

Direct Visualization of Active Valence Electrons in Carbon Allotropes

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ABSTRACT: Direct visualization of active valence electrons is presented. It makes clear the nature of chemical bonds. Each active valence electron builds negatively charged shape due to their delocalization. The article shows that it is the active valence electron that creates the van der Waals force, which bonds layers of crystalline graphite together. Easy quantum mechanical explanation of the electron cloud densitometry is given. Accordance with this effect, an atom begins to illuminate, depicting its own shape. The electron cloud densitometry image made clear a carbon atom with all six electrons. The presence of the active valence electrons is shown in electron cloud densitometry images of activated carbon, graphite, graphene and diamond.

KEYWORDS: Active valence electron, Electron cloud densitometry, Visual chemistry, Activated carbon, Graphite, Graphene, Diamond, Musokhranov coke.

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I. INTRODUCTION

In 1873, the 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 due to polarization and weaker than covalent and ionic bonds. This force plays a major role in carbon allotropes. So in the Encyclopedia Britannica under the watchword "Structure of carbon allotropes" we can read "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". The prominent quantum chemist Coulson in his book from 1961 entitled Valence [2] wrote on page 391: "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 aim of the study is, as firmly shown by electron cloud densitometry there are the active valence electrons in nature which 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 together. The presence of the active valence electrons in activated carbon, graphite, graphene and diamond will be shown in electron cloud densitometry images.

II. THEORY

The active valence electron quantum mechanical theory is given below.

In 1927, Heitler and London [6] performed a quantum mechanical calculate the hybridization of the 1s molecular orbitals of the H₂ 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 would be logical to carry out these calculations for hybridization double bonds.

Here is the active valence electron theory, which 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. Let us prove this statement.

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

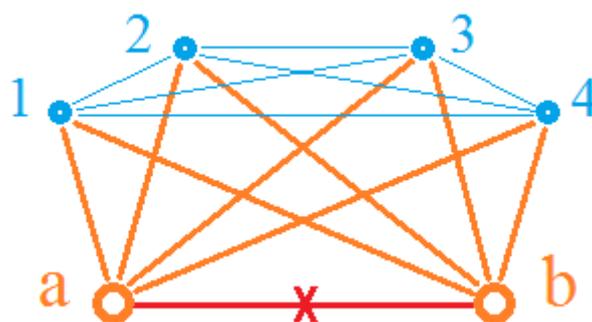


Fig. 1. Atom *a* with exchange electrons 1, 2 and *b* with exchange electrons 3, 4 take part in double hybridization

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 atom *a* are described by the wave functions $\varphi a(1)$ and $\varphi a(2)$ and the exchange electrons 3 and 4 of atom *b* are described by the wave functions $\varphi b(3)$ and $\varphi b(4)$.

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 $\Psi 1$ 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 will change when the exchange electrons are swapped.

Let us construct a function $\Psi 2$ 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 $s = 1/2$, and for 3 $s = -1/2$.

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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 or σ -bonds exist and π -bonds do not. It follows that π -bonds and the van der Waals force are 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 electron is the true valence electron in the outer shell associated with an atom, and that can participate in the formation of a chemical bond.

The active valence electrons in activated carbon, graphite, graphene and diamond are visualized by the electron cloud densitometry as below.

III. 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 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 see 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]. O.P. Kucherov and S.E. 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.

Here is a brief but comprehensive presentation of this theory.

Consider two objects of quantum mechanics: a) an atom with inner and valence electrons; b) 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 $\Psi(x,y,z)$, 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 $dx dy dz$:

$$P(x,y,z) = |\Psi(x,y,z)|^2 dx dy dz \tag{4}$$

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 $\sqrt{j}(x,y,z) = \text{constant}$.

The wave function of the atomic electron is $\phi(x,y,z)$ and the square module of this function determines the electron cloud density $\rho(x, y, z)$ in the volume $dx dy dz$:

$$\rho(x,y,z) = |\phi(x, y, z)|^2 dx dy dz \tag{5}$$

Let's 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 $|\Psi(x,y,z)|^2 dx dy dz$ 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 the expression (6) from z_{min} to z_{max} 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, we obtained that 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.

