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Computer Simulation of the Electrotransport Characteristics of the "Au – Bipyridine – Au" Nanocontact

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In the framework of the density functional theory, using the method of non-equilibrium Green's functions (DFT + NEGF) and in the local density approximation, the electrotransport characteristics of the "Au – Bipyridine – Au" nanocontact were studied. The calculation is implemented in the program Atomistix ToolKit with Virtual NanoLab. The current-voltage, *dI*/*dV* characteristics, the transmission spectrum and the density of states of the nanocontact are calculated. It is shown that the transmission spectra of the nanocontact are reminiscent of the spectrum of resonant tunnel structures. A shift in transmission spectra was detected when a bias voltage was applied, which is explained by a voltage drop along the molecular transition. It is shown that DDOS at negative energy (– 6 ÷ – 1 eV) is significantly higher than at positive energy. In the bias voltage range – 3 ÷ – 0.5 V, a noticeable current oscillation is observed. It is shown that a multitude of areas with negative differential resistance, possibly due to resonant tunneling of quasiparticles, appear on the current-voltage characteristic of the nanosystem. The same changes are observed on the *dI*/*dV*-characteristic. The results obtained may be useful for calculating new promising electronic devices of molecular electronics.

Keywords: Electron transport, Nanocontact, Bipyridine, Negative differential resistance, Current-voltage characteristic.

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1. INTRODUCTION

At present, the development of exotic materials with controlled electrophysical properties is becoming more and more relevant for creating new types of electronic devices in micro- and nanoelectronics [1, 2]. They differ in their fundamentally new electrophysical properties from traditional semiconductor materials and on their basis develop new trends in electronics. Such areas of electronics include superconducting electronics (see e.g. [3-5]), organic electronics (see e.g. [6, 7]), molecular electronics [8], single electronics [9, 10], and others, where the working objects are nanoscale structures.

It is known that the effects of the rectified voltage, negative differential resistance, spin filtration, and others occur in nanostructures [11]. One of the most attractive materials for molecular electronics is Bipyridine (systematic name: 2-pyridin-2-ylpyridine, chemical formula: $C_{10}H_8N_2$) [12]. The structure of the Bipyridine molecule is shown in Fig. 1.

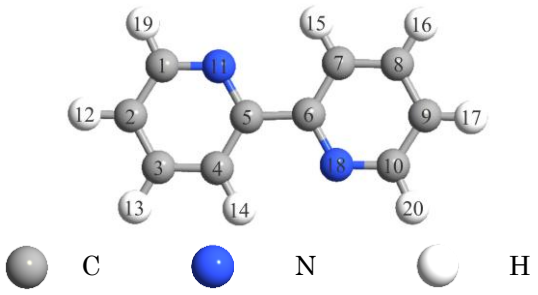

Fig. 1 – Bipyridine molecule structure

In [13], in the framework of the self-consistent non-equilibrium Green method in combination with the density functional theory (DFT), the electrotransport properties of a 4.4-bipyridine molecule located between two Au_111 surfaces were investigated. In this work, using the TRANSIESTA 17 package, it was found that the behavior of electron transport strongly depends on the interface configuration and good agreement with experimental measurements can be achieved by lengthening the simulated molecular transition.

In this paper, an attempt was made using computer simulation using Atomistix ToolKit with Virtual NanoLab to determine the electrical characteristics of the "Au – Bipyridine – Au" nanocontact.

2. SIMULATION MODEL AND METHODS

In this paper, the "Au – Bipyridine – Au" nanocontact consisting of 196 atoms is considered. The Bipyridine molecule is located between two gold (Au_111) surfaces. The Bipyridine molecule is connected to the gold electrodes through 12 and 17 hydrogen atoms (see Fig. 1) by replacing them with gold atoms. The geometry of the studied nanocontact is shown in Fig. 2a-c. The total length of the nanocontact is ~ 50 Å. The electrodes were obtained by expanding the central region along the C axis by ~ 7.064 Å. The distance between the electrodes is ~ 35.79 Å, where the central region of the nanocontact of 142 atoms is located. The region of active scattering includes the Bipyridine molecule and three surface layers of Au_111. This area is in Fig. 2a and marked in green.

