the desired electronic properties is performed by carefully choosing the substituents that control structures parameters and packing of anthracene-based materials [7–10] and thus crucially result in efficiency of conductivity. Due to very small bandwidths of such organic media the charge-transfer processes at room temperature are usually described by the electron-hopping mechanism between neighboring molecules and are strongly dependent on the ionization potential (IP), electron affinity (EA), reorganization

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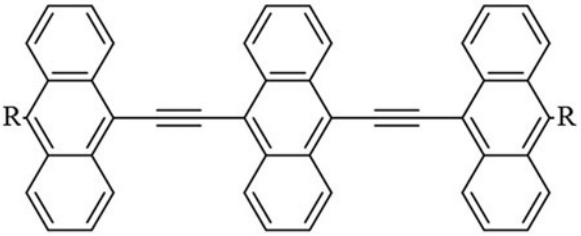

M1: R=H; **M2**: R=$(CH_2)_4$; **M3**: R=$(CH_2)_{10}$; **M4**: R=2–Ethylhexyl;
M5: R= Ethyl acetate (–COO–CH_2–CH_3)

Figure 1. Structure of the molecule under consideration and its functionalizations [13–15].

energy of the individual subunits and the coupling between the molecules packed in the solid state characterized by the transfer integral value [11, 12]. Since the molecular parameters governing charge transport cannot be simply assessed at the sight of molecular structure, just the systematic quantum chemical studies can provide invaluable information with a prerequisite for design, prediction and improvement of the important features of optoelectronic devices.

The aim of present paper is to investigate, on the basis of the parameters obtained by quantum-chemical calculations, the conformational and electronic properties of 9,10-teranthrylene-ethynylene chromophore, firstly reported in references [13–15], in which three neighboring anthracenes are linked by two ethynylene bounds and functionalized by five different chemical groups R in their terminal position (Fig. 1): unsubstituted (**M1**), *n*-butyl (**M2**), *n*-decyl (**M3**), 2-ethylhexyl (**M4**), ethyl acetate (**M5**). These compounds have been considered as reliable organic semiconductors in solution processed field-effect transistor devices. Remarkably, some of them showed increased mobility by four orders of magnitude when the deposited film was annealed before contact deposition [15] requiring a systematic theoretical study to understand deeper the optoelectronic process in such materials. In the present paper, the density functional theory (DFT) formalism is applied to all structures above being in their neutral and first ionized states in order to find an influence of substitution type on the energetics of ions and coupled charge-transfer properties. Evolution of intermolecular transfer integrals are estimated within the co-facial dimer model as a function of relative displacement of subunits.

2. Computational methodology

The three-dimensional geometries, the total energies, the highest occupied molecular orbitals (HOMO) and the lowest unoccupied molecular orbitals (LUMO), as well as their energy levels, are obtained for the isolated **M1**–**M5** and **ANT** molecules in their neutral, anionic, and cationic charge states using the quantum-chemical calculations (the **ANT** molecule is used as a benchmark structure). The procedure of full geometry optimization and electronic structure calculations are performed at the density functional theory (DFT) level with the hybrid B3LYP of three parameter Becke functional (B3) [16] and the functional of Lee, Yang, and Parr (LYP) [17] which includes both local and non-local correlations and provides reasonable agreement with experimental data for the wide class of materials. The split-valence 6–31+G(d) basis set, which are a valence double zeta set augmented with *d* polarization functions and *s* and *p* diffuse functions for each atom except for hydrogen, is used in all calculations that are performed by Gaussian'03 program package with energy convergences parameter of 10^{-4} eV. The calculation of radical cation states are carried out by the unrestricted DFT scheme. Analytic

second derivative calculations, which yield the harmonic vibrational frequencies, are carried out at the relaxed geometries to ensure that each optimized conformation has no imaginary frequencies and thus corresponds to a global minimum on the potential energy hypersurface.

The main parameters for charge transport at the molecular level are the reorganization energies due to the oxidation and reduction of the molecule and the electronic coupling between adjacent molecules characterized by transfer integrals. The Marcus–Hush intramolecular reorganization energy for the self-exchange reaction of a molecule and its ion is decomposed into the two parts $E_r^{+/-} = E_{r1}^{+/-} + E_{r2}^{+/-}$ for hole (+) or electron (–) transfer, correspondingly, and can be determined quantum-chemically from the individual relaxation process for the cationic and anionic species that require the knowledge of their relaxed geometries and energies. $E_{r1}^{+/-}$ corresponds to the difference between the energies of the neutral molecule at neutral and ion (cation/anion) geometry, while $E_{r2}^{+/-}$ is the difference between vertical and adiabatic IP/EA for cation/anion charge state. The adiabatic ionization potential (IP_a)/[adiabatic electron affinity (EA_a)] refers to the formation of the molecular ion (cation/anion) in its ground vibrational state and is defined by the difference between the energies of the ion (cation/anion) at the optimized ion geometry and the neutral molecule at its neutral geometry, whereas the vertical ionization potential (IP_v)/[vertical electron affinity (EA_v)] represents a Franck–Condon vibrational ground state to ionization (cation/anion) without any changes in geometry and is characterized by the difference between the total energies of the ion (cation/anion) at neutral geometry and the neutral molecule at its neutral geometry.

