Abstract of the doctoral thesis

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titled:

„Analysis of the electron-phonon structure and thermodynamic properties of potential two-dimensional superconductors"

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For the first time observed in 1911, the phenomenon of superconductivity consists in the disappearance of electrical resistance and the acquisition of the properties of a perfect diamagnet in a material cooled below a certain characteristic temperature, called the critical temperature (T_c). This discovery is now considered to be one of the most important in the history of physics and despite over a century of history, it still arouses great interest in the scientific community. The scope of this doctoral dissertation includes theoretical studies of the properties of the electronic structure and phonon structure, electron-phonon mass enhancement parameter (λ) and thermodynamics of the superconducting state in selected two-dimensional systems. I have focused on the possibility of inducing a superconducting state in systems based on graphene or blue phosphorene (a two-dimensional allotrope of phosphorus) which in their pure form do not exhibit a phase transition to a superconducting state. However, there are several commonly accepted methods for modifying the crystal structure of such systems, which may result in the appearance of a Cooper pair condensate indicating a phase transition.

In my research I have decided to analyse the following systems: graphene monolayers XC_6 and XC_8 and double graphene layers C_6XC_6 with an admixture of an atom of element which belong to first or second group of the periodic table (X = K, Ca, Rb or Sr), as well as blue phosphorene double layer systems P_8CaP_8 with introduced calcium atoms between the surfaces. In the first step I have performed calculations using the methods of the electron density functional theory (DFT) which allowed to obtain information on: electronic properties of the studied systems, dynamic stability of their crystal structures and spectral functions of the electron-phonon interaction $\alpha^2F(\omega)$. Then I have determined the basic physical parameters characterizing the superconducting state of strongly correlated systems including: transition temperature, superconducting band gap, specific heat jump and thermodynamic critical field, with the use of the formalism of Eliashberg's equations. The obtained results allowed me for comparison with the general predictions of the BCS theory.

All the stable structures I have studied exhibit conductive properties due to the presence of many available electronic states at the Fermi energy ϵ_F level. This is a very promising result in terms of usefulness in electronics, especially when comparing this

result to the electronic properties of the primary systems of the graphene monolayer (semimetal) and the blue phosphorene monolayer (semiconductor with a 2 meV indirect energy gap). Also, basing on the conclusions of the BCS theory, the critical temperature depends on the density of electron states on the Fermi surface $N(\epsilon_F)$. A different behaviour can be seen in the phonon structure diagram where each impurity element causes an increase in the phonon density function (PhDOS) in the region of the smallest frequencies, which in turn translates into rise of the electron-phonon coupling constant λ. This, in addition to the results of the electronic structure, suggests the possible greatest increment in the electron-pairing interactions potential in systems intercalated with calcium atoms, notably in the graphene bilayers C_6XC_6. Obtained values of the pairing kernel λ equal to: 0.86, 1.18, 0.93 and 0.85 confirm that, respectively for the systems: C_6KC_6, C_6CaC_6, C_6RbC_6 and C_6SrC_6. For single-layered structures the results show values of 0.23, 0.35, 0.26, 0.27 for KC_6, CaC_6, RbC_6, SrC_6 and 0.34, 0.42, 0.29, 0.17 for KC_8, CaC_8, RbC_8, SrC_8. The strength of electron coupling interactions in the blue phosphorene bilayers is at the level of 0.759 and 0.798 in the configurations AA and AA'. All C_6XC_6 layers can be considered as strongly correlated structures due to the value $\lambda \approx 1$. Such a level of the coupling constant had made me determine the thermodynamic properties of the superconducting state in C_6XC_6 and P_8CaP_8 layers using the formalism of the Eliashberg's equations. I have obtained only the critical temperature in XC_6 and XC_8 systems using the Allen-Dynes formula because of low λ values. This is an approach that gives only the value of T_c while neglecting the influence of strong-coupling interactions. For this reason the critical temperatures may be underestimated in comparison to the results of the Eliashberg's theory approach, as is the case in the C_6XC_6 systems. The structures of the graphene bilayers allow for the induction of the superconducting state at the following temperatures: 8.67 K, 14.56 K, 5.47 K and 8.74 K, respectively for the dopant: K, Ca, Rb and Sr. However, the originally derived formalism of the Eliashberg's equations assumes that the parameter $\lambda\omega_D/\epsilon_F$ of the material should be 0 or very close to it, while its values in the C_6XC_6 compounds are: 0.079, 0.081, 0.093 and 0.062. In order to compare the values and determine the necessity of first-order Migdal's theory corrections application I have calculated the transition temperatures with *vertex corrections* introduced to the formalism. This modification lead to a slight decrease of all graphene bilayers T_c except for C_6RbC_6. The transition temperatures of a single graphene layers indicate the possibility of superconducting state occurrence only in the systems with a calcium atom in the cell, regardless of its concentration; their critical temperatures are: 0.81 K and 1.86 K for CaC_6 and CaC_8, respectively. Double layered systems of blue phosphorene P_8CaP_8 can boast a two-digit critical temperature result: 11.63 K and 11.74 K for AA and AA' configurations.

The results proves the significant impact of the dopant on the electronic structure of examined systems and show that each scheme of dopant atom placement affects the shape of the phonon density of states function in the low frequency region. This area directly translates into the highest electron-phonon interaction potential values and has a decisive impact on increasing the possibility of superconducting state induction in the analysed materials.

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