The unique properties of two-dimensional (2D) materials such as graphene [1] and materials with a structure similar to graphene [2] cause interest in connection with the possibility of applying such materials in quantum electronics, semiconductor technique and quantum computing systems. The study of impurity centers in such materials is one of the fundamental areas of modern nanoscience. The paper presents the calculation of the energy of singlet and triplet states of two-electron systems such as exchange-coupled pairs of shallow hydrogen-like impurities and D--centers in 2D graphene-like structures with ion-covalent bond. The calculations were carried out by the variational method with using the Gaussian system of functions. Similar functions were previously used to calculate the energy of the singlet and triplet states of the 2D hydrogen molecule [3]. The parameters of the electron– phonon coupling were determined using the dielectric characteristics calculated in [2] with using the modified method of binding orbitals of binary 2D *ANB8–<sup>N</sup>* compounds.  $\frac{E}{\sqrt{2}}$ Two-electron systems in two-dimensional<br>  $\frac{E}{\sqrt{2}}$  the channel in  $\frac{1}{\sqrt{2}}$  ( $\frac{1}{\sqrt{2}}$  iii)  $\frac{1}{\sqrt{2}}$  ( $\frac{1}{\sqrt{$ **EVO-PLEC**<br> **EXAMPLE TOST**<br> **EXAMPLE TOST**<br> **EXAMPLE TOST**<br> **EXAMPLE TOST**<br> **EXAMPLE TOST**<br> **EXAMPLE TOST**<br> **EXAMPLE TON**<br> **EXAMPLE** Two **- electron sympatric interpretation**  $\mathbf{R} = \mathbf{R} \times \mathbf{R}$ <br>
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*<sup>2</sup>Taras Shevchenko National University of Kyiv;* 

# **INTRODUCTION**

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Newsate of In crystals with parameters characterizing the intermediate electron-phonon coupling  $(1 < \alpha < 2)$ ,  $0.06 < \eta < 0.9$ ), accounting for the interaction of electrons with optical phonons leads to a significant decrease in the energy of the ground state and a significant increase in the binding energy of two-electron centers. For exchangecoupled pairs of impurity centers, the phonon component of the Heisenberg exchange has an antiferromagnetic character and is comparable in magnitude to the energy of the Coulomb exchange interaction calculated without taking into account the polaron component of the energy. Oneelectron WF **Ψ(r)** can be used to construct twoelectron functions of the singlet and triplet states in the framework of the Heitler-London and the molecular orbital methods. **EXERCISE THE RESULTE OF EXERCISE AND RESULTE AND RES** In the second control of the second control o

We consider two  $D^0$  centers in the phonon field of a 2D crystal. The energy  $E_{12}$  of the ground state of the considered system has the form:

**References** 

:  ${C_i, a_{1i}, a_{2i}, a_{3i}}$   $N_{12}$   $N_{12}$   $N_{12}$  $\{J_{12}\},\,J_{12}=\frac{12}{N}\frac{12}{N}\frac{C}{N}\frac{1}{N}\frac{C}{N^2},\,(4)$   $F^{\dagger}F^{\dagger}F^{\dagger}F^{\dagger}F^{\dagger}F^{\dagger}F^{\dagger}F^{\dagger}F^{\dagger}F^{\dagger}F^{\dagger}F^{\dagger}F^{\dagger}F^{\dagger}F^{\dagger}F^{\dagger}F^{\dagger}F^{\dagger}F^{\dagger}F^{\dagger}F^{\dagger}F^{\dagger}F^{\dagger}F^{\dagger}F^{\dagger}F^{\dagger}F^{\dagger}F$  $12 \t 10$   $12 \t 12$  $2 = N$   $N$   $N$   $N$   $2$   $(1)$   $E_{i} = E^{0} + E_{i} - E_{i}$  $\{a_{1i}, a_{2i}, a_{3i}\}\$   $IV_{12}$   $IV_{12}$   $IV_{12}$ 2  $\{a_{3i}\}\qquad I\mathbf{V}_{12} \qquad IV_{12} \qquad IV_{12} \qquad V_{13}$  $12 + C + f$  (A)  $12 - 111111$   $0.12$   $0.912$  $a_{3i}$   $N_{12}$   $N_{11}$  $E_{12} = \min \{J_{12}\}, J_{12} = \frac{I_{12}}{I_{12}} + \frac{V_C}{I_{12}} + \frac{V_f}{I_{12}}$ , (4)