Computer simulation of the electrotransport characteristics of the "Au – Bipyridine – Au" nanocontact was

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carried out within the framework of the DFT using the non-equilibrium Green's function (NEGF) method in the local density approximation (LDA) [14].

Simulation of characteristics is implemented in the program Atomistix ToolKit with Virtual NanoLab [15]. (The basic equations of this method are described in detail in our previous works [16, 17]).

The current-voltage characteristic (CVC) of the nanostructure is calculated on the basis of the well-known Landauer equation, which indicates the fundamental relationship of the electric current with the transmission spectrum:

$$I(V_L,\ V_R,\ T_L,\ T_R) = \frac{2e}{h}\int_{-\infty}^{+\infty} T(\varepsilon)\left[f\left(\frac{\varepsilon-\mu_R}{k_B T_R}\right) - f\left(\frac{\varepsilon-\mu_L}{k_B T_L}\right)\right] d\varepsilon\,, \tag{1}$$

where e is the electron charge, h is the Planck constant, ε is the energy, $T(\varepsilon)$ is the transmission function (spectrum), $f(\varepsilon)$ is the Fermi function of quasiparticle energy distribution, k_B is the Boltzmann constant, T_L, T_R are the current temperatures of the left and right electrodes, μ_R, μ_L are the electrochemical potentials of the left and right electrodes.

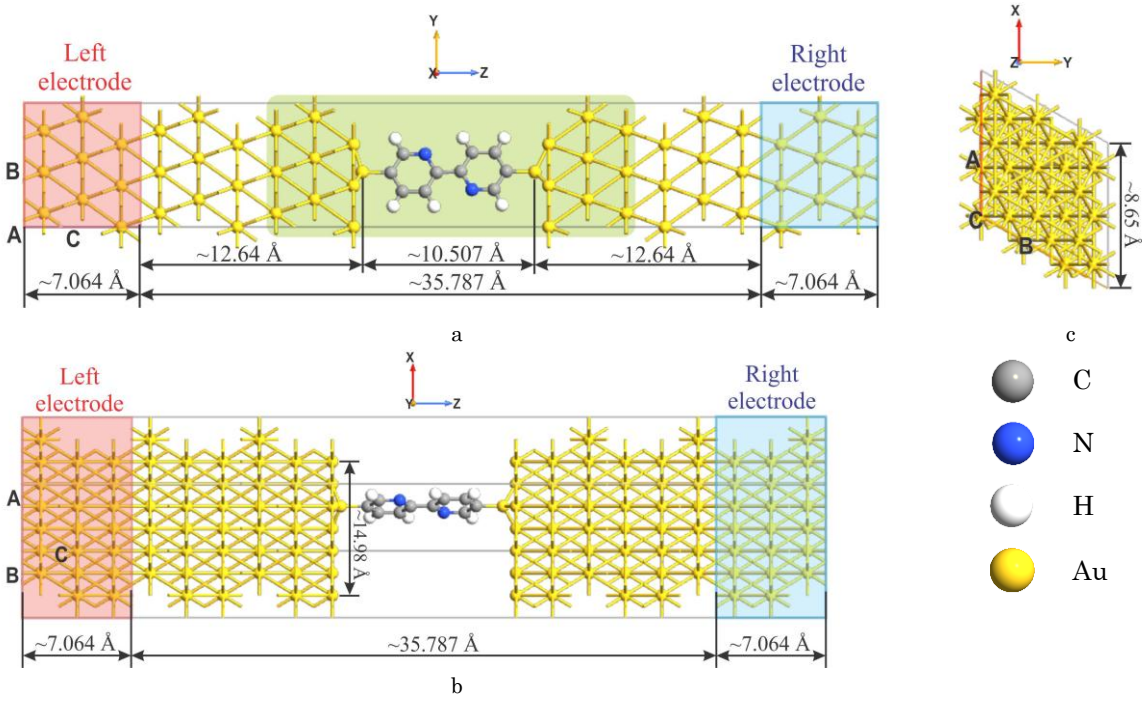


Fig. 2 – The geometry of"Au – Bipyridine – Au" nanocontact: a) Z-Y plane; b) Z-X plane; c) X-Y plane

To describe the interatomic interaction and optimization of the Bipyridine and Au structures, we used the ReaxFF_SiCNH [18] and EAM_Au_Sheng_2011 [19] potentials, respectively.

