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COMPUTER MODELING OF STRUCTURE AND CALCULATION OF THE SHORT-RANGE ORDER PARAMETERS DISORDERED TWO-LAYERS AB GRAPHENE

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Computer modeling in modern science is an important method of research if the conducting of an experiment is impossible or requires a large amount of resources. Through modeling, a researcher can observe and draw conclusions about which factors influence certain material properties. Computer modeling of structure disordered two-layers graphene allows to study the effect of defects on electron properties to understand how to change the structure of the materials to obtain the characteristics that are necessary for further use.

The short-range order parameter can be obtained both experimentally and theoretically [1], and can serve a qualitative and quantitative characteristic of the defect structure of a material. Earlier, we carried out automation of short-range order parameters calculations for single-layer graphene [2], bcc, fcc, and simple cubic lattices [3]. The received data had a qualitative and quantitative match with the experimental data. Using the same method and experimentally determined locations of defects in the structure, similar software was developed for two-layers AB graphene.

The program is written the Java programming language. To model the structure of two-layers AB graphene with defects, a freely distributed Jmol applet was used, which allows to visualize structures with short-range order at the atomic level. When the program is opened, the crystal lattice of two-layers AB graphene appears in front of the user. In the upper right part of the program window there is a button that allows you to select the location of atoms of different sort: in the upper layer, above the layer, or between the layers.

Figure 1 shows a screenshot of the program window. The yellow color indicates the places where atoms of different sort may be located. If one of the yellow spheres is selected by the user, it changes color to red and bonds with the nearest carbon atoms appear. After entering information on the location of defects in the structure, one can move to the calculations of the short-range order parameter for the first and second coordination spheres. In the lower right part of the window there is a button “Short range”. After clicking this button, the data on the short-range order values for the given configurations of defects will appear in the sidebar.

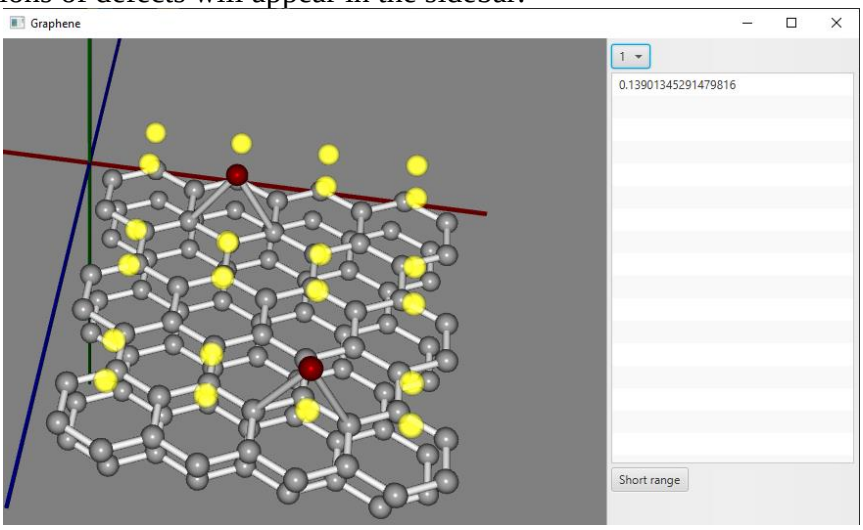

Fig.1. The program window, which shows the option choice of the location of impurity atoms above the layer. The placement of the yellow spheres is a possible choice for the location of an atom of a different sort above the layer, the placement of the red spheres is selected for the calculation of a different sort atoms, the gray spheres are carbon atoms.

In the present program the calculated data of the short-range order parameters are different depending on configurations of defects and have different values both in magnitude and in sign. The results of the program were used to describe the electronic relaxation time, the density of electronic states and the electrical resistance of two-layers AB graphene. Through to the data on the values of the order parameters for specific disordered structures that were obtained in the process of program work, it became possible to predict what configuration of defects lets to open the gap in the density of states and which ones lead to the metallization of two-layers graphene.

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