It should be noted that 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 electrostatics.

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

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

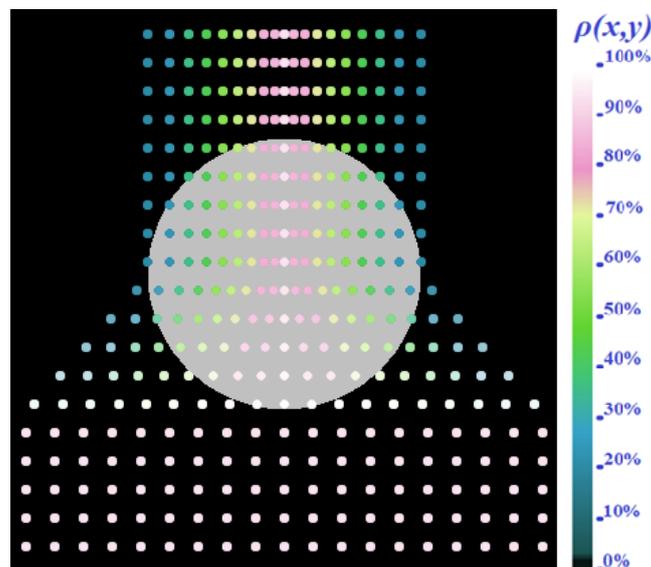


Fig. 2. Electron cloud attracts the electron beam in proportion to its own density $\rho(x,y)$. The density scale is shown on the right

The property of the electron cloud to shift the electron beam is shown in Figure 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.

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 the 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. Next we will demonstrate this with examples of activated carbon, graphite, graphene and diamond.

IV. ACTIVATED CARBON

Widespread activations of carbon are chemical [4], physical [11], mechanical [12] and al.

Amorphous carbon was 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 density images obtained on a high resolution electron microscope (JEOL JEM-2100F) using the method [10], Patent of Ukraine No.115602, with 10 pm resolution.

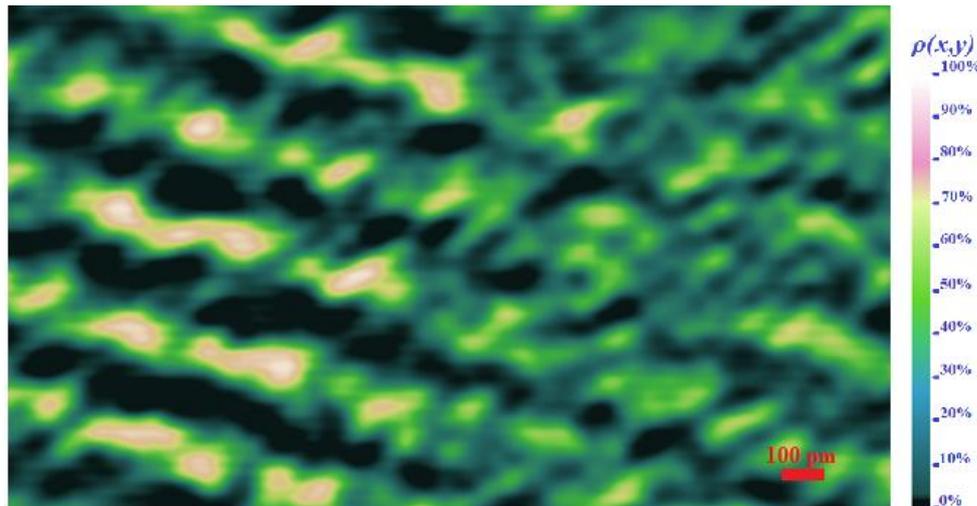


Fig. 3. Electron cloud density image of sp^2 hybridized carbon in crystalline graphite (left) and activated carbon without hybridization (right)

The electron cloud density image (Figure 3) shows the result of the activation. Carbon atoms in crystalline graphite (left) form layers by covalent chemical bonds sp^2 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.