3. RESULTS AND DISCUSSION

The results of the calculation of the local density of states (LDOS) of the nanocontact are presented in Fig. 3. As shown, at the Au – Bipyridine interface, a surge of LDOS ~ 110 eV^{-1} $Å^{-3}$ is observed.

The evolution of the transmission function (spectrum) of the "Au – Bipyridine – Au" nanocontact with increasing bias voltage from – 3 V to 3 V is shown in Fig. 4a, b. Since the transport characteristics of the nanocontact are determined by the transmission method, we consider the behavior of the transmission function at $V_{bias} = 0$. At zero bias voltage, 14 distinct peaks are observed in the transmission spectrum at energies of – 5.4 eV, – 4.92 eV, – 4.08 eV, – 3.48 eV, – 2.52 eV, – 2.04 eV, – 1.32 eV, – 0.96 eV, – 0.36 eV, 2.04 eV, 2.52 eV, 3.12 eV, 3.72 eV and 5.4 eV.

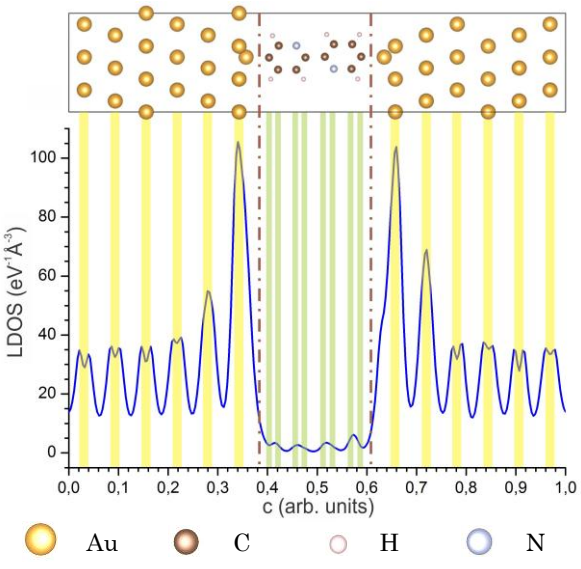


Fig. 3 – LDOS of the "Au – Bipyridine – Au" nanocontact

As shown in Fig. 4a, b, the transmission spectrum peaks shift when a bias voltage is applied, and a decrease in the spectrum amplitude is observed relative to $V_{bias} = 0$. Perhaps this spectrum behavior depends on the spatial distribution of the renormalized molecular orbitals and the voltage drop along the molecular transition [13].

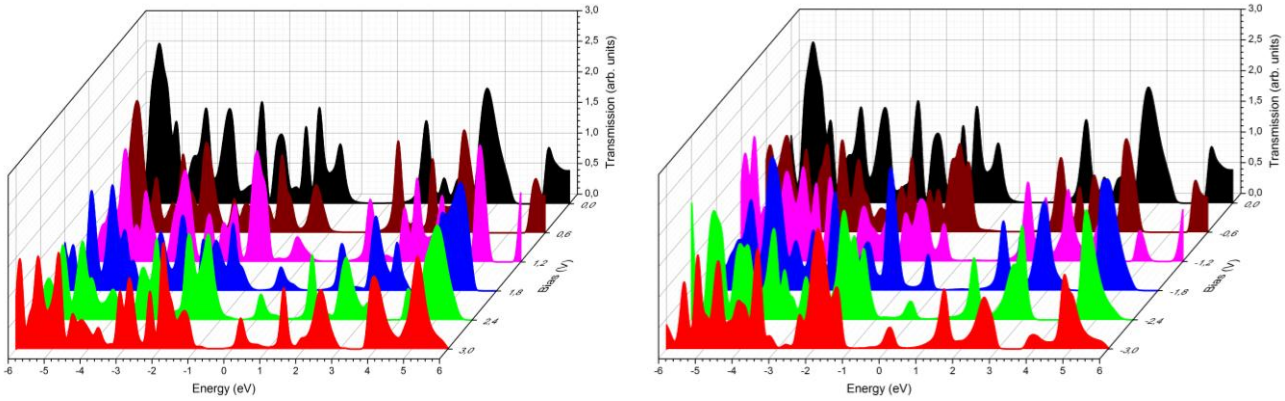
The transmission spectra of the nanocontact with maximum and minimum values resemble a spectrum of resonant tunneling structures [20]. In our view, a possible resonant tunneling can be caused by small dimensions of the central part of the nanoscale junction as shown in Fig. 2. It is the effect of resonant tunneling that determines the behavior of the electronic transport in investigated nanostructures.