The energy-splitting in dimer (ESD) model [18], which is based on Koopmans' theorem, is used to estimate the transfer integral for hole (electron) as half energetic splitting of the HOMO and HOMO–1 (LUMO and LUMO+1) energy levels of a molecular dimer constructed from identical neutral molecules at the optimized geometry. It is well established that packing in the solids often involves displacements of adjacent molecules along their long or short molecular axes. Thus, the evolution of the hole and electron transfer integrals is computed using the intermediate neglect of differential overlap (INDO) semi-empirical Hamiltonian [19] starting from a perfectly co-facial dimer, with the two molecules superimposed at a fixed distance of 3.2 Å (close to recently observed for solution-sheared pentacene-based thin film [20]) and then increasingly displaced a molecule along two orthogonal axes in molecular plane. It is known [21] that the INDO method typically provides transfer integrals of the same order of magnitude as those obtained with DFT-based approaches which naturally are much expensive in computational time and resources. To prove this statement the evolutions of transfer integrals for pure **ANT** dimer are calculated and compared within three conceptually different levels of theory; that are, the DFT/B3LYP/6–31+G(d,p), the Møller–Plesset perturbation technique MP2/6–31+G(d,p) and the INDO methods.

3. Results and discussions

The DFT approach is applied to find the relaxed free space geometries and molecular energy levels of **M1**–**M5** (Fig. 1) and **ANT** ($C_{14}H_{10}$) in their neutral and charged states. From comparative reason the **ANT** molecule is considered as a benchmark structure to check our methodology and, then, to analyze the data obtained for the rest anthracene-based molecules under consideration. The calculations show that optimized **M1**–**M5** conformations are characterized by the similar twisted space configurations of *ter*-anthrylene-ethynylene backbone where side anthracene units are tilted at dihedral angle of about 37° in respect to the central unit due to the steric hindrance. Figure 2 represents the evolution of total energy

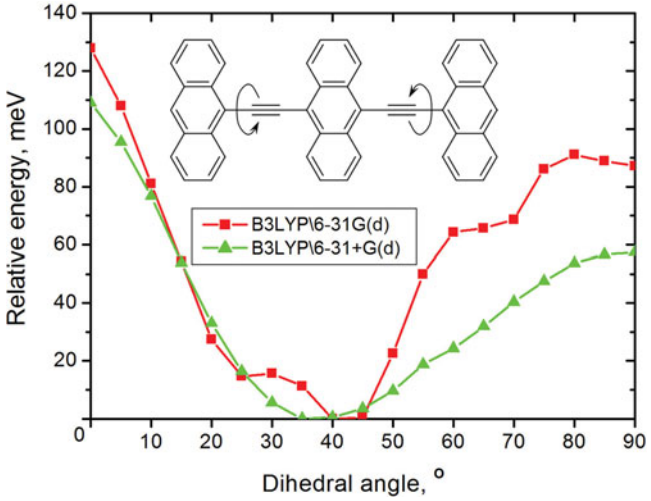

Figure 2. Difference of total energy of neutral *ter*-anthrylene-ethynylene core **M1** as function of torsion dihedral angle (see inset) of side anthracenes calculated at the DFT/B3LYP level with 6–31+G(d) and 6–31G(d) basis set (data for the last basis set adapted from ref. [14]); 0° value of dihedral angle defines the co-planar conformation.

change as a function of torsion dihedral angle according to the schema presented in inset. The profile obtained in present work with using higher 6–31+G(d) basis set slightly differs from the result (adapted from our early study [14]) performed with 6–31G(d) set that reveals a minima at ∼45°. The relative energy differences between the molecular conformations with different torsional angles are found to be fairly small (∼0.11 eV) and, thus, the co-planar conformation may be easily stabilized by the van der Waals interactions in solvent or as a result of self-assemble in a close-packed manner of adsorption on the metallic or organic substrates.

