

## TRANSPORT PROPERTIES OF PENTACENE, HEXACENE AND THEIR BN ANALOGUES

Stevan Armaković<sup>1\*</sup>, Sanja J. Armaković<sup>2</sup>, Svetlana S. Pelemiš<sup>3</sup>,  
Blanka Škipina<sup>4</sup>, Igor Hut<sup>5</sup>

<sup>1</sup>University of Novi Sad, Faculty of Sciences, Department of Physics,  
Trg Dositeja Obradovića 4, Novi Sad, Serbia

<sup>2</sup>University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry  
and Environmental Protection, Trg Dositeja Obradovića 3, Novi Sad, Serbia,

<sup>3</sup>University of East Sarajevo, Faculty of Technology, Zvornik, Karakaj bb,  
Zvornik, Republic of Srpska

<sup>4</sup>University of Banja Luka, Faculty of Technology, Banja Luka,  
Vojvode Stepe Stepanovića 73, Republic of Srpska

<sup>5</sup>University of Belgrade, Department of Biomedical Engineering, Faculty of Mechanical  
Engineering, Kraljice Marije 16, Belgrade, Serbia

**Abstract:** We have investigated transport properties of higher acenes pentacene and hexacene and compared it with the transport properties of their BN analogues. Charge hopping from one structure to another was investigated through calculations of reorganization energies based on DFT and Marcus semiempiric approach, while the investigation of charge transport along the investigated structures was based on DFT calculations and non-equilibrium Green's function (NEGF) method. Attention was also paid to the energy separation between the lowest excited singlet (S1) and triplet (T1) state, which is quantity that is important for the field of thermally activated delayed fluorescence (TADF). The obtained results indicate that both groups of investigated structures have certain advantages and drawbacks. According to the reorganization energies and I-V characteristics, pentacene and hexacene have better properties, while from the aspect of TADF, BN analogues of pentacene and hexacene have better properties.

**Keywords:** Acenes, DFT, optoelectronics, reorganization energies, TADF, NEGF, transport properties.

### 1. INTRODUCTION

From the aspect of organic electronics, acenes are very important  $\pi$ -conjugated molecules that consist of linearly fused benzene rings. These molecules are considered to be the basis of modern organic light-emitting diodes (OLED) and field effect transistors (FET), due to their fantastic transport properties [1–7]. This class of materials is also known as organic semiconductors [8].

The smallest and most studied acenes are benzene, naphthalene and anthracene [9]. Pentacene molecule, consisting of five benzene rings, has attracted great attention as an active semiconducting material for application in organic field effect transistors (OFET). Herringbone structure in which the face of one molecule is close to the edge of another is typical

for bulk crystals that pentacene forms, while the bulk solid consists of a stack of these layers [10, 11]. From the aspect of practical applications it is important to emphasize that intermolecular spacing of pentacene layers can be manipulated by parameters such as substrate temperature, deposition rates and thickness of a layer [12]. Pentacene is reported to have charge carriers mobility of beyond  $10 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ , which is the value that can be compared even with amorphous silicon devices [1]. However, a precise mechanism of charge transport in organic materials is rather complex. Semiconducting organic molecules such as pentacene are fully conjugated and thanks to the strong covalent bonds the overlap between  $\pi$ -orbitals along the molecule induces a continuous cloud over the whole molecule in which electrons are localized. Pentacene forms a film with desirable morphology thanks to which a good intermolecular overlap between the

\* Corresponding author: stevan.armakovic@df.uns.ac.rs

molecules exist, which consequently leads to high mobilities that are measured.

Higher acenes are molecules that consist of more than five linearly fused benzene rings. Although electronic properties of pentacene are well known, specific properties of higher acenes are much less known by the scientific community. Higher acene with six benzene rings, hexacene, attracted attention from crystallographic aspect. However, its investigation has been made difficult due to its low stability and solubility [13]. Although hexacene and its higher homologues are not stable, their existence can be demonstrated in suitable matrixes [14,15], while this acene and heptacene (higher acene with seven linearly fused benzene rings) can be synthesized through photochemical bis-decarbonylation of bridged R-diketones (Strating-Zwanenburg reaction).

