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Electron Cloud Densitometry of Inner and Valence Electrons in Carbon Allotropes

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Abstract: Electron cloud densitometry of carbon allotropes is presented in this study. Carbon consists of two inner and four valence electrons. The valence electrons in carbon are hybridized or active. Each active valence electron builds a negatively charged shape due to their delocalization. It is proved that the active valence electron creates the van der Waals force, which bonds layers of crystalline graphite together. An easy quantum mechanical explanation of the electron cloud densitometry is given in this study. In accordance with this effect, an atom begins to illuminate, depicting its shape. Electron cloud densitometry images show the inner and valence electrons in the applied functional materials, such as activated coke, graphite, graphene, and diamond.

Keywords: Electron cloud densitometry, Visual chemistry, Activated coke, Graphite, Graphene, Diamond.

1. Introduction

Solid carbon exists in several allotropic forms: graphite, diamond, graphene, nanotubes, fullerenes, coke, vitreous carbon, and so on. In 1873, van der Waals discovered a force [1] that was later named after him. The van der Waals force includes attraction between atoms, molecules, and surfaces. They are active owing to polarization and weaker than covalent and ionic bonds. This force plays a major role in carbon allotropes. The Encyclopedia Britannica under the watchword "Structure of carbon allotropes" defines it as "the interlayer distance (337 pm) is sufficiently large to preclude localized bonding between the layers; the bonding between layers is probably by van der Waals interaction". A prominent quantum chemist Coulson entitled valence [2] as "the distance between successive planes is 335 pm, a value so large that it can only arise from van der Waals forces". The Van der Waals force is present in the monolayer graphene [3]. The Van der Waals force is present in the activated carbon [4] embodied in both charcoal and coke [5].

The study aims to show that by electron cloud densitometry, there are active valence electrons in nature that builds negatively charged shape due to their delocalization. The active valence electrons create the van der Waals force, which, in particular, connects the layers of crystalline graphite.

2. Theory

The active valence electron quantum mechanical theory is given below.

In 1927, Heitler and London [6] performed a quantum mechanical calculation of the hybridization of the 1s molecular orbitals of the H_2 molecule. The success of this theory led to a series of studies in the field of chemical bonds and Pauling's creation of the monograph “the Nature of Chemical Bonds” [7]. In 2021, O.P. Kucherov [8] extended these quantum mechanical calculations to heavy atoms, such as silicon. Thus, it is logical to carry out these calculations of hybridization double bonds.

The active valence electron theory states that if there is already a hybridization created by electrons ***1*** and ***2*** between two atoms ***a*** and ***b***, then additional hybridization created by electrons ***3*** and ***4*** is impossible. This statement is proved as follows.

Let the hybridization create a system consisting of the atom a with two electrons ***1, 2*** and atom ***b*** with two electrons ***2, 3*** (Fig. 1).

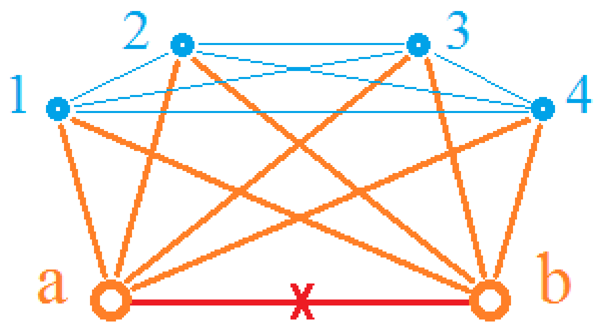


Fig. 1. Atom *a* with exchange electrons *1, 2* and *b* with exchange electrons *3, 4* take part in double hybridization.

Hybridization is a purely quantum mechanical exchange phenomenon that occurs in the presence of symmetry with respect to the point ***X***, which bisects the distance ***ab*** between atoms. The exchange electrons ***1*** and ***2*** of an atom ***a*** are described by the wave functions ***φa(1)*** and ***φa(2)*** and the exchange electrons ***3*** and ***4*** of atom ***b*** is described by the wave functions ***φb(3)*** and ***φb(4).***

According to the principle of superposition, the wave function of a system of four bound electrons is the product of their wave functions.

$$\Psi 1 = \varphi a(1)\times\varphi a(2)\times\varphi b(3)\times\varphi b(4) \quad (1)$$

However, the function ***Ψ1*** is not unique for the system of two atoms. There is the principle of quantum mechanics according to which identical particles cannot be distinguished. Therefore, nothing changes when the exchange electrons are swapped.