Further we investigate the changes to frontier orbitals that take place upon substitution R. The calculations reveal that no significant difference is found in the HOMO and LUMO energies as well as their shapes with both the change in torsion dihedral angle and the change in type of chemical functionalization R. The profiles of frontier molecular orbitals are presented in Fig. 3 whereas the energy levels are shown in Table 1. The spatial distributions of electron densities of HOMO and LUMO for **M1**–**M5** compounds are characterized by very similar shapes and are mostly localized on the anthracene subunits (Fig. 3) and on the ethynylene groups, defining the absorption and emission processes which may mainly be attributed to the centered π–π^* transition. The significant role of ethynylene radicals in optoelectronic properties of organic structures also can be confirmed by our early study of charge transmission mechanisms through the localized states that are associated directly with π–electrons located mainly at the triple and double bonds of a linear molecule [22]. The DFT calculated shapes of frontier wave functions are in good agreement with the bright contrast areas on the STM images obtained for **M2**–**M4** compounds [14] reflecting the π-conjugated nature of three-anthracene cores. Note that different types of side functionalization R force the formation of close-packed assemblies with various molecular arrangements that may affect the optoelectronic properties of such multi-layer organic arrays.

As can be seen from Table 1, **ANT** molecule is characterized by HOMO and LUMO energies of –5.51 eV and −1.96 eV, respectively, and by the highest HOMO-LUMO gap (HLG) of 3.54 eV in the series that coincide with the results of DFT calculations presented in [23]. The **M2**–**M4** structures demonstrate the almost equal values for their HOMO, LUMO and

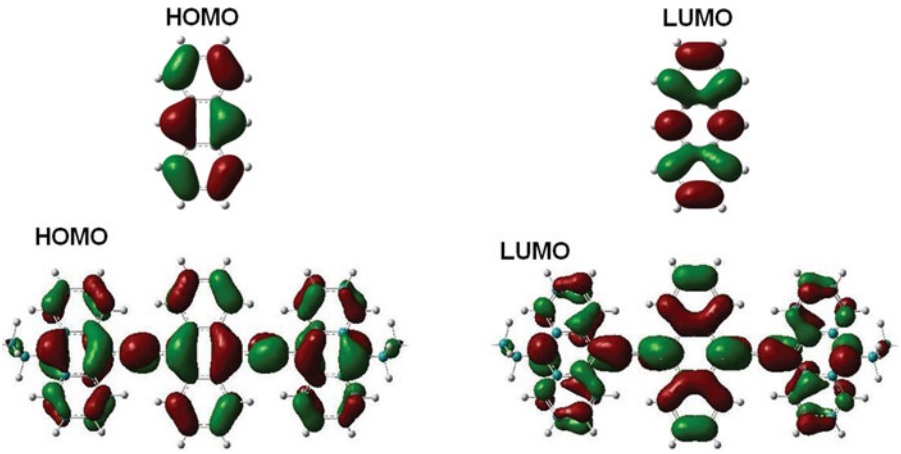

Figure 3. Calculated (DFT/B3LYP/6–31+G(d)) shapes of frontier wave functions HOMO and LUMO of **ANT** (top panel) and **M1**–**M5** (bottom panel) molecules (Fig. 1) in neutral form (the shapes are similar for all **M1**–**M5** structures).

HLG around -4.98 eV, −2.68 eV and 2.3 eV, respectively, and thus no effects of substitution type are observed. Unsubstituted **M1** and functionalized **M5** compounds show a decrease in both HOMO and LUMO energies providing larger HLG values of 2.41 eV and 2.37 eV, correspondingly. The HLG calculated for **M2**–**M5** structures (see Table 1) are consistent with the results of electrochemical investigations and optical gaps reported in [13, 14, 15].

The estimated values for IPs, EAs (both vertical and adiabatic) and the magnitudes for the intramolecular reorganization energies are collected in Table 2. All the **M1**–**M5** molecules demonstrate the positive EA values that are almost four times higher than that obtained for **ANT**. It is clearly seen that **M1**–**M4** molecules are characterized by minor influence of substitution type providing similar values for IPs and EAs, respectively, and **M5** structure has slightly larger values due to higher polarity of its ethyl acetate functionalization. The reorganization energies for both hole E_r^+ and electron E_r^- transfer calculated for **M1**–**M5** are systematically higher in comparison with those of **ANT**, thus the structure relaxation becomes stronger when the conjugate core is extended by additional **ANT**s and the functional groups R are substituted. The calculations reveal that **M5** molecule has the highest magnitudes of the reorganization energies in the series that are about 0.05 eV and two times higher for E_r^+ and

Table 1. The energy levels (in eV) of wave functions which can be involved into the lowest transitions calculated for the molecules in neutral form within DFT/B3LYP/6-31+G(d) method. Available experimental data for HLG are presented in bottom row.