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## **BASIC RELATIOS**

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# **Systems in two Tes with ion-C**<br>
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ydrogen atom e<br>  $\frac{8}{\pi}$ <br>  $\int_{\frac{1}{(C,a)}}^{\infty} \frac{r}{2} c_i \exp(-a_i r^2)$ ,<br>
Parameters of the Canal Canal Canal Canal Canal Canal C **ructures with ion-covalent bond<br>
1.1.**<sup>1</sup>, Venger E.F.<sup>1</sup>, Kashyrina Ya.O.<sup>2</sup>, Roik O.S.<sup>2</sup><br>
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**Kashirina N.I. 1 , Venger E.F.<sup>1</sup> , Kashyrina Ya.O. 2 , Roik O.S. 2** The set of t Venger E.F.<sup>1</sup>, Kashyrina Ya.O.<sup>2</sup>, Roik O.S.<sup>2</sup><br>Example: The Value of Ultraine Respiring 1506@gmail.com Venger E.F.<sup>1</sup>, Kashyrina Ya.O.<sup>2</sup>, Roik O

*1***V.** *Lashirina N.I.<sup>1</sup>, Venger E.F.<sup>1</sup>, Kashyrina Ya.O.<sup>2</sup>, Roik O.S.<sup>2</sup><br>17. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine, <u>kashirina1506@gmail.com</u> ;* 

$$
\Phi_{12} = \Psi_{12} \exp(-S_1 - S_2), \quad S_1 = \sum_k f_k (a_k^+ - a_k) \qquad \begin{array}{c} \text{AgC} \\ \text{CdF} \end{array}
$$
\n
$$
S_2 = \sum_{k,j} g_k(\mathbf{r}_1, \mathbf{r}_2) \exp(-i\mathbf{kr}_i) a_k^+ + H.c.
$$
\n
$$
g_k = \varphi_k (\exp(-i\mathbf{kr}_1) + \exp(-i\mathbf{kr}_2)) \qquad \text{Table}
$$

1 *i N*



The strong coupling energy of BP in a 2D crystal is

where the first, second and third terms of the left part eq. (4) for  $J_{12}$ , correspond to the kinetic energy, the Coulomb energy, the total contribution of the phonon field and electron-phonon interaction, respectively;  $N_{12}$  - is the normalization integral:

Fig. 1. Two center coordinates system.

The electron WF is determined by:

$$
P_{12} \equiv \Psi_{12}(r_1, r_2, r_{12})
$$

### **CONCLUSIONS**

$$
E_{12} = \langle \Phi_{12} | H_{12} | \Phi_{12} \rangle \qquad (1) \quad \text{IN I ERMEDIALE COUF}
$$
\n
$$
H_{12} = -\frac{1}{2} (\Delta_1 + \Delta_2) + H_C + H_{2e-f} + H_f \qquad (2) J_{12i} = \frac{2T_{12}}{N_{12}} + \frac{2\alpha V_C}{(1-\eta)N_{12}} + \frac{2\alpha V_C}{(1-\eta)
$$

**2D Hydrogen atom** effective Rydberg  
\n
$$
\Psi_{ex}(r) = \left(\frac{8}{\pi}\right)^{1/2} \alpha \exp(-2\alpha r), \qquad R = \frac{Ry}{\hbar c}
$$
\n
$$
\Psi(r) = \frac{1}{\sqrt{N(C, a)}} \sum_{i=1}^{n} C_i \exp(-a_i r^2), \qquad \text{Exchange-C}
$$

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Yenger E.F.<sup>1</sup>, Kashyrina Ya.O.<sup>2</sup>, Roik O.S.<sup>2</sup><br>
Yenger E.F.<sup>1</sup>, Kashyrina Ya.O.<sup>2</sup>, Roik O.S.<sup>2</sup><br>
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Yenger atom **r Systems in two-dimensional**<br> **Proper E.F.', Kashyrina Ya.O.**<sup>2</sup>, Roik O.S.<sup>2</sup><br> **repared to the COVAL COVAL COVAL COVAL COVERTS IS THE INTERNATIONAL CONTRACT Physics, NAS of Ukraine, kashirina 1506@gmail.com;<br>
Fifty o ON Systems in two-dimensional**<br> **CLUIES With ion-covalent bond**<br>
Venger E.F.<sup>1</sup>, Kashyrina Ya.O.<sup>2</sup>, Roik O.S.<sup>2</sup><br>
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The R parameter in Tab \* 4 2 3 2 2 2 1 0 *R m e Ry* **IONAL TEPLO FOR A SURFACE CONSUMBERED SET AND NASUREMARY SAMPLE 15 PRACTICLE AND SURFACE SURFACE (SP) =**  $a^2n^2/(1-n)^2$ **<br>
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also pairs in covalent 2D crystals can THE STATE AND STATE AND STATE AND STATE AND STATE AND STATE AND STATED THE STATE INTO THE STATE IN THE STATE AND STATED THE STATED AND STATED THE CAUGATION CONTINUIS TO THE CAULISATION OF THE CAUGATION CONTINUIS (CONTINU** The energy of exchange-coupled pairs in covalent 2D crystals can be determined based on the calculation of the energy of a 2D hydrogen molecule [3]. To calculate the value of the effective Rydberg, one should use the crystal parameters. In the case when the crystal has an addition of ionic bonds, the calculations should be performed taking into account the electron-phonon interaction with l optical phonons. Table V. Lists the energy calculations for singlet and triplet exchange-coupled pairs of shallow hydrogen-like centers in 2D crystals, as well as various contributions to the total energy (designations  $T_2$ ,  $V_c$ ,  $V_f$  and  $V_{fi}$  correspond to the first, second, third and fourth terms in equation (5).