Let us construct a function ***Ψ2*** in which electrons ***1*** and ***3*** change places.

$$\Psi 2 = \varphi a(3)\times\varphi a(2)\times\varphi b(1)\times\varphi b(4) \quad (2)$$

This means that electrons ***1*** and ***3*** have the same energies and all quantum numbers ***n, l, m***, but differ only in the spin direction. That is, for ***1 s = ½,*** and for ***3 s = -½.***

Let us construct a function ***Ψ3*** in which electrons ***1*** and ***2*** change places.

$$\Psi 3 = \varphi a(2)\times\varphi a(1)\times\varphi b(3)\times\varphi b(4) \quad (3)$$

This means that electrons ***1*** and ***2*** have the same energies and all quantum numbers ***n, l, m***, but differ only in the spin direction. That is, for electron ***1 s = ½,*** and for electron ***2 s = -½.***

As a result, the electrons ***2*** and ***3*** must have the same all quantum numbers ***n, l, m, s*** which is prohibited by the Pauli principle. That is, a single bond is possible but a double bond is impossible. It follows the van der Waals forces as an active valence electron that are not bound to other atoms by hybridization or ionization. Their elongated shape creates the active dipole moment and weakly attracts positive charges. The active valence electrons in activated coke, graphite, graphene, and diamond are visualized by the electron cloud densitometry as below.

3. Experiment

The following describes the technology of electron cloud densitometry of atoms and chemical bonds.

The body of valence electrons cannot be seen with either an optical microscope or a transmission electron microscope. Classical physics does not allow this for two reasons. First, electrons do not have the bodies we want to see. Second, both optical and electron waves exceed the size of an atom.

However, quantum mechanics allows us to observe the real shape of the inner and valence electrons. Quantum mechanics teaches that the electrons that revolve around the nucleus of an atom have the shape of a cloud and that cloud has a density [9]. Kucherov and Lavrovsky [10] invented electron cloud densitometry, the essence of which is that an electron beam, passing through an atom, receives information about the shapes of electron clouds. Below is a brief but comprehensive presentation of this theory.

Consider two objects of quantum mechanics: a) an atom with inner and valence electrons and b) an external electron beam. The quantum mechanical objects have the properties of waves and particles at the same time. The objects are waves.

The basis of quantum mechanics is the statement that the wave function ***Ψ(x,y,z),*** with coordinates ***x, y, z,*** describe the state of the system and the square modulus of this function determines the probability to find the system in the volume ***dxdydz.***

$$P\,(x,y,z)=|\Psi\,(x,y,z)|2dxdydz. \tag{4}$$

The wave function of the electron beam $\sqrt{j}$ is a plane wave, it is given by the current density and does not depend on the coordinates $\sqrt{j(x,y,z)} = constant$.

The wave function of the atomic electron is $\varphi(x,y,z)$ and the square module of this function determines the electron cloud density $\rho(x, y, z)$ in the volume ***dxdyd.***

$$\rho(x,y,z)=|\varphi(x, y, z)|2dxdydz. \tag{5}$$

Let us find the electron cloud density $\rho(x,y,z)$ by taking advantage of the fact that the objects have the properties of particles. The objects are particles.The quantum mechanics particles obey the principle of superposition: the probability of meeting at a certain point $|\Psi(x,y,z)|2dxdydz$ is equal to the product of the probabilities of each particle to get to this point.

$$P(x,y,z)= |\sqrt{j}|2 \times | \Phi(x,y,z)|2 \tag{6}$$

In this case, the following integral of Eq. (6) from ***zmin*** to ***zmax*** defines the probability $I(x,y)$ to find the electron at point ***x, y*** of the microscope screen.

$$J(x,y) = j\times\rho(x, y) \tag{7}$$

Thus, the plane wave amplitude $J(x,y)$ is proportional to the electron cloud density $\rho(x,y)$ or the thickness of the electron cloud of the atom at the point of the beam passage. The cloud changes the current not by absorption or amplification, but by spatial shift due to the principle of superposition. This is a purely quantum effect, it is absent in electrodynamics.

The theory set out above is accurate and not approximated in any way.

