Report on the Real Structure of Benzene Molecules and the Thickness of Graphene

Ning Wang

Guangdong Pharmaceutical University

Dulun Wang (✉ gzwdl@163.com)

Guangdong Pharmaceutical University

Research Article

Keywords: Benzene Molecules, Thickness of Graphene

Posted Date: September 21st, 2021

DOI: <https://doi.org/10.21203/rs.3.rs-900329/v1>

License: © ⓘ This work is licensed under a Creative Commons Attribution 4.0 International License.

[Read Full License](#)

Report on the Real Structure of Benzene Molecules and the Thickness of Graphene

Ning Wang¹, Dulun Wang^{2*}

¹College of Medical Information Engineering, Guangdong Pharmaceutical University,

No. 280 Wai-huan East Road, Guangzhou, China

² School of Life Sciences and Biopharmaceutics Guangdong Pharmaceutical
University, China

No. 280 Outer Wai-huan East Road, Guangzhou, China

Ning_wang@gdpu.edu.cn, gzwdl@163.com*

*corresponding author

Abstract

The problem of the benzene molecular structure has not been solved for a long time. This research proposes a new concept of covalent bonds based on the existing theory: each electron shared by the nucleus corresponds to a half-valent bond, and a half-valent bond can be formed between interval carbon atoms of the benzene ring. A new theory was established. Quantum mechanical calculations results can quantitatively explain experimental results, such as the hydrogenation heat and ultraviolet spectroscopy of benzene. It has solved more than one hundred years of difficult problems. The design of the new structural forms of benzene molecules shows half-valent bonds with dotted lines, which have a wide range of adaptability, and shows the structural forms and reaction formulas of more than dozens of benzene homologs and derivatives. Under the guidance of the new theory, the stacked three-dimensional structure of benzene was explored. The thickness of the three-layer benzene tube is calculated to be almost equal to the thickness of the graphene. Therefore, it is speculated that graphene may be a three layer structure.

Introduction

Since Kaikule proposed the benzene molecular plane structure of cyclohexatriene, which was inconsistent with the experimental results, many people have also proposed some related structures, which were also unsuccessful. In particular, the experimental results of the hydrogenation heat and the ultraviolet spectrum of benzene that cannot be quantitatively explained are called the mystery of a century^{1,2,3}.

Solving the problem of benzene molecular structure must follow the valence bond theory of chemical bonds^{4,5}. The nature of chemical bonds is that the nuclei share electrons. In the existing valence bond theory, the nucleus shares a pair of opposite spin electrons to form one valence bond⁶. This definition is not suitable for the reality of benzene and some other molecules. Moreover, the theory does not prove that the shared electrons must be paired and the spins must be reversed^{7,8}. Therefore, here is an attempt to discard the above two insufficient and nonessential conditions. In new theory, it is defined as the atom nucleus share every electron all counted as a half-valent bond. In this way, the theory can be adapted to all molecular structures.

According to the existing molecular orbital theory, the $2s$ and $2p$ orbitals of every carbon atom in the benzene ring may be hybridized into a $3 sp^2$ orbital and a p_z orbital alone. Six sp^2 orbitals in 6 carbon atoms form a regular hexagonal ring using 6 σ bonds. The other 6 σ bonds are connected outside the ring to the hydrogen atom. The remaining 6 unhybridized p_z orbitals are linearly combined into 6 molecular orbitals. Among them, there are 3 bonding orbitals and 3 anti-bonding orbitals. Their 6 p electrons are all on the bonding orbital, and each orbital can accommodate 2 electrons with opposite spin directions. The 3 anti-bonding orbitals are unoccupied and vacant. The molecular structural energy is low, so the structure is stable^{9,10}. The 6 carbon nuclei of the benzene ring share 6 electrons, forming 6 half-valent π bonds and connected into a large half-valent π bond ring. It is the ground state of the benzene molecule.