Wave function	**M1**	**M2**	**M3**	**M4**	**M5**	**ANT**
LUMO+3	− 0.78	− 0.72	− 0.72	− 0.72	− 0.88	0.17
LUMO+2	− 2.03	− 1.96	− 1.95	− 1.95	− 2.16	− 0.23
LUMO+1	− 2.24	− 2.19	− 2.18	− 2.18	− 2.42	− 0.67
LUMO	− 2.71	− 2.68	− 2.68	− 2.68	− 2.87	− 1.96
HOMO	− 5.12	− 4.98	− 4.98	− 4.98	− 5.24	− 5.51
HOMO–1	− 5.56	− 5.45	− 5.44	− 5.44	− 5.67	− 6.74
HOMO–2	− 5.83	− 5.78	− 5.78	− 5.78	− 5.93	− 7.18
HOMO–3	− 6.88	− 6.82	− 6.82	− 6.82	− 6.99	− 8.31
			HOMO – LUMO gap (HLG)			
Theory	2.41	2.30	2.30	2.30	2.37	3.54
Experiment	–	2.2[13]	2.2[13]	2.19[14]	2.4[15]	3.43[23]

Table 2. Calculated (DFT/B3LYP/6–31+G(d)) values of the ionization potentials ($IP_{a/v}$), electron affinities ($EA_{a/v}$) and reorganization energies ($E_r^{+/-}$) (in eV).

Energy, eV	M1	M2	M3	M4	M5	ANT
IP_a	5.949	5.802	5.875	5.790	6.035	7.024
IP_v	6.065	5.892	5.878	5.874	6.161	7.091
EA_a	1.914	1.880	1.872	1.887	2.181	0.527
EA_v	1.764	1.776	1.775	1.788	1.962	0.433
E_{r1}^{+}	0.083	0.081	0.082	0.084	0.099	0.068
E_{r1}^{-}	0.106	0.100	0.106	0.108	0.183	0.099
E_{r2}^{+}	0.116	0.090	0.087	0.085	0.126	0.067
E_{r2}^{-}	0.150	0.104	0.098	0.098	0.220	0.095
E_r^{+}	0.199	0.171	0.169	0.169	0.225	0.135
E_r^{-}	0.256	0.204	0.203	0.206	0.403	0.194

E_r^{-}, respectively, than those of **M1**–**M4**. Note that all structures under study systematically demonstrate higher value of reorganization energy for electrons than for holes that make them more favorable for holes transport than for electron one. The obtained data for **ANT** are in good agreement with the results of theoretical [23–25] and experimental studies [26, 27].

In the following, we consider the evolution of transfer integrals values as a function of relative position of molecular subunits in the dimers. We first investigate the co-facial dimer constructed from two neutral **ANT** molecules with fixed 3.2 Å distance between their planes, and then shifted one of the molecules along short or long molecular axis (see insets on Fig. 4). The results for transfer integrals calculated within ESD model at the INDO, B3LYP/6–31+G(d,p) and MP2/6-31+G(d,p) levels of theory are presented in Fig. 4. The perfectly co-facial (unshifted) configuration naturally provides a highly symmetric reference point leading to the largest electronic splitting, but are exceptional in actual structures. For shifts along the short molecular X-axis (Fig. 4a) the HOMO splitting exhibits two extreme points, while the LUMO splitting does not change sign and decrease gradually as the translation proceeds. The displacement along the long Y-axis (Fig. 4b) progressively reduces the wave function overlap and lead to the strong oscillations in the curves with different periodicity observed for electron and holes transfer integrals that can be related by molecular geometry and bonding/antibonding interactions between frontier molecular wave functions in dimer. The obtained evolutions of energy splitting for **ANT** dimer (Fig. 4) are qualitatively consistent

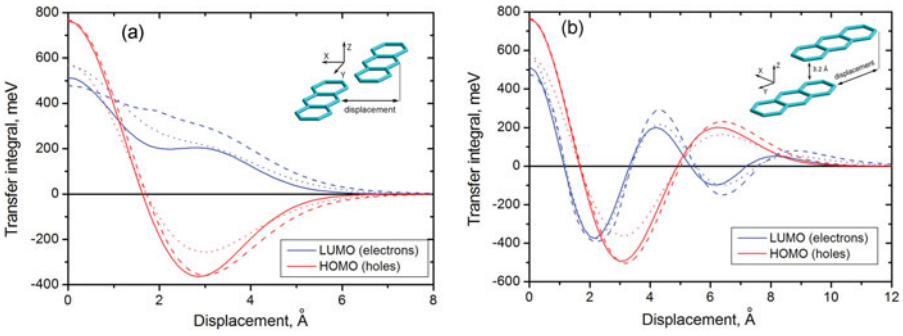

Figure 4. Evolution of transfer integrals for electrons (blue) and holes (red) as a function of the displacement along short X (a) and long Y (b) axis for **ANT** co-facial dimer (see inset) with a π-stacking distance of 3.2 Å. Results of calculations within INDO – solid curves, B3LYP/6-31+G(d,p) – dotted curves, MP2/6-31+G(d,p) – dashed curves.

