Graphene model as a lattice of hydrogen-like atoms with shielded ions in the strong bond approximation

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The simplest graphene model is an approximation of independent hydrogen-like atoms with a shielded ion. In [1], on the basis of the Thomas-Fermi theory, the distribution of electrons in shielded atoms of ions with an arbitrary charge of the nucleus was obtained. This electron distribution was used in [2-3] in the carbon atom model to calculate the emission characteristics of graphene. At the same time, it was assumed that of the four valence electrons, three electrons that are connected have little effect on the emission process. It was shown that the centrally symmetric field of the shielded ion is inhomogeneous in radius. Therefore, in the variational calculation of the electron energy, the total energy operator was modified according to [4]. The degeneracy condition was obtained for this operator and the ground state energy was calculated. In [5], this model, taking into account the Coulomb interaction of an electron with a shielding shell, was used to calculate the photo-ionization energy of light atoms from the ground state. In the presented paper, the distribution of shielding electrons in the model of an atom with a finite ion shielding radius - r_i is obtained. The radius r_i is determined from the condition of equality of the centripetal binding forces with the ion and the centrifugal field forces of the nearest lattice atoms. In [6], this model was used for a self-similar solution of the self-consistent problem of the evolution of the quantum state of a weakly bound electron during demoralization from the ion shielding shell Fig. 1.

References

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Figures

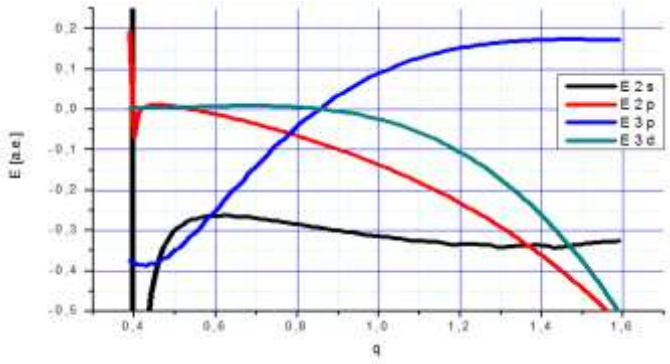

Figure 1: Dependence of the binding energy of the electron of the carbon atom in the 2s, 2p and 3p states on the effective charge of the ion at two values of the lattice step.