When getting energy outside the system, 1 electron in each bonding orbital

transitions to the anti-bonding orbital and occupies it. All electrons become the same spin¹¹. The active electrons increase the mutual repulsion between adjacent p_z orbital electrons, and the steric hindrance effect⁹ causes one of the p_z orbitals to turn to the opposite phase of the benzene ring plane. Since then, the positive and negative phases each have three interval carbon atom p_z orbitals, forming a new neighboring relationship of triangular rings. In each phase, there are three interval carbon nuclei sharing three electric π electrons, forming three half-valent π bonds and their bond rings. This is the excited state of the benzene molecule. Only in the excited state can molecules participate in chemical reactions. Such a valence bond follows the tetravalent requirement of carbon, so it satisfies the saturation of the covalent bond⁴. The half-valent bond ring of the benzene molecule the movement of electrons produces a ring current and its induced magnetic field to make the molecular structure more stable.

This series of concepts formed a new theory of the planar structure of benzene molecules. When the ring planes of the excited states of two benzene molecules are flipped and stacked, these two rings are completely symmetrical. The 3 p_z orbital of the interval carbon atoms of the benzene ring can be completely docked, and the electron cloud overlaps to form 3 σ bonds. A two layer ring structure can be synthesized out. However, this two-layer structure is unstable, and it is also easy to form a three-layer benzene tube. The top and bottom of this three-layer benzene tube are exactly the same as a benzene molecular structure, so it is a stable three-dimensional structure. It can be called a three layer unit benzene tube. It is even possible to form a multilayer benzene tube. Surprisingly, the thickness of the three-layer unit benzene tube is equivalent to the thickness of a layer of graphene. Given that the structure of graphene is similar to a fused ring compound of benzene, referring to the general physical and chemical properties of graphene, it is suspected that graphene may have a three-layer structure.

Method

To verify the correctness of the new theory of the benzene molecular structure, an equivalent electronic model of the benzene ring was established, carrying out the coordinate table transformation and over to a hydrogen atom model. Then, the equivalent electronic wave function and wave equation are established. The variational method was used to solve the energy eigenvalues of the equation and calculate the equivalent electron energy levels and transition energies^{7,12,13} The equivalent electronic ground state and excited state transition energy are used to quantitatively explain the hydrogenation heat and ultraviolet spectrum of benzene, as well as the bond length of the benzene ring. The calculated value is compared with the experimental result to verify the correctness of the new theory of the planar structure of the benzene molecule. The comparison of the calculated thickness of the three-layer benzene tube with the thickness of the graphene documented in the data shows the basis for suspicion that graphene is also a three-layer structure.

Quantitative interpretation of the hydrogenation heat of benzene

In the benzene ring, 6 p_z electrons revolve around the carbon nucleus where they are located, and the movement of each electron has an arc in the same direction along the benzene ring. They will be connected in an arc to form a circle. The overall behavior is similar to a circular motion of an equivalent electron along the circumscribed circle of a benzene ring. Generate the pulse loop current and corresponding magnetic field. The ground state and the excited state are the two energy levels of the equivalent electron. In this way, an equivalent electronic model of benzene was established. To make the model transition to the hydrogen-like atom model⁷ and determine its kinetic energy and potential energy, the wave function and Schrodinger equation¹² were established. However, the kinetic energy of the equivalent electron is not known. The only amount that can be inferred is the work done by the electron to circumscribe a

circle around the benzene ring.

$$W_B = 2\pi f_B r_B \quad (1)$$

The question is whether it is possible for W_H to be seen as kinetic energy. First, the certain distance of a circle around it, that is, when the perimeter is written in the form of integral, and the force is also written in the form of differential:

$$l = 2\pi r_H = \int_0^{t_0} u dt, \quad f_H = m \frac{du}{dt} \quad (2)$$

So get

$$W_H = 2\pi f_W r_H = m \frac{du}{dt} \int_0^{t_0} u dt = m \int_0^{u_0} u du = \frac{1}{2} m u_0^2 \quad (3)$$