The figure shows a sharp change in chemical bonds as a result of activation (right). The green covalent chemical bonds sp^2 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.

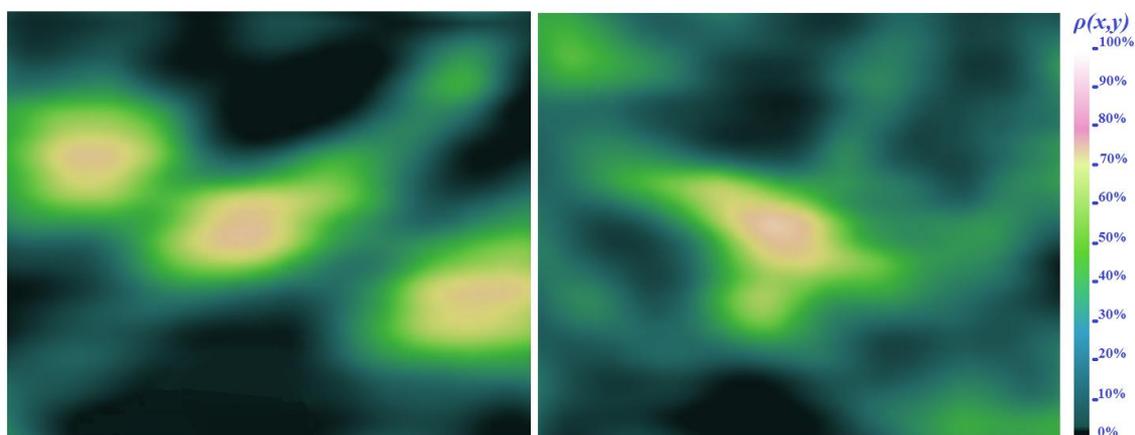
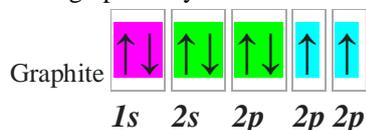


Fig. 4. Electron cloud density images of a single carbon atom in a graphite crystal (left) or in an active coal (right). In each state, the atom has two inner pink electrons and four valence electrons. The difference is that the left atom has two green covalent and two blue active electrons, and the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

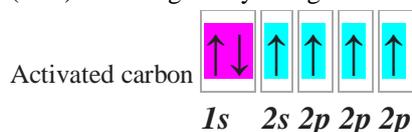
The electron cloud density image (Figure 4, left) shows a single carbon atom in crystalline graphite with all its own six electrons. The two inner electrons have the shape of a pink ball. The two covalent bond electrons green create strong sp hybrids in the form of the infinity sign ∞ with two neighboring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



Each carbon atom in crystalline graphite is known to have three sp^2 hybrids, but Figure 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 (Figure 4, right) shows a single carbon atom in activated carbon 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:



The active valence electrons create the van der Waals force; it is what makes coal active.

The fact of disappearance of covalent bonds during mechanical activation of graphite is confirmed by decrease and expansion of the Raman vibrational bands sp^2 and sp^3 -hybridization [13].

In addition, it should be noted that the active valence electrons have opened up new materials with extraordinary technological properties. For example, cheap Musokhranov coke [14].

V. GRAPHENE

The electron cloud densitometry was used to study images of single-layer graphene Figure 5.