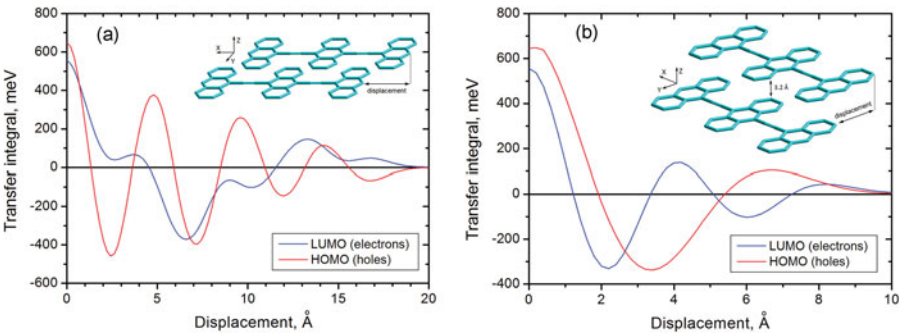

Figure 5. Evolution of INDO calculated transfer integrals for electrons (blue) and holes (red) as a function of the displacement along X (a) and Y (b) axis for **M1** co-facial dimer (see inset) with a π-stacking distance of 3.2 Å.

with corresponding results for the tetracene [28]. The INDO calculations demonstrate good predictive quality, which is comparable with that provided by the approaches of higher level such as DFT or MP2, and thus can be considered as good first-order approximation approach for further estimations of magnitudes of transfer integrals within the ESD model.

The same methodology is applied to **M1** dimer constructed from two identical neutral **M1** structures at co-planar (non-twisted) conformation, thereby effectively considering π-conjugated *ter*-anthrylene-ethynylene core only without any substituents. Figure 5 displays the INDO calculated evolutions of transfer integrals for positive and negative charge carriers with increasing displacement. The transfer integrals are found to have the same order of magnitude for both **ANT** and **M1** dimers and are characterized by almost higher value of HOMO amplitude than LUMO one, predicting more efficient mobility for hole rather than for electron. Due to the presence of three anthracenes in **M1** core and hence the extended molecular size in comparison with **ANT** the appearance of oscillating curves both for electrons and holes integrals is observed in Fig. 5a for the translations along X-axis. The displacement along Y axis (Fig. 5b) demonstrates the same periodic trend in the behavior of HOMO and LUMO splitting as for **ANT** dimer (Fig. 4b) but only with a little difference in amplitudes caused by the symmetry deviations in the shapes of frontier wave functions of *ter*-anthrylene-ethynylene backbone. The oscillation periods for electron and hole transfer integrals are found to be different so as even small shift, consequently, can encourage a situation where the coupling for electrons becomes dominant and hence electrons may occur to be more mobile than holes.

4. Concluding remarks

The results of our theoretical work indicate that electronic characteristics of **M1**–**M5** are mainly defined by π-conjugated three-anthracene core and slightly depend on the substituents type. The realization of co-planar conformation is assumed. Calculated HLG is in reasonable agreement with the available experimental results, given that our calculations consider isolated molecules in vacuum, whereas the measurements were performed on a solid. The estimated reorganization energies of positive and negative charge carriers in *ter*-anthrylene-ethynylene derivatives are found to be systematically higher than in anthracene. The amplitude of transfer integrals that govern charge transport in π-conjugated materials are shown to be extremely sensitive to parameters of molecular arrangement that can be forced by substituent type, method of deposition etc. The co-facial configuration naturally provides

largest values of transfer integrals. If persistent and amenable to high-quality multi-layer formation with possible co-planar π-π overlapping stabilized by substituents of special type, *ter*-anthrylene-ethynylene based compounds may find perspective application in organic electronic devices due to their reduced HLG, predicted reorganization energies, and also expected by our calculations higher hole mobility rather than electron one. The results of this study can be effectively used to design, prior to chemical synthesis, new anthracene-based derivatives whose transport properties are affected by specific arrangements guided by different chemical functionalizations.

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