Despite the problems with synthesis of higher acenes, research of the acene family from the theoretical aspect predicts a set of specific properties [16–18]. Besides benzene as a building block of acenes, borazine can be viewed as a building block of acene boron-nitride (BN) analogues. Benzene and borazine are typical representatives of planar aromatic organic and inorganic molecules, containing six  $\pi$ -electrons which are delocalized over the six-membered ring [19,20]. Taking into account that boron and nitrogen atoms together with BN units are frequently used for modifications of carbonaceous materials, in this work we decided to investigate the transport properties of pentacene, hexacene and their BN analogues. For this work we were also motivated by our results concerning oxidation/reduction potentials, reorganization energies and  $\Delta E(S_1 - T_1)$  values reported in [7]. The mentioned parameters are important for transport properties in optoelectronic devices, while further we decided to investigate the charge and heat transport properties through calculation of  $I-V$  curves and thermoelectric coefficients.

## 2. COMPUTATIONAL DETAILS

Density functional theory (DFT) calculations of optoelectronic properties were performed with Jaguar 8.8. program and corresponding optoelectronics module as implemented in Schrodinger Material Suite 2015-2 [21,22]. Optoelectronic properties are calculated within the screening method [22]. Concerning the oxidation and reduction potential, OP and RP respectively, they were calculated employing the following equation:

$$\text{OP (or RP)} = S \times \text{OE} + I \quad (2)$$

where S, OE and I denotes slope, orbital energy and intercept, respectively. The values of S and I were

obtained by linear regression against experimental OP and RP over a wide range of relevant organic molecules [22]. For OP, the value of orbital energy corresponds to the value of highest occupied molecular orbital (HOMO) energy from the neutral molecule, while for RP the value of orbital energy corresponds to the value of the lowest unoccupied molecular orbital (LUMO) energy from the neutral molecule. These values were developed using B3LYP with the default basis set, which is MIDI! in this case, meaning that these values are not suitable for other functionals and basis sets. For OP and RP the value of slopes and intercepts respectively were  $-17.50$  and  $-22.50$  V and  $-2.17$  and  $-0.35$  V [22]. Results concerning oxidation/reduction potentials, reorganization energies and TADF of pentacene, hexacene and their BN analogues have been taken from our previously published paper [7].

In order to investigate charge and heat transport properties of pentacene and hexacene these structures were modeled as device systems presented in Figure 3. Concretely, charge and heat transport properties of investigated device systems have been simulated employing the Quantum Wise Atomistix Toolkit (ATK) [23,24], which utilizes the self-consistent non-equilibrium Green's functions and the density functional theory. Initially, the structures were optimized by the ATK until the atomic forces were less than  $0.01\text{eV}/\text{\AA}$ , without any constraints. Generalized gradient approximation (GGA) with Perdew-Burke-Ernzerh (PBE) functional with Double Zeta Polarized (DZP) basis set has been used for optimization of device systems. Transport simulations with ATK were done employing the self-consistent extended Hückel method with Cerda type of Hückel basis sets [25]. For both optimization and transport calculations mesh grid of k space was set to  $1 \times 1 \times 100$ , while the electronic temperature was set to 300 K. Phonon subsystem of pentacene and hexacene devices has been investigated employing the Tersoff 2010 CH potentials [26,27]. For BN analogues of pentacene and hexacene devices phonon subsystem has been investigated employing the potentials of Marian et al. [28].

## 3. RESULTS AND DISCUSSIONS

### 3.1. Oxidation and reduction potentials

One of the main drawbacks of pentacene includes poor stability and low solubility in organic solvents [29–32]. It is easily oxidized in the air, while its poor solubility can be attributed to the strong intermolecular forces because of  $\pi$ -stacking [29]. Oxidation and reduction properties of molecules can be assessed

through calculation of reduction and oxidation potentials, which can be interpreted as the tendency of structure to gain/lose electrons and thus become oxidized/reduced. For RP, the more positive/less negative potential, the more likely the reduction is to occur, while for OP the more negative/less positive the potential is, the more likely oxidation is to occur. Calculated OP and RP for investigated structures are given in Figure 1.

cur, while for OP the more negative/less positive the potential is, the more likely oxidation is to occur. Calculated OP and RP for investigated structures are given in Figure 1.