It seems that at the end point of the circle, W_H and kinetic energy E_k can be equal

$$W_H = E_k \quad (4)$$

It can also be said that at this point, it is possible to change the equivalent electron model to a hydrogen atom-like model. Similarly, at this point, the kinetic energy E_K and the potential energy V_H of the electrons outside the hydrogen nucleus are also equal.

$$W_H = E_K = V_H = \frac{e^2}{4\pi\epsilon_0 r_H} \quad (5)$$

$$2\pi f_W r_H = \frac{e^2}{4\pi\epsilon_0 r_H}, \quad f_W = \frac{e^2}{8\pi^2 \epsilon_0 r_H^2} \quad (6)$$

Obviously, it has the following relationship with the general form of force in the hydrogen atom mode:

$$f_H = \frac{e^2}{4\pi\epsilon_0 r_H^2} \quad (7)$$

Comparing (6) with (7), the force of the rotation of work done along the benzene ring is less than the force of the electromagnetic field, $f_H = 2\pi f_w$. To make the force of the former equal to the latter, the only way to change the radius is. If is set

$$f_B = \frac{e^2}{4\pi\epsilon_0 r_B^2} = \frac{e^2}{8\pi^2 g \epsilon_0 r_H^2} \quad (8)$$

and g has nothing to do with r . We get

$$r_B^2 = 2\pi g r_H^2 \quad (9)$$

This clearly shows that the difference between the two expressions of force is mainly reflected in the radius r . If r in (9) is regarded as a coordinate transformation, this transformation can make the equivalent electron model further transition to the hydrogen-like atom mode¹³.

With reference to (7), (8) and (9), the potential energy of the equivalent electron can also be written more in the general form¹⁴:

$$V_B = \int \frac{e^2}{8\pi^2 g \epsilon_0 r^2} dr = -\frac{e^2}{16\pi^2 g \epsilon_0 r} = \frac{e^2}{8\pi^2 b \epsilon_0 r} \quad (10)$$

$$b = -2g$$

In (10), V_B is the equivalent electronic potential energy of the benzene ring, e is the electronic charge, and ϵ_0 is the vacuum permittivity.

Therefore, as the equivalent electronic coordinate transformation of the benzene ring, refer to (9) and (10), which can be written as a general transformation form:

$$r_B^2 = 2\pi b r^2 = 2\pi b (x^2 + y^2 + z^2)$$

$$r_B = r(x, y, z)\sqrt{2\pi b} \quad (11)$$

Based on the abovementioned equivalent electrons, a reciprocating circular motion is made along the benzene ring, and the abovementioned conditions are met only at the end of a circle. Therefore, in the new coordinate system, it is reasonable to set the motion period to $2n\pi$. According to these conditions, resimulate the Schrodinger wave function⁷, from (4) (10) (11), Planck's formula and De Broglie's formula⁷, establish the equivalent electronic wave function. then

$$\Psi = e^{-i2n\pi(vt - \frac{r\sqrt{2\pi b}}{\lambda})} = e^{-i\frac{2n\pi}{h}Et} \psi, \quad \psi = e^{i\frac{2n\pi}{h}pr\sqrt{2\pi b}} \quad (12)$$

$$E_K = h\nu = \frac{1}{2}mu^2, \lambda = \frac{h}{p}, p = mu, u = \lambda\nu, E_K = E - V$$

In the wave function (12), n is a natural number, λ is the wavelength, ν is the frequency, r is the radius of the benzene ring, h is the Planck constant, p is the electron momentum, m is the static mass of the electron, u is the electron velocity, E_K is the kinetic energy, E is the total energy, and V is the potential energy. With reference to (10), (12) and Schrodinger's equation^{7,12}, the three-dimensional wave equation of the equivalent electron can be obtained:

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} = \frac{16n^2\pi^3bm}{h^2}(E - V)\psi \quad (13)$$