Law 1. *Thus, the interaction of the electric beam with electron clouds in accordance with the principle of quantum mechanical superposition obeys the Kucherov law:* ***the current passed by an electron cloud is proportional to the density of that cloud.***

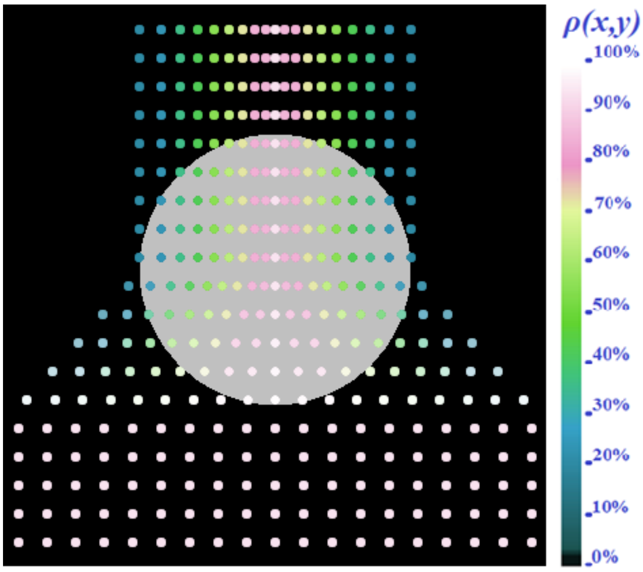


Fig. 2. Electron cloud attracts the electron beam in proportion to its own density $\rho(x,y)$. The density scale is shown on the right.

The property of the electron cloud to shift the electron beam is shown in Fig. 2. When the object under study has the size of an atom, electron rays pass through the atom without absorption. However, as a result of the quantum superposition, electron clouds attract an electron beam without changing their speed and direction. On the periphery, where the electron cloud is absent, the rays completely disappear. The intensity of the rays increases in the center, where the thickness of the electron cloud reaches a maximum. As a result, the atom begins to illuminate, depicting its internal construction.

The electron cloud densitometry of different materials clearly shows the following. The inner electrons have a pink ball around the nucleus. All carbon atoms, both without hybridization and with $sp/sp^2/sp^3$ hybrids, have green constructions in the form of the infinity sign ∞. The active valence electrons have an elongated negatively-charged blue structure. This is demonstrated with the examples of activated coke, graphite, graphene, and diamond.

4. Activated coke

Widespread activations of carbon are chemical [4], physical [11], or mechanical [12]. Amorphous carbon is synthesized by mechanical activation (MA) treatment of spectrally pure (99.99%) graphite in a Fritsch Pulverisette P6 ball mill in SiN vial and milling balls in argon gas atmosphere (400 RPM, the mass ratio of balls and a sample of 30:1, the energy density of 2.42 W/g). Specific energies (doses) transferred to the samples during grinding for 10 hrs were 87.1 kJ/g. The electron cloud densitometry images are obtained with a high-resolution electron microscope (JEOL JEM-2100F) by using the method in Ref. [10] with 10 pm resolution.

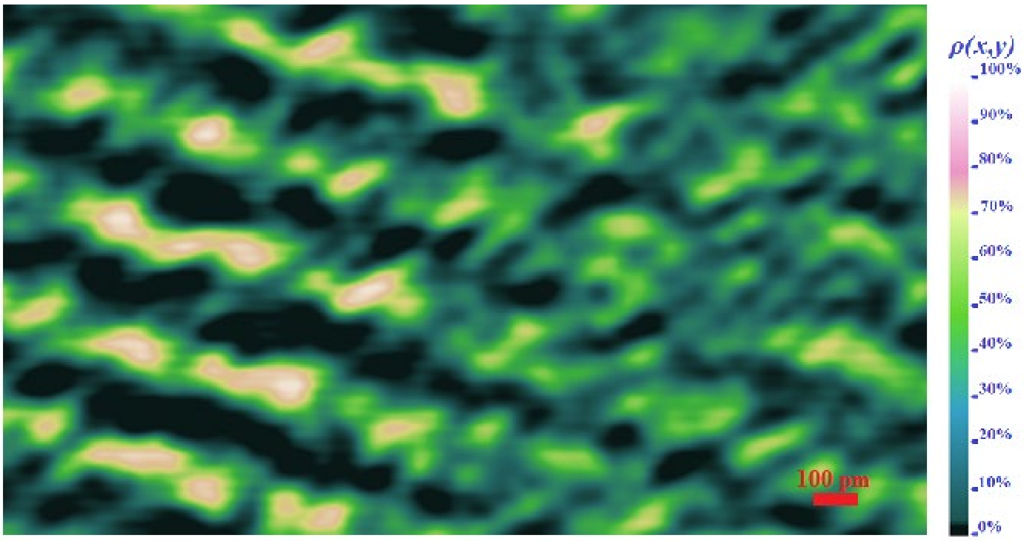


Fig. 3. Electron cloud density image of ***sp²*** hybridized carbon in crystalline graphite (left) and activated coke without hybridization (right).