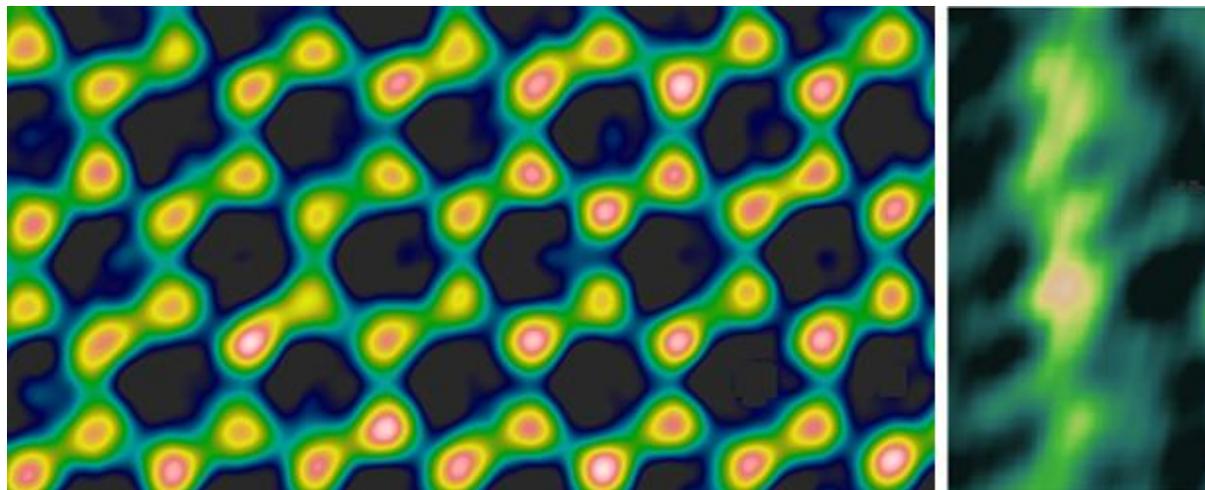
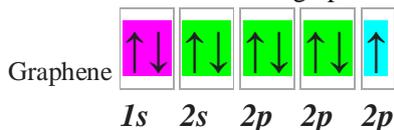


Fig. 5. Electron cloud densitometry images of single-layer graphene, front view (left) and side view (right). The two inner electrons create a pink ball around the nucleus, the three sp^2 electrons create strong green hybrids; the one blue active electron is pulled to the side from each atom, as both images show

The electron cloud density image (Figure 5) shows the hexagonal planar sp^2 hybrid constructions in the form of the infinity sign ∞ with three neighboring atoms. The active valence electron (blue) builds negatively charged shape due to their delocalization and occur laterally from graphene layer. This is clearly seen in both figures.

Each carbon atom in graphene has three green sp^2 hybrids and one blue active electron:



The spatial 3d model of graphene is shown in Figure 6. This and the next spatial 3d model are created using the molecular graphics program VMD [15].

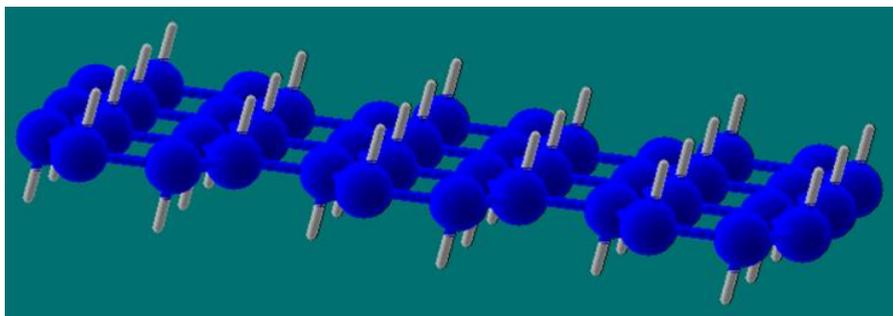


Fig. 6. Spatial 3d model of graphene. The layer of carbon atoms are connected by strong sp^2 hybrids and the gray active electrons are elongated out of the plane

Each carbon atom in spatial 3d model is bonded by sp^2 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.

VI. DIAMOND

Figure 7 shows the spatial 3d model of a crystal lattice of diamond with tetrahedral structure. The carbon atoms have sp^3 hybrids inside and sp^2 hybrids with one active electron on a surface.