Substitute (10) into (13) to get

$$-\frac{h^2}{16n^2\pi^3bm}\left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2}\right) - \frac{e^2}{8\pi^2b\epsilon_0r}\psi = E\psi \quad (14)$$

Equation (14) is converted to the spherical coordinate equation

$$-\frac{h^2}{16n^2\pi^3bm}\left[\frac{1}{r^2}\frac{\partial\psi}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\psi^2}\right]-\frac{e^2}{8\pi^2b\epsilon_0r}\psi=E\psi \quad (15)$$

To solve the energy eigenvalue E in equation (15), the Lagrange undetermined coefficient method is applied^{13,14}. The Hamiltonian operator¹⁴ is used in the algorithm, which must meet the following conditions:

$$H\psi = E\psi, \quad \delta\left(\int\psi^*H\psi du - \eta\int\psi^*\psi du\right) = 0 \quad (16)$$

$$(H - \eta)\psi = 0, \quad \delta\eta(\psi) \equiv \delta\left(\frac{\int\psi^*H\psi du}{\int\psi^*\psi du}\right) = 0 \quad (17)$$

In (16) and (17), H is the Hamiltonian quantity, E is the energy eigenvalue, and η is the undetermined coefficient. Since only the r part of (15) is involved, H can be

$$\begin{aligned} H &= -\frac{h^2}{16n^2\pi^3bm}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\right]-\frac{e^2}{8\pi^2b\epsilon_0r} \\ &= -\frac{h^2}{16n^2\pi^3bm}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) - \frac{e^2}{8\pi^2b\epsilon_0r} \end{aligned} \quad (18)$$

Suppose: the variational function is $\psi = e^{-ar}$, and a is a positive real number. Through (16), (17) and (18), the undetermined coefficient η can be calculated by the variational method as follows:

$$\eta = \frac{-4\pi\int_0^\infty e^{-ar}\left\{\left[\frac{h^2}{16n^2\pi^3bm}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) + \frac{e^2}{8\pi^2b\epsilon_0r}\right]e^{-ar}\right\}r^2dr}{4\pi\int_0^\infty r^2e^{-2ar}dr}$$

$$\begin{aligned}
&= \frac{-\frac{h^2 a^2}{16n^2 \pi^3 b m} \int_0^\infty r^2 e^{-ar} dr + \left(\frac{h^2 a}{8n^2 \pi^3 b m} - \frac{e^2}{8\pi^2 b \epsilon_0} \right) \int_0^\infty e^{-ar} r dr}{\int_0^\infty e^{-2ar} r^2 dr} \\
\eta &= \frac{h^2 a^2}{16n^2 \pi^3 b m} - \frac{e^2 a}{8\pi^2 b \epsilon_0}
\end{aligned} \tag{19}$$

by (16) , (17) and (19)

$$\begin{aligned}
\frac{d\eta}{da} &= \frac{h^2 a}{8n^2 \pi^3 b m} - \frac{e^2}{8\pi^2 b \epsilon_0} = 0 \\
a &= \frac{n^2 \pi m e^2}{\epsilon_0 h^2}
\end{aligned} \tag{20}$$

Substituting (20) into (19), the coefficient η to be determined is

$$\eta = \frac{h^2}{16n^2 \pi^3 b m} \left(\frac{n^2 \pi m e^2}{\epsilon_0 h^2} \right)^2 - \frac{e^2}{8\pi^2 b \epsilon_0} \left(\frac{n^2 \pi m e^2}{\epsilon_0 h^2} \right) = -\frac{n^2 m e^4}{16\pi b \epsilon_0^2 h^2} \tag{21}$$

From (16), (17), (18), (19) and (21), the calculated energy eigenvalue¹⁴ is

$$E = -\frac{n^2 m e^4}{16\pi b \epsilon_0^2 h^2} \tag{22}$$

In formula (22), E is the eigenvalue of the equivalent electron energy, but it is still not clear that it is the lowest value. It can be calculated only after turning it into an energy level formula.