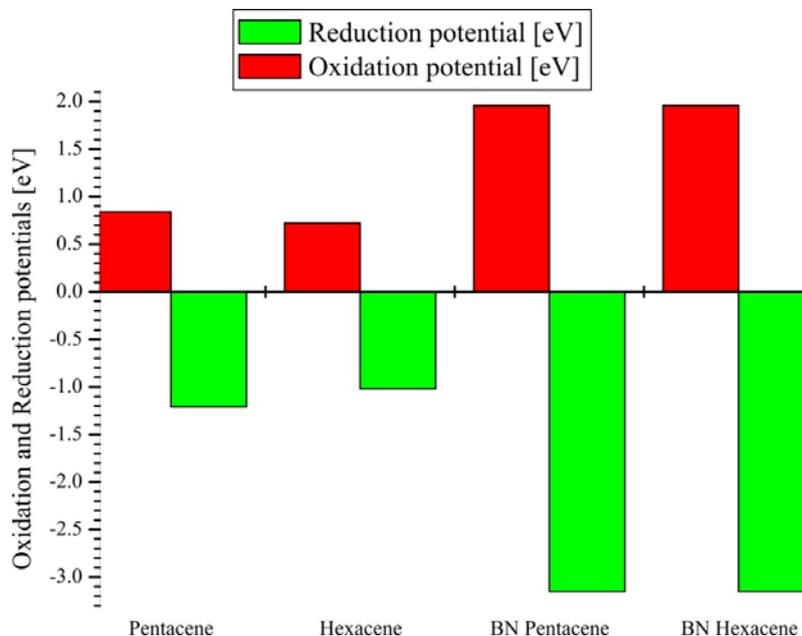


Figure 1. Oxidation and reduction potentials of investigated structures [7]

According to the definition of OP and RP it can be seen from the obtained results that pentacene and hexacene have similar OP and RP values. However, when it comes to the OP and RP of BN analogues of pentacene and hexacene it can be seen that their values significantly differ comparing to their all carbon relatives. These values also indicate that BN analogues are significantly less prone to oxidation and reduction than pentacene and hexacene, leading to their significantly higher stability over pentacene and hexacene.

Luminescence, electroluminescence and electronic properties of different materials are strongly affected by oxygen quenching, which occur when they are exposed to air. Thus, improved OP and RP indicate that BN analogues of pentacene and hexacene could be significantly less prone to the effects of oxygen quenching.

### 3.2. Reorganization energies

Significantly high charge mobilities and efficient charge injection properties are the main quantities that are considered as crucial parameters determining the efficiency of electronic materials [33]. From the aspect of practical applications, charge transfer from one organic molecule to another is very important. This type of charge transport can be investigated within the Marcus semi-empirical ap-

proach, according to which charge hopping rate,  $k_{ET}$ , which regulates the charge carrier mobility, can be expressed as [34, 35]:

$$K_{ET} = \frac{4\pi^2}{h} \frac{1}{\sqrt{4\pi\lambda k_B T}} t^2 \exp\left[\frac{-\lambda}{4k_B T}\right], \quad (1)$$

where  $\lambda$  is reorganization energy, while  $t$  represents the charge transfer integral (or charge coupling). Equation (1) tells that in order to achieve as good performance of electric material as possible, reorganization energy should be minimized while charge coupling should be maximized.

Reorganization energies can be calculated according to following formulas:

$$\lambda_1 = E^0(G^*) - E^0(G^0), \quad (2)$$

$$\lambda_2 = E^*(G^0) - E^*(G^*), \quad (3)$$

$$\lambda_i = \lambda_1 + \lambda_2, \quad (4)$$

where  $E^0(G^0)$  and  $E^*(G^*)$  are the ground state energies of the neutral and ionic states, respectively.  $E^0(G^*)$  is the energy of the neutral molecule at the optimal ionic geometry, while  $E^*(G^0)$  is the energy of the charged state at the optimal geometry of the neutral molecule. Obtained results for reorganization energies of pentacene, hexacene and their BN analogues are given in Figure 2.

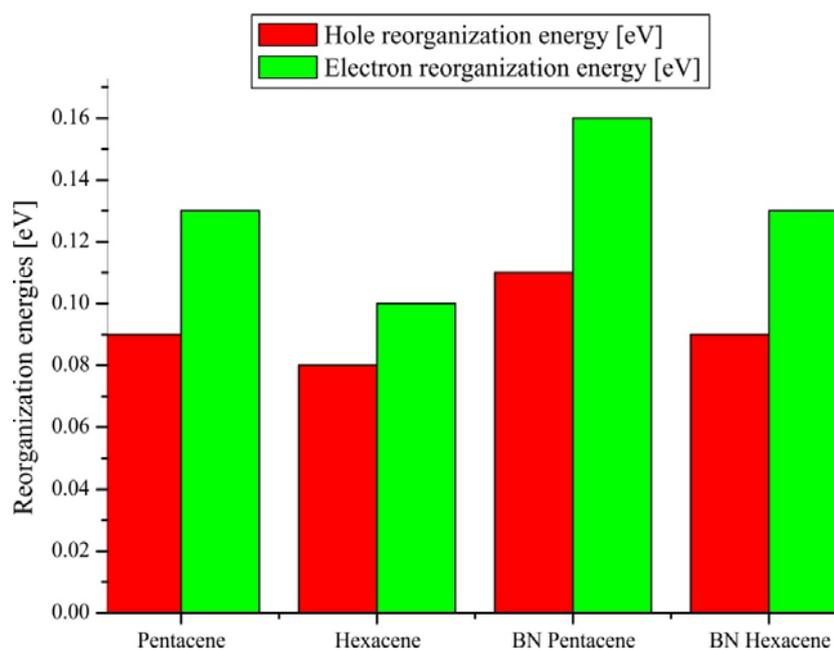


Figure 2. Hole and electron reorganization energies of investigated structures [7]

Pentacene and hexacene obviously possess very low values of reorganization energies, especially for holes, with values even below 0.1 eV, which is very important for practical optoelectronic applications. Reorganization energies of BN analogues of pentacene and hexacene are not as good as for pentacene and hexacene. However, the values of HRE are comparable to pentacene and hexacene, while BN hexacene structure has value of HRE below 0.1 eV, namely 0.09 eV. On the other hand, ERE are somewhat higher than for pentacene and hexacene. Nevertheless, these values can be considered as very competitive with values obtained for other perspective organic molecules, when it comes to the applications in optoelectronic devices.

### 3.3. Thermally activated delayed fluorescence

The importance of the TADF mechanism lies in the fact that it might enable the improvement of efficiency of OLED without employment of phosphorescent metal-organic complexes. In OLED singlet and triplet excitons are formed in 1:3 ratio, according to spin statistics. Unfortunately, only singlet excitons are responsible for light emitting, while triplet excitons relax by releasing heat. To overcome this drawback, phosphorescent emitters such as iridium or platinum based complexes are usually used for manufacture of high efficiency OLED [36–38]. The usage of precious metals however leads to the production challenges such as high pricing, because of which chances for OLED to have more significant role in the market are low [39].

One of the crucial parameters that determines the effectiveness of the TADF mechanism is certainly the energy separation between the lowest excited singlet ( $S_1$ ) and triplet ( $T_1$ ) state,  $\Delta E(S_1 - T_1)$ . If  $\Delta E(S_1 - T_1)$  has a suitably low value, then singlet state  $S_1$  can be populated thermally at ambient temperature from the energetically lower-lying triplet state. If  $\Delta E(S_1 - T_1)$  is larger than ca.  $3 \times 10^3 \text{ cm}^{-1}$  (or 0.37 eV) a thermal population of the singlet state  $S_1$  is not effective. Therefore in this work we calculated  $\Delta E(S_1 - T_1)$  values for pentacene, hexacene and their BN analogues and obtained interesting results. Namely, for pentacene and hexacene  $\Delta E(S_1 - T_1)$  had the value which was by far above the desired threshold of 0.37 eV, 1.41 eV and 1.33 eV, respectively [7]. On the other hand,  $\Delta E(S_1 - T_1)$  values of BN analogues of pentacene and hexacene were 0.25 eV and 0.30 eV, respectively, which are much lower than values obtained for their all carbon relatives [7]. Additionally, these values are below 0.37 eV, which is very desirable for the TADF mechanism and indicates the potential for practical applications of BN analogues of higher acenes in the devices based on optoelectronic properties of organic molecules.

### 3.4. Charge and heat transport

Since according to the previously presented results in this work, BN analogues possess certain advantages over their all carbon relatives, we decided to investigate the charge and heat transport properties of

these structures. In order to do so, we calculated the  $I-V$  curves in order to charge transport properties and we have also calculated the electron and phonon thermoelectric coefficients in order to gain an insight into the heat transport properties. For the investigation of transport properties in ATK package, the following

device systems has been built and considered, Figure 5. Left and right electrodes are indicated with L and R, respectively, the central scattering region is indicated with C, while Figure 4 contains calculated  $I-V$  for device systems presented in Figure 3.

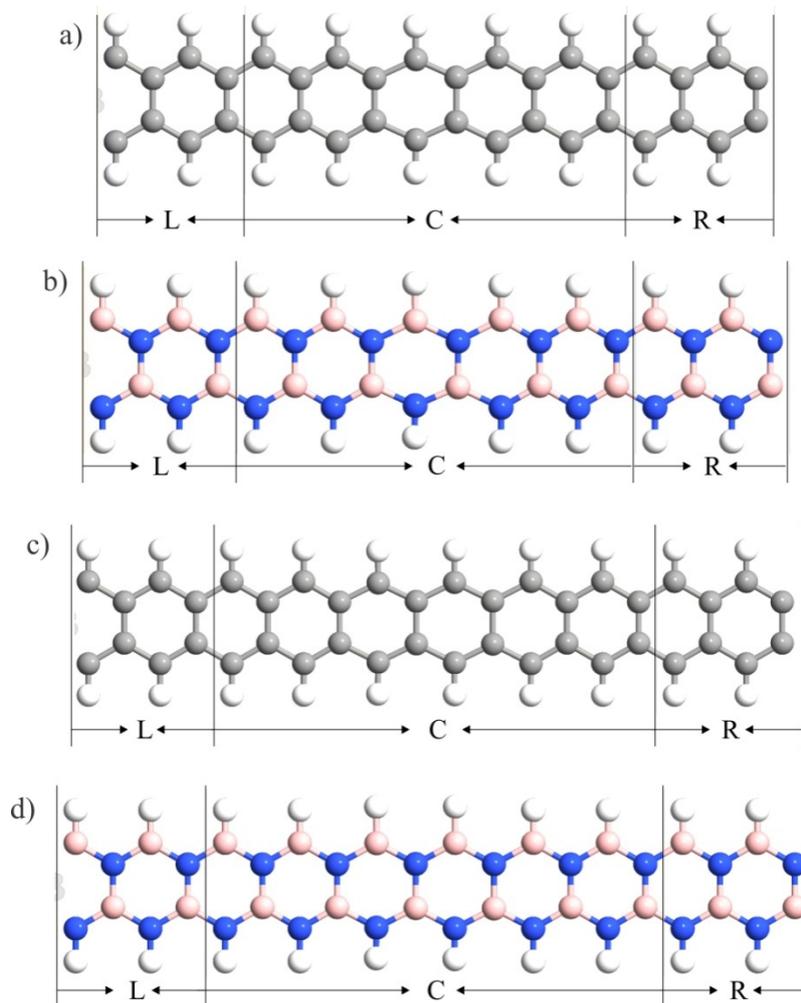


Figure 3. Investigated device systems

The results presented in Table 1 indicate that electron subsystems of investigated device systems are very similar in terms of electron conductivity, which is not surprising taking into account that replacement of two carbon atoms by one boron and nitrogen atom leads to the formation of systems that are isoelectronic with their all-carbon analogues. However, the phonon subsystem of investigated device systems significantly differs. In cases of pen-

tacene and hexacene  $k_{ph}$  is still higher than the  $k_e$ , meaning that phonons are principally responsible for heat conductivity. Contrary to this,  $k_{ph}$  of BN analogues of pentacene and hexacene is lower than the  $k_e$ , meaning that in these cases electrons are more important in terms of heat conductivity. Consequently, it can be concluded that heat conductivity of BN analogues of pentacene and hexacene is lower than of pentacene and hexacene.

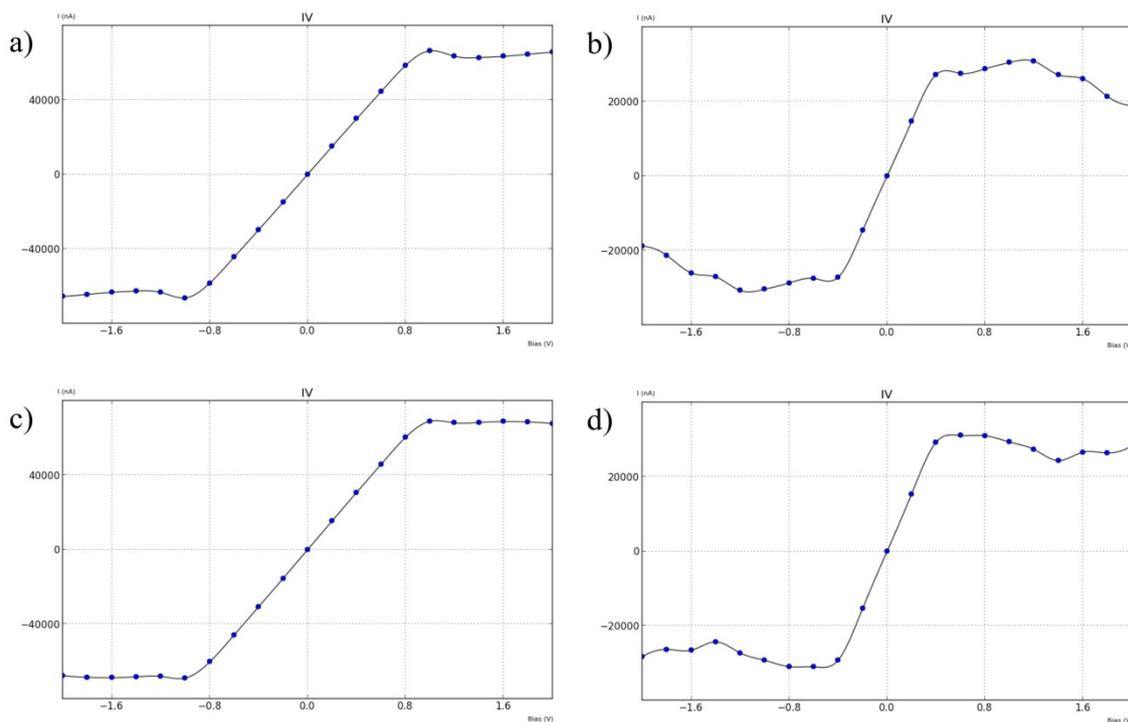


Figure 4. *I-V* curves of the investigated device systems  
 a) pentacene, b) BN pentacene, c) hexacene and d) BN hexacene

As it can be clearly seen, the device systems based on pentacene and hexacene have much better charge transport properties than device systems based on their BN analogues. In the case of pentacene and hexacene, the peak value of current is achieved at bias voltage of 1 V, while in the case of BN analogues this value is achieved at around 0.5 V. This means that in terms of current intensity device systems based on pentacene and hexacene are much

better because much stronger current is calculated in these cases, however, the response is much faster in the case of BN analogues, because peak current intensity is achieved at much lower bias voltage.

An insight into the heat transport properties of investigated structures can be obtained after the inspection of calculated thermoelectric coefficients: electron, phonon and total conductivity,  $k_e$ ,  $k_{ph}$  and  $k$ , respectively, presented in Table 1.

Table 1. *Thermoelectric coefficients of investigated structures*

Device system	$k_e$ [W/K]	$k_{ph}$ [W/K]	$k = k_e + k_{ph}$ [W/K]
Pentacene	$5.526 \times 10^{-10}$	$7.919 \times 10^{-10}$	$1.344 \times 10^{-9}$
Hexacene	$5.661 \times 10^{-10}$	$8.387 \times 10^{-10}$	$1.405 \times 10^{-9}$
BN-Pentacene	$5.494 \times 10^{-10}$	$3.214 \times 10^{-10}$	$8.708 \times 10^{-10}$
BN-Hexacene	$5.666 \times 10^{-10}$	$5.322 \times 10^{-10}$	$1.099 \times 10^{-9}$

#### 4. CONCLUSIONS

We have investigated transport properties of pentacene, hexacene and their BN analogues employing DFT calculations and NEGF method. Initially we were interested in optoelectronic properties and we have calculated important properties that might serve to assess the overall potential of investigated structures for practical applications. Calculations of OP and RP indicated that BN analogues of pentacene and hexacene might be much less prone to oxidation and reduction than pentacene and hex-

acene, which indicates their significantly higher stability. The investigation of reorganization energies indicated that both HRE and ERE of hexacene are lower than pentacene and that both of these two parameters are somewhat higher for BN analogues of pentacene and hexacene, but still low enough to be considered competitive with other organic molecules.  $\Delta E(S_1 - T_1)$  value of BN analogues of pentacene and hexacene is much lower than for regular pentacene and hexacene and something that is even more important it is well below the desired threshold of 0.37 eV. *I-V* curves revealed that in terms

of current intensity, pentacene and hexacene are much better than their BN analogues, however peak current intensity of BN analogues is achieved for much lower bias voltage thanks to which BN analogues could be much more responsive. Finally, thermoelectric coefficients indicated that electron conductivity is very similar for all investigated devices. On the other hand,  $k_{ph}$  is higher for pentacene and hexacene, while for their BN analogues it is lower than  $k_e$ . Consequently, total thermal conductivity is lower for BN analogues of pentacene and hexacene.

## 5. ACKNOWLEDGMENTS

This work has been done thanks to the support received from Schrödinger Inc. This work has been done within the projects of the Ministry of Education and Science of Republic of Serbia grant no. OI171039 and TR34019.

## 6. REFERENCES

- [1] X. K. Chen, et al., *A promising approach to obtain excellent n-type organic field-effect transistors: introducing pyrazine ring*, The Journal of Physical Chemistry C, Vol. 115-43 (2011) 21416-21428.
- [2] C. Tang, S. VanSlyke, *Organic electroluminescent diodes*, Applied Physics Letters, Vol. 51-12 (1987) 913-915.
- [3] P. K. Ho, et al., *Molecular-scale interface engineering for polymer light-emitting diodes*, Nature, Vol. 404-6777 (2000) 481-484.
- [4] H. Katz, *Organic molecular solids as thin film transistor semiconductors*, J. Mater. Chem., Vol. 7-3 (1997) 369-376.
- [5] G. Horowitz, M. E. Hajlaoui, *Mobility in polycrystalline oligothiophene field-effect transistors dependent on grain size*, Advanced Materials, Vol. 12-14 (2000) 1046-1050.
- [6] C. R. Newman, et al., *Introduction to organic thin film transistors and design of n-channel organic semiconductors*, Chemistry of materials, Vol. 16-23 (2004) 4436-4451.
- [7] S. Armaković, S.J. Armaković, V. Holodkov, S. Peleliš, *Optoelectronic properties of higher acenes, their BN analogue and substituted derivatives*, Materials Chemistry and Physics, Vol. 170 (2016) 210-217.
- [8] J. T. Kintigh, A. Robust, et al., *High-Temperature Organic Semiconductor*, The Journal of Physical Chemistry C, Vol. 118-46 (2014) 26955-26963.
- [9] A. R. Reddy and M. Bendikov, *Diels-Alder reaction of acenes with singlet and triplet oxygen-theoretical study of two-state reactivity*, Chemical communications, Vol. 11 (2006) 1179-1181.
- [10] J. E. Northrup, M. L. Tiago, S. G. Louie, *Surface energetics and growth of pentacene*, Physical Review B, Vol. 66-12 (2002) 121404.
- [11] R. Campbell, J. M. Robertson, J. Trotter, *The crystal structure of hexacene, and a revision of the crystallographic data for tetracene*, Acta crystallographica, Vol. 15-3 (1962) 289-290.
- [12] B. Park, *Electronic and structural properties of pentacene at organic/inorganic interfaces*, ProQuest 2008.
- [13] M. M. Payne, S. R. Parkin, J. E. Anthony, *Functionalized higher acenes: hexacene and heptacene*, Journal of the American Chemical Society, Vol. 127-22 (2005) 8028-8029.
- [14] A. R. Murphy, J. M. Frechet, *Organic semiconducting oligomers for use in thin film transistors*, Chemical reviews, Vol. 107-4 (2007) 1066-1096.
- [15] C. Tönshoff, H. F. Bettinger, *Photogeneration of octacene and nonacene*, Angewandte, Chemie International Edition, Vol. 49-24 (2010) 4125-4128.
- [16] P. V. R. Schleyer, et al., *The acenes: is there a relationship between aromatic stabilization and reactivity?*, Organic letters, Vol. 3-23 (2001) 3643-3646.
- [17] K. B. Wiberg, *Properties of some condensed aromatic systems*, The Journal of Organic Chemistry, Vol. 62-17 (1997) 5720-5727.
- [18] K. Houk, P. S. Lee, M. Nendel, *Polyacene and cyclacene geometries and electronic structures: bond equalization, vanishing band gaps, and triplet ground states contrast with polyacetylene*, The Journal of organic chemistry, Vol. 66-16 (2001) 5517-5521.
- [19] A. K. Phukan, et al., *Structure, reactivity and aromaticity of acenes and their BN analogues: A density functional and electrostatic investigation*, Inorganic chemistry, Vol. 43-19 (2004) 5824-5832.
- [20] V. I. Minkin, M. N. Glukhovtsev, B. Simkin, *Aromaticity and antiaromaticity*, J. Wiley & Sons. 1994.
- [21] A. D. Bochevarov, et al., *Jaguar: A high-performance quantum chemistry software program with strengths in life and materials sciences*, International Journal of Quantum Chemistry, Vol. 113-18 (2013) 2110-2142.
- [22] Schrödinger Release 2015-2: Jaguar, version 8.8, Schrödinger, LLC, New York, NY, 2015.

- [23] M. Brandbyge, et al., *Density-functional method for nonequilibrium electron transport*, Physical Review B, Vol. 65–16 (2002) 165401.
- [24] J. Taylor, H. Guo, J. Wang, *Ab initio modeling of quantum transport properties of molecular electronic devices*, Physical Review B, Vol. 63–24 (2001) 245407.
- [25] J. Cerda, F. Soria, *Accurate and transferable extended Hückel-type tight-binding parameters*, Physical Review B, Vol. 61–12 (2000) 7965.
- [26] N. Juslin, et al., *Analytical interatomic potential for modeling nonequilibrium processes in the W–C–H system*, Journal of Applied Physics, Vol. 98–12 (2005) 123520.
- [27] L. Lindsay, D. Broido, *Optimized Tersoff and Brenner empirical potential parameters for lattice dynamics and phonon thermal transport in carbon nanotubes and graphene*, Physical Review B, Vol. 81–20 (2010) 205441.
- [28] C. M. Marian, M. Gastreich, *A systematic theoretical study of molecular Si/N, B/N, and Si/B/N (H) compounds and parameterisation of a force-field for molecules and solids*, Journal of Molecular Structure: THEOCHEM, Vol. 506–1 (2000) 107–129.
- [29] D. Lehnher, R. R. Tykwinski, *Oligomers and Polymers Based on Pentacene Building Blocks*, Materials, Vol. 3–4 (2010) 2772–2800.
- [30] J. E. Anthony, *Functionalized acenes and heteroacenes for organic electronics*, Chemical Reviews, Vol. 106–12 (2006) 5028–5048.
- [31] J. E. Anthony, *The larger acenes: versatile organic semiconductors*, Angewandte Chemie International Edition, Vol. 47–3 (2008) 452–483.
- [32] M. Bendikov, F. Wudl, D. F. Perepichka, *Tetrathiafulvalenes, oligoacenes, and their buckminsterfullerene derivatives: The brick and mortar of organic electronics*, Chemical reviews, Vol. 104–11 (2004) 4891–4946.
- [33] G. García, et al., *Poly (arylenethynyl-thienoacenes) as candidates for organic semiconducting materials. A DFT insight*, Organic Electronics, Vol. 13–12 (2012) 3244–3253.
- [34] L. Wang, et al., *Computational methods for design of organic materials with high charge mobility*, Chemical Society Reviews, Vol. 39–2 (2010) 423–434.
- [35] V. Coropceanu, et al., *Charge transport in organic semiconductors*, Chemical reviews, Vol. 107–4 (2007) 926–952.
- [36] M. Baldo, et al., *Excitonic singlet-triplet ratio in a semiconducting organic thin film*, Physical Review B, Vol. 60–20 (1999) 14422.
- [37] C. Adachi, et al., *Nearly 100% internal phosphorescence efficiency in an organic light-emitting device*, Journal of Applied Physics, Vol. 90–10 (2001) 5048–5051.
- [38] M. Baldo, et al., *Very high-efficiency green organic light-emitting devices based on electrophosphorescence*, Applied Physics Letters, Vol. 75–1 (1999) 4–6.
- [39] M. P. Gaj, et al., *Highly efficient Organic Light-Emitting Diodes from thermally activated delayed fluorescence using a sulfone-carbazole host material*, Organic Electronics, Vol. 16 (2015) 109–112.



## ТРАНСПОРТНА СВОЈСТВА ПЕНТАЦЕНА, ХЕКСАЦЕНА И ЊИХОВИХ ВН АНАЛОГА

**Сажетак:** Истраживали смо транспортна својства представника ацена, пентацена и хексацена и упоређивали их са транспортним својствима њихових ВН аналогних структура. Прелаз наелектрисања са једне на другу структуру истражен је преко прорачуна енергија реорганизације на основу *DFT* и Маркусовог полумеморијског приступа, док су се истраживања транспорта наелектрисања дуж структура заснивала на *DFT* прорачунима и методу неравнотежних Гринових функција (*NEGF*). Пажња је била посвећена и енергетском размаку између најнижег побуђеног синглетног (S1) и триплетног (T3) стања, што је величина важна за област термално активираних одложених флуоресценције (*TADF*). Добијени резултати индицирају да обе групе истражених структура имају одређене предности и мане. Према енергијама реорганизације и I–V карактеристикама, пентацен и хексацен имају боља својства, док са аспекта *TADF*-а, боља својства имају ВН аналози.

**Кључне ријечи:** ацени, *DFT*, оптоелектроника, енергије реорганизације, *TADF*, *NEGF*, транспортна својства.