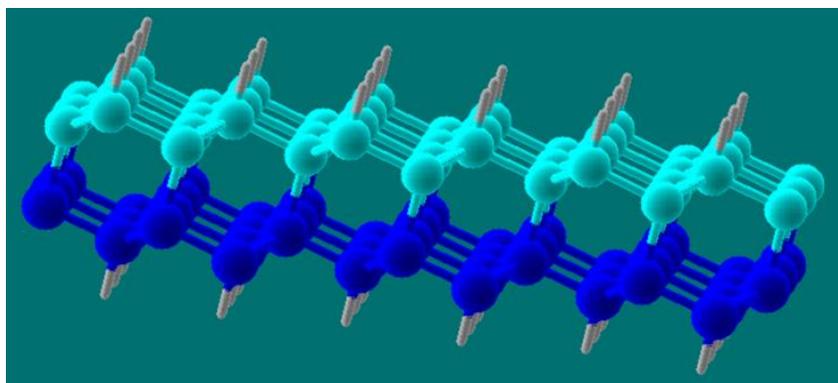
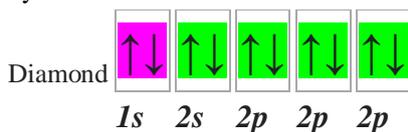
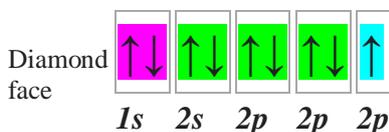


Fig. 7. Spatial 3d model of diamond. The carbon atoms are connected by sp^3 hybrids inside and by sp^2 hybrids outside. The gray active valence electrons at the diamond facets are pulled to the sides

Carbon atoms are connected by strong sp^3 hybrids in the diamond inside. Each carbon atom has four sp^3 hybrids and has no active electrons:



However, on the diamond face, the fourth carbon atom is cut off; therefore, every fourth adjacent covalent electron becomes active. So each carbon atom has three sp^2 hybrids and one active electron:



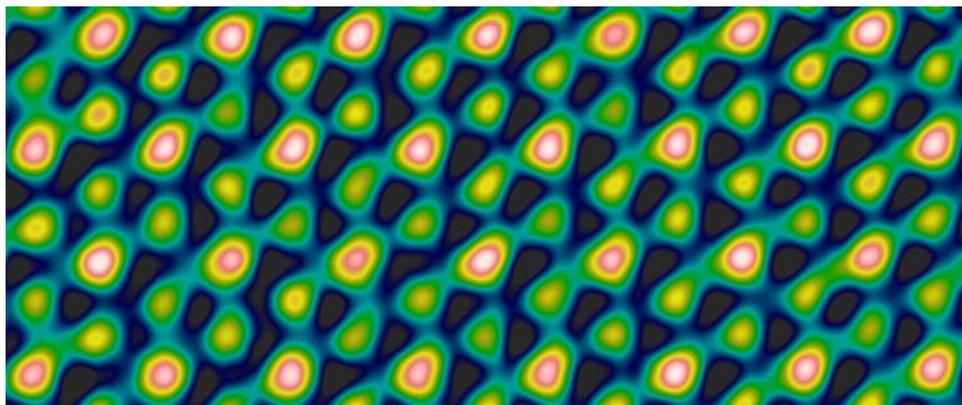


Fig. 8. Electron cloud densitometry image of the diamond face. The carbon atoms are connected by green strong sp^2 hybrids. The active valence electrons at the diamond facet are white points

Figure 8 shows the electron cloud densitometry image of the diamond face with tetrahedral structure. The carbon atoms have sp^2 hybrids of green. But, every third atom lies on the surface and has the active electron on it. This makes it brighter than other atoms, and the active electron amplifies its center to white.

VII. CONCLUSION

Easy quantum mechanical explanation of the electron cloud densitometry is given. Accordance with this effect, an atom begins to illuminate, depicting its own shape. The electron cloud densitometry image made clear a carbon atom with all six electrons.

As firmly shown by electron cloud densitometry there are the active valence electrons in nature which 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 together.

The active valence electrons were visualized in graphite, graphene, diamond and rudenite. Each active valence electron builds negatively charged long sleeve due to their delocalization.

Summarizing the above, we can conclude that the electron cloud densitometry gives rise of visual chemistry.

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