$$E_n = \frac{n^2 E_H}{2\pi b}, (n = 0, 1, 2), \tag{23}$$

$$E_H = -\frac{m_e e^4}{8\epsilon_0^2 h^2} = -13.606(eV) = 313.755(kcal/mol) \quad (24)$$

In (23), E_H is the lowest energy level of extranuclear electrons of hydrogen atom⁷. E_n is the energy level of the equivalent electron. n is number of energy levels. It is also the two states of the benzene molecule. When $n = 2$, the energy level is E_2 and is the lowest energy level. It is the ground state and cannot participate in chemical reactions. When $n = 1$, the energy level is E_1 , which must be an excited state. Can participate in chemical reactions? When in an excited state, the electrons further increase their energy, benzene hydrogenates to form cyclohexane, the electrons escape, and the benzene ring does not exist. If you regard it as an extreme state of energy level, it can only be $n=0$, and the energy level is $E_0=0$. These energy levels are as follows:

$$E_0 = 0$$

$$E_1 = \frac{E_H}{2\pi b} = -2.165/b(eV) \quad (25)$$

$$E_2 = 4E_1 = -8.658/b(eV) \quad (26)$$

Its transition energy should be

$$\Delta E_1 = E_0 - E_1 = 2.165/b(eV) \quad (27)$$

$$\Delta E_2 = E_1 - E_2 = 3E_1 = 6.493/b(eV) \quad (28)$$

where ΔE_2 is the transition energy of the ground state. ΔE_1 is the transition energy of the excited state.

The transition energy of the equivalent electronic in excited state was used to quantitative interpretation the experimental results of the hydrogenation heat of benzene^{4,14}. In (27), the excited state transition energy ΔE_1 , value $2.165/b$ (eV)

(49.926/ b *kcal/mol*), is equivalent to the hydrogenation heat released by the hydrogenation of benzene to cyclohexane. The experimental value of the heat of hydrogenation of benzene is 2.160 *eV* (49.802 *kcal/mol*), and it is calculated that $b=1.00231$. Even if coefficient b is not taken into account, the error rate is only 0.231%. It is accurate enough. The experimental value of the heat of hydrogenation of benzene, which is a century-old mystery, is quantitatively explained here.

If the tiny b is not counted, the hydrogenation heat of benzene is a constant composed entirely of basic physical constants¹², denoted as B_H .

$$B_H = \Delta E_1 = \frac{me^4}{16\pi\epsilon_0^2 h^2} \quad (29)$$

$$\Delta E_2 = E_1 - E_2 = \frac{hc}{\lambda} = -\frac{me^4}{16\pi\epsilon_0^2 h^2} (n_1^2 - n_2^2) = 3B_H$$

$$\frac{3me^4}{16\pi\epsilon_0^2 h^3 c} = \frac{3}{2\pi} R_\infty, \quad R_\infty = \frac{2\pi}{hc} B_H \quad (30)$$

$$R_\infty = \frac{me^4}{8\epsilon_0^2 h^3 c} = 1.097 \times 10^7 (m^{-1})$$

In (30), the ground state transition energy ΔE_2 is related to the ultraviolet light energy absorbed by the benzene molecule, and combined with (27) and (28), the Rydberg constant R_∞ can also be calculated.

Quantitatively explains of the ultraviolet spectrum of benzene

General benzene *UV* spectrum^{15,16} image, superimposed image of a large number of benzene molecules. It shows a strong single peak at 184 *nm*, a strong dentate peak at

203-212 *nm*, and a weak dentate peak at 230-270 *nm*. In the infrared spectrum, there are skeleton vibration peaks at 6250 *nm* and 6670 *nm* and *C-H* stretching vibration peaks at 3230 *nm* and 3300 *nm*.

To interpret these spectra, first use the Planck formula

$$E = \frac{hc}{\lambda} \quad (31)$$

Calculate the energy corresponding to the wavelength. In (31), *E* is the energy, λ is the wavelength of the absorption peak, *h* is the Planck constant, and *c* is the speed of light. Substituting the value in, the calculation results are shown in Table 1.