The results of the calculation of the Device Density of States (DDOS) "Au – Bipyridine – Au" are presented in Fig. 5.

As shown, the features of the transmission spectrum appear in the DDOS of the structure under consideration at the same energy values, since these values are directly proportional, i.e. $T(\varepsilon) = D(\varepsilon - U)2\pi\gamma_1\gamma_2/\gamma$ (where U is the self-consistent potential, γ is the Luttinger parameter) [20]. The density of the state of a nanodevice at negative energy is substantially greater (approximately 4.6 times) than at positive energy.

The main peaks at 172.67 eV^{-1}, 154.42 eV^{-1} are observed at – 3.96 eV and – 1.44 eV, respectively. With positive energy, the maximum value of density of states 37.44 eV^{-1} appears at 5.64 eV.

The results of simulation of CVC and differential conductivity are shown in Fig. 6. As shown, there is a strong oscillation characteristics, forming peaks of – 8.48 μA, – 5.16 μA, – 5.16 μA, – 0.936 μA with the application of a negative voltage of – 2.39 V, – 1.95 V, – 1.29 V, – 0.67 V, respectively. The current minima – 10 μA, – 9.28 μA, – 6.15 μA occur at – 2.22 V, – 1.62 V and – 1.07 V, respectively.



a b

Fig. 4 – Evolution of the transmission spectrum of the "Au – Bipyridine – Au" nanocontact with increasing bias voltage V_{bias} : a) 0 ÷ 3 V; b) 0 ÷ – 3 V

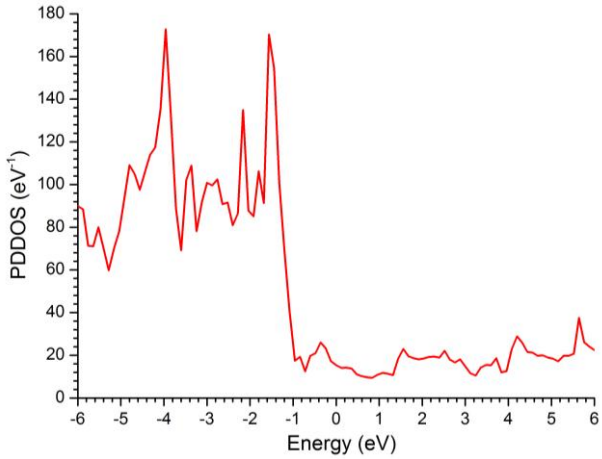


Fig. 5 – DDOS of "Au – Bipyridine – Au" nanocontact

When a positive voltage is applied in the range from 0 to 0.9 V, the current rises quasi-exponentially to a value of 7.9 μA. After that, there is a slow current drop to 5.83 μA with $V_{bias} = 1.61$ V. In the range of 1.61 V ÷ 2.4 V, the current rises again to 10.6 μA and quickly drops to 9.88 μA with $V_{bias} = 2.55$ V. Noticeable changes in the CVC form the areas of negative differential voltage.

The features of the CVC of the nanocontact are clearly manifested in their differential conductivity (Fig. 6). The maximum differential conductivity of 42.44 μS is observed at a bias voltage of 2.75 V, and the maximum negative differential conductivity of – 18.9 μS is at a bias voltage of – 1.79 V.

At a negative bias voltage, the dI/dV spectrum has a strongly oscillating character. The differential conductivity maxima of 26.57 μS, 28.63 μS, 20.73 μS and 23.83 μS occur at V_{bias} equal to – 2.53 V, – 2.09 V, – 1.48 V and – 0.89 V, respectively. The minima of differential conductivity are observed as dips – 10.38 μS, – 13.8 μS, – 18.9 μS, – 6.84 μS, – 1 μS when a voltage is applied of – 2.72 V, – 2.31 V, – 1.79 V, – 1.17 V, – 1.17 V, – 0.63 V, respectively.