The electron cloud density image (Fig. 3) shows the result of the activation. Carbon atoms in crystalline graphite (left) form layers by covalent chemical bonds ***sp²*** hybrids with have green constructions in the form of the infinity sign ∞ in accordance with the theory [8]. The blue active valence electrons that form the Van der Waals forces bound the layers.

Figire 4 shows a sharp change in chemical bonds as a result of activation (right). The green covalent chemical bonds ***sp²*** hybrids in the form of the infinity sign ∞ become blue active valence electrons and the crystalline structure is distorted. All active valence electrons have an elongated negatively-charged blue form and create amorphous chaos.

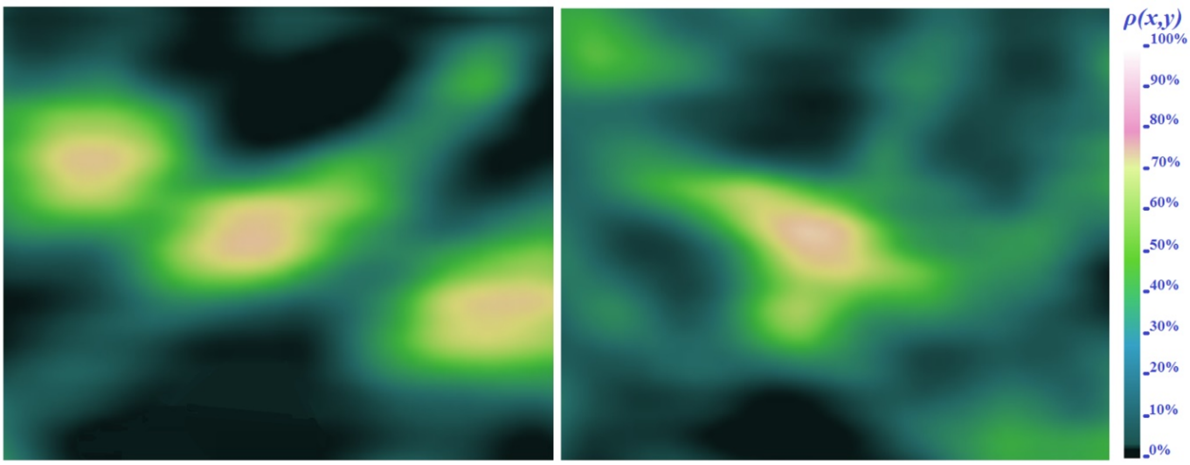


Fig. 4. Electron cloud densitometry images of a single carbon atom in a graphite crystal (left) and activated coke (right). In each state, the atom has two inner pink electrons and four valence electrons. The difference is that the left atom has two green covalent and two blue active electrons, and the right atom has four blue active electrons.

The electron cloud density image (Fig. 4, left) shows a single carbon atom in crystalline graphite with six electrons. The two inner electrons have the shape of a pink ball. The two covalent bond electrons green create strong ***sp*** hybrids in the form of the infinity sign ∞ with two neighboring atoms. The two active valence electrons (blue) builds negatively charged shapes due to their delocalization and occur laterally from the graphite layer.

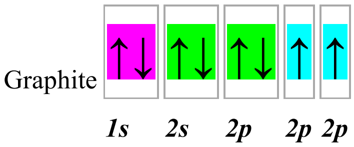


Fig. 5. Valence electrons in graphite layer.

Each carbon atom in crystalline graphite is known to have three sp^2 hybrids, but Fig. 3 shows the edge of the crystal therefore the third hybrid atom is lacking. Classical carbon atoms in crystalline lattice with three sp^2 hybrids will be shown below by the example of graphene.

The space between the layers is mostly black, signifying zero density of the electron clouds.

The electron cloud density image (Fig. 4, right) shows a single carbon atom in activated coke with all its own six electrons. The two inner electrons have the shape of a pink ball. Four active valence electrons (blue) build negatively charged clouds elongated in different directions.

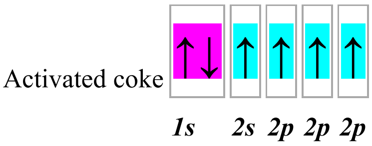


Fig. 6. Valence electrons in activated coke.