Table 1 The energy corresponding to the peak wavelength of the infrared and ultraviolet spectra of benzene

Ultraviolet spectrum		Infrared spectrum	
Wavelength (<i>nm</i>)	energy <i>E</i> (<i>eV</i>)	Wavelength (<i>nm</i>)	energy <i>E</i> (<i>eV</i>)
184	$E_{184} = 6.786$	3230	$E_{3230} = 0.387$
203	$E_{203} = 6.151$	3300	$E_{3300} = 0.379$
212	$E_{212} = 5.890$	6250	$E_{6250} = 0.200$
230	$E_{230} = 5.429$	6670	$E_{6670} = 0.187$
270	$E_{270} = 4.625$		

Note: The energy *E* subscript is the peak of the spectral wavelength, and the character as a whole represents the energy of the corresponding wavelength.

Simplified calculation by Huckel's^{7,17} molecular orbital theory, the wave function and energy level of the benzene molecular orbital are:

$$\begin{aligned}
\psi_1 &= \frac{1}{\sqrt{6}}(\phi_1 + \phi_2 + \phi_3 + \phi_4 + \phi_5 + \phi_6), \quad \varepsilon_1 = \alpha + 2\beta \\
\psi_2 &= \frac{1}{\sqrt{12}}(2\phi_1 + \phi_2 - \phi_3 - 2\phi_4 - \phi_5 + \phi_6), \quad \varepsilon_2 = \alpha + \beta \\
\psi_3 &= \frac{1}{\sqrt{4}}(\phi_2 + \phi_3 - \phi_5 - \phi_6), \quad \varepsilon_3 = \alpha + \beta \\
\psi_4 &= \frac{1}{\sqrt{4}}(\phi_2 - \phi_3 + \phi_5 - \phi_6), \quad \varepsilon_4 = \alpha - \beta \\
\psi_5 &= \frac{1}{\sqrt{12}}(2\phi_1 - \phi_2 - \phi_3 + 2\phi_4 - \phi_5 - \phi_6), \quad \varepsilon_5 = \alpha - \beta \\
\psi_6 &= \frac{1}{\sqrt{6}}(\phi_1 - \phi_2 + \phi_3 - \phi_4 + \phi_5 - \phi_6), \quad \varepsilon_6 = \alpha - 2\beta
\end{aligned} \tag{32}$$

According to the new theory of benzene molecular structure, combining (27) and (28), ground state and excited state energy levels, the corresponding (32) is

$$E_1 = \varepsilon_1 + \varepsilon_2 + \varepsilon_3 + \varepsilon_4 + \varepsilon_5 + \varepsilon_6 = 6\alpha = -2.165(eV) \tag{33}$$

$$E_2 = 2(\varepsilon_1 + \varepsilon_2 + \varepsilon_3) = 6\alpha + 8\beta = -8.660(eV) \tag{34}$$

$$\Delta E_2 = E_1 - E_2 = 6.493(eV) = -8\beta \tag{35}$$

from (27) , (29) , (33) get

$$\alpha = -0.361(eV) = -\frac{m_e e^4}{6 \times 16 \pi^2 \varepsilon_0^2 h^2} (eV) \tag{36}$$

from (29) (30) (35) , get

$$\beta = -0.812(eV) = -\frac{(1-2^2)m_e e^4}{-8 \times 16 \pi^2 \varepsilon_0^2 h^2} (eV) \tag{37}$$

In (36), the Coulomb integral α coincides with the negative value of the half-valent π bond energy between the carbon atoms in the benzene ring. Moreover, both α and β are constants composed of basic physical constants, which are composed of (36) and (37), and the relationship between the two is obtained

$$6\alpha = \frac{3}{8}\beta = -\frac{m_e e^4}{16\pi^2 \epsilon_0^2 h^2} (eV), \quad