With a positive bias voltage, the highs of 16.28 μS, 1.43 μS, 2.65 μS, 16.81 μS, 42.44 μS appear at 0.63 V, 1.3 V, 1.72 V, 2.25 V, 2.75 V, respectively. The dI/dV minima of – 4.69 μS, – 3.7 μS, 0.22 μS, and 7.45 μS occur when V_{bias} is equal to 1.09 V, 1.49 V, 1.88 V, and 2.47 V, respectively.

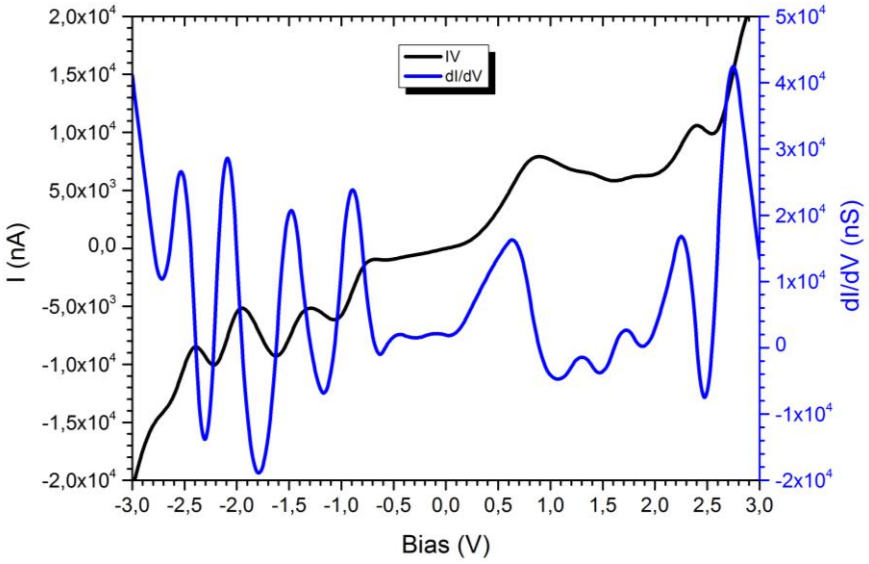


Fig. 6 – Current-voltage and *dI/dV* characteristics of the "Au – Bipyridine – Au" nanocontact

4. CONCLUSIONS

Thus, in this work, within the framework of the density functional theory, the basic electrical characteristics (density of states, transmission spectra at various values of bias voltage, CVC, differential conductivity) of the "Au – Bipyridine – Au" nanocontact are studied.

It is shown that the CVC of the nanocontact is characterized by a sharp increase in the tunneling current at certain voltage values, possibly due to resonant tunneling of quasiparticles, and many sections of negative differential resistance are observed on the CVC.

It was revealed that the *IV* and *dI/dV* characteristics of the nanocontact at a negative bias voltage oscillate. The evolution of the transmission spectrum of a nanostructure with an increase in the bias voltage (from – 3 to 3 V) is shown, and the behavior of the transmission spectrum with sharp resonance peaks is evidence of the effect of resonant tunneling in the nanostructures under consideration. It is shown that when a bias voltage is applied, the transmission spectra shift, which is explained by the voltage drop along the molecular transition. At the Au – Bipyridine interface a surge of LDOS ~ 110 $eV^{-1}Å^{-3}$ is observed. It is shown that the DDOS value at negative energy from – 6 eV to – 1 eV is approximately 4.6 times greater than the DDOS value at a positive voltage.

The obtained results can be useful for building novel electronic devices in the field of molecular electronics.