The active valence electrons create the van der Waals force and makes coal active. The disappearance of covalent bonds during mechanical activation of graphite is confirmed by the decrease and expansion of the Raman vibrational bands sp^2 and sp^3 -hybridization [13]. In addition, the active valence electrons have opened up new materials with extraordinary technological properties. For example, cheap Musokhranov coke [14].

5. Graphene

The electron cloud densitometry was used to study images of single-layer graphene Fig. 7.

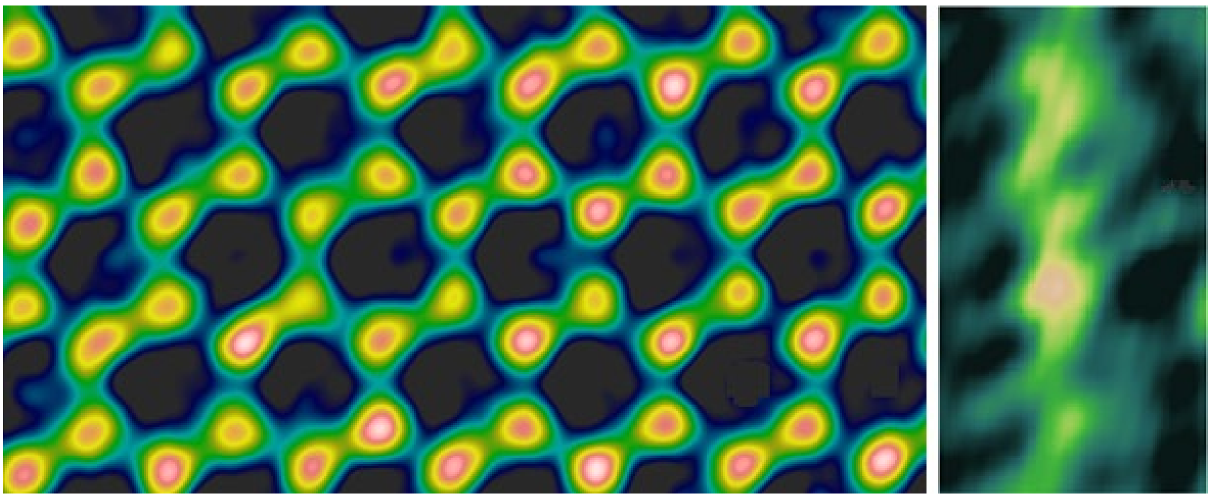


Fig. 7. Electron cloud densitometry images of single-layer graphene, front view (left) and side view (right). The two inner electrons create a pink ball around the nucleus, the three ***sp²*** electrons create strong green hybrids; the one blue active electron is pulled to the side from each atom, as both images show.

The electron cloud density image (Fig. 7) shows the hexagonal planar ***sp²*** hybrid constructions in the form of the infinity sign ∞ with three neighboring atoms. The active valence electron (blue) builds a negatively-charged shape due to their delocalization and occurs laterally from the graphene layer. This is seen in both Figs. 8–10.

Each carbon atom in graphene has three green ***sp²*** hybrids and one blue active electron.

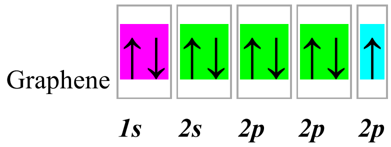


Fig. 8. ***sp²*** hybrids in graphene.

The spatial 3d model of graphene is shown in Fig. 9. This and the next spatial 3d model are created using the molecular graphics program VMD [15]. Each carbon atom in the spatial 3d model is bonded by ***sp²*** hybrids to three adjacent atoms in a way that creates a hexagonal lattice. The active valence electron has an elongated negatively charged gray shape and goes away from the graphene layer.

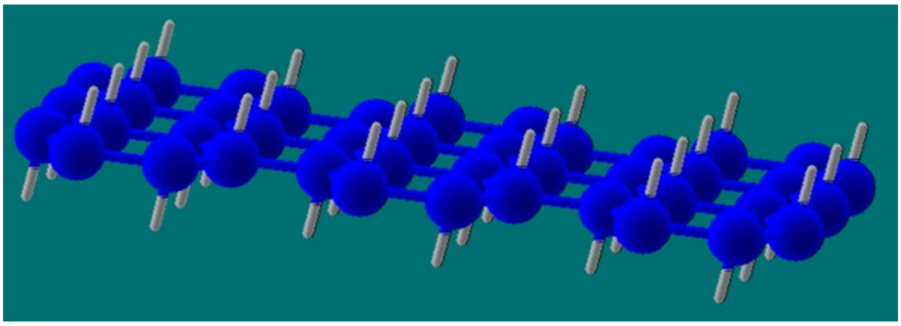


Fig. 9. Spatial 3d model of graphene. The layer of carbon atoms are connected by strong ***sp²*** hybrids and the gray active electrons are elongated out of the plane.