**Table VI. Lists the energy calculations for singlet (***S***=0) and triplet (***S***=1) states of 2D shallow helium-like centers (***Z***=2) in crystals, as well as various contributions to the total**  energy  $E_{2}$ .





$$
\text{B}\text{P in a 2D crystal is} \qquad \text{in 2D systems: } E_{H}^{-}/E_{H} = 0.11992
$$
\n
$$
\frac{T_{12}}{N_{12}} + \frac{V_{C}}{N_{12}} + \frac{V_{f}}{N_{12}^{2}}, \text{ (4)} \qquad \text{E}_{b}^{-} = E^{0} + E_{p} - E^{-}, E_{b}^{0} = E_{p} - E_{b}^{0}, E_{p} \ge -\frac{\pi\alpha}{2}
$$
\n2.

**Table I. Parameters of the approximate WF 2D H**







**Table II. Approximate Ψ(r) and exact Ψex(r) values of the WF of a 2D H**

*Eex*= −2*E<sup>h</sup>* , *E<sup>H</sup> (Ψ)* = −1.9999762*E<sup>h</sup>*

 $(1)$  $\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$  $\sum V_k \left\{ \begin{matrix} \sum_{i=1}^{k} |X_i| & i \mathbf{w}_1 \end{matrix} \right\}$   $\sum V_k = \min \left\{ J_{12i} \right\}$ *k E*<sup>2</sup> min*J*12*i* **INTERMEDIATE COUPLING**  $(1-\eta)N_{12}$   $(1-\eta)N_{12}^2$   $(1-\eta)N_{12}^2$  AgCl  $\frac{0}{1-\eta}$  $\frac{12}{1}$   $\frac{200}{C}$   $\frac{1}{1}$   $\frac{200}{P}$ 2  $\sim$  2i,  $\sim$   $\sim$ 12 Agui  $2T_{12}$   $2\alpha V_C$   $2\alpha V_{ph}$   $s_L$   $(5)$  AgBr  $\frac{1}{1}$  $i = \frac{1}{M}$   $(1$  $C_{+}$   $\frac{2\alpha V_{ph}}{ph}$   $\frac{1}{2} S I_{-}$  (5)  $T_{12}$   $2\alpha V_c$   $2\alpha V_{ph}$   $5\alpha V_{p}$   $6\alpha V_{p}$   $1\alpha V_{p}$   $1\alpha V_{p}$   $1\alpha V_{p}$   $1\alpha V_{p}$   $1\alpha V_{p}$ 



**Table IV. Results of calculations in 2D systems of the ground-state energies of** *D***<sup>0</sup> and** *D* **– - centers,** *E* **0 , and**  *E* **– , respectively. Binding energies are denoted** *E<sup>B</sup>* **. All energies are in units of** *ħω*

**Table III. Material parameters**

The values highlighted in yellow correspond to three-

For all the parameters given in the Table IV, the polaron energy calculated using the Buimistrov-Pekar method is  $E_p$  =  $-\pi a/2$  (weak electron-phonon coupling), which is typical for crystals with a ion- covalent bond, when the covalent component of the bond predominates and the conditions for polaron self-trapping are not fulfilled.

$$
R = \frac{Ry^*}{\hbar \omega} = m^* e^4 \bigg/ \bigg( 2\varepsilon_0^2 h^3 \omega \bigg) = \alpha^2 \eta^2 \bigg/ \big( 1 - \eta \big)^2
$$

 The *R* parameter in Table III determines the ratio of the effective Rydberg to the energy of longitudinal optical phonons:

# **Exchange-Coupled Pairs of Paramagnetic Centers in 2D Crystals**





Table VI shows the energy of the helium-like center. These values correspond to the limiting value of an exchange-coupled pair energy at a distance between the Coulomb centers  $R_{12}=0$ , without taking into account the energy of the Coulomb centers repulsion. As an example, crystals with a fairly significant ionic value (1<  $\alpha$  < 2, 0.3<  $\eta$  < 0.5). The  $R_m$  is the equilibrium distance between Coulomb for the singlet term.