REFERENCES

1. J.C. Cuevas, E. Scheer, *Molecular Electronics (An Introduction to Theory and Experiment)*, 848 (World Scientific: 2017).
2. N. Agrait, A.L. Yeyati, J.M. van Ruitenbeek, *Phys. Rep.* **377**, 81 (2003).
3. K.K. Likharev, *Physica C* **482**, 6 (2012).
4. A.I. Braginski, *J. Supercond. Nov. Magn.* **32**, 23 (2019).
5. D. Sergeyev, *Russ. Phys. J.* **59**, 456 (2016).
6. Y. Kanbur, M Irimia-Vladu., E.D. Głowacki, G. Voss, M. Baumgartner, G. Schwabegger, L. Leonat, M. Ullah, H. Sarica, S. Erten-Ela, R. Schwödiauer, H. Sitter, Z. Küçükyavuz, S. Bauer, N.S. Sariciftci, *Organ. Electron.* **13**, 919 (2012).
7. Z. Bao, J. Locklin, *Organic Field-Effect Transistors*, 640 (CRC Press, New York: 2007).
8. M.C. Petty, T. Nagase, H. Suzuki, H. Naito, *Molecular Electronics.* In: Kasap S., Capper P. (eds) *Springer Handbook of Electronic and Photonic Materials. Springer Handbooks* (Springer, Cham: 2017).
9. K. Moth-Poulsen (eds), *Handbook of Single-Molecule Electronics*, 448 (Jenny Stanford Publishing, New York: 2016).
10. E.S. Soldatov, V.V. Kolesov, *RENSIT,* **4(2)**, 71 (2012).
11. X. Li, D Zou, B. Cui, Y. Li, M. Wang, D. Li, D. Liu, *Phys. Lett. A* **382**, 2475 (2018).
12. A. Srivastava, B. Santhibhushan, V. Sharma, K. Kaur, Md. Sh. Khan, M. Marathe, A. de Sarkar, M.Sh. Khan, *J. Electron. Mater.* **45**, 2233 (2016).
13. X. Wu, Q. Li, J. Huang, J. Yang, *J. Chem. Phys.* **123**, 184712 (2005).
14. M. Brandbyge, J.-L. Mozos, P. Ordejon, J. Taylor, K. Stokbro, *Phys. Rev. B* **65**, 165401 (2002).
15. *Atomistix ToolKit. Manual Version 2015.1.*, QuantumWise A/S, 840 (2015).
16. D. Sergeyev, K. Shunkeyev, *Russ. Phys. J.* **60**, 1938 (2018).
17. D. Sergeyev, *J. Nano-Electron. Phys.* **10**, 03018 (2018).
18. O. Böhm, *AQcomputare GmbH* (2015).
19. H.W. Sheng, M.J. Kramer, A. Cadien, T. Fujita, M.W. Chen, *Phys. Rev. B* **83**, 134118 (2011).
20. S. Datta, *Quantum Transport: Atom to Transistor,* 404 (Univ. Press, Cambridge: 2005).

Комп'ютерне моделювання електротранспортних характеристик наноконтакту "Золото – Біпіридин – Золото"

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У рамках теорії функціоналу щільності, використовуючи метод нерівноважних функцій Гріна (DFT + NEGF), і в наближенні локальної щільності, були вивчені електротранспортні характеристики наноконтакту "Золото – Біпіридин – Золото". Розрахунок реалізований у програмі Atomistix ToolKit з використанням забезпечення Virtual NanoLab. Розраховуються вольт-амперні характеристики, характеристики *dI*/*dV*, спектр пропускання і щільність станів наноконтакту. Показано, що спектри пропускання наноконтакту нагадують спектр резонансних тунельних структур. При застосуванні напруги зміщення виявлено зсув спектрів пропускання, що пояснюється падінням напруги на молекулярному переході. Показано, що DDOS при від'ємній енергії (– 6 ÷ – 1 еВ) значно вище, ніж при додатній енергії. У діапазоні напруг зсуву – 3 ÷ – 0.5 В спостерігається помітне коливання струму. Показано, що на вольт-амперній характеристиці наносистеми з'являється безліч областей з від'ємним диференціальним опором, можливо, внаслідок резонансного тунелювання квазічастинок. Такі ж зміни спостерігаються і на характеристиці *dI*/*dV*. Отримані результати можуть бути корисними для розрахунку нових перспективних електронних пристроїв молекулярної електроніки.

Ключові слова: Електронний транспорт, Наноконтакт, Біпіридин, Негативний диференціальний опір, Вольт-амперна характеристика.