6. Diamond

Fig. 10 shows the spatial 3d model of a crystal lattice of diamond with a tetrahedral structure. The carbon atoms have ***sp³*** hybrids inside and ***sp²*** hybrids with one active electron on a surface.

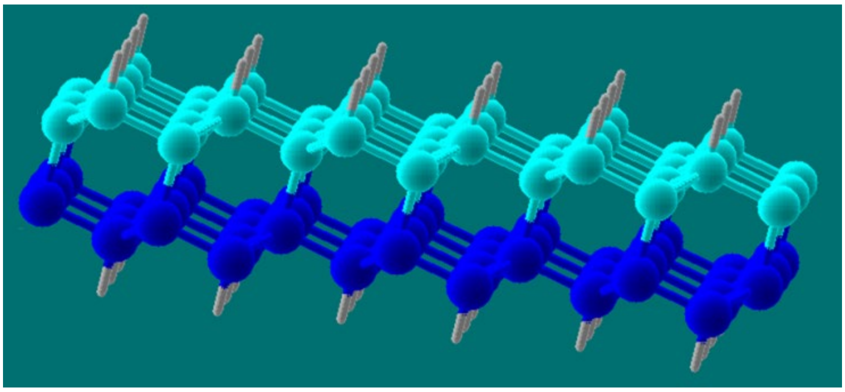
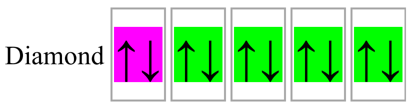


Fig. 10. Spatial 3d model of diamond. The carbon atoms are connected by ***sp³*** hybrids inside and by ***sp²*** hybrids outside. The gray active valence electrons at the diamond facets are pulled to the sides.

Carbon atoms are connected by strong ***sp³*** hybrids in the diamond inside. Each carbon atom has four ***sp³*** hybrids and has no active electrons:

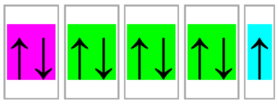


1s 2s 2p 2p 2p

Fig. 11. ***Sp³*** hybrids in diamond.

However, on the diamond face, the fourth carbon atom is cut off; therefore, every fourth adjacent covalent electron becomes active. Thus, each carbon atom has three ***sp²*** hybrids and one active electron.

Diamond face



1s 2s 2p 2p 2p

Fig. 12. ***sp²*** hybrids in diamond face.

Fig. 13 shows the electron cloud densitometry image of the diamond face with a tetrahedral structure. The carbon atoms have ***sp²*** hybrids of green. However, every third atom lies on the surface and has an active electron in it. This makes it brighter than other atoms, and the active electron amplifies its center to white.

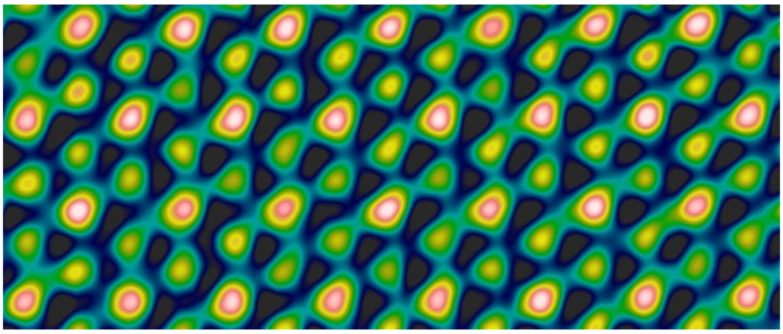


Fig. 13. Electron cloud densitometry image of the diamond face. The carbon atoms are connected by green strong ***sp²*** hybrids. The active valence electrons at the diamond facet are white points.

7. Conclusions

A Quantum mechanical explanation of the electron cloud densitometry is given. In accordance with this effect, an atom begins to illuminate and show its shape. The electron cloud densitometry image shows a carbon atom with all six electrons. As firmly shown by electron cloud densitometry, there are the active valence electrons in nature that builds negatively charged shape due to their delocalization. The active valence electrons create the van der Waals force, which, in particular, connects the layers of crystalline graphite. The active valence electrons are visualized in activated coke, graphite, graphene, and diamond. Each active valence electron builds a negatively charged long sleeve due to its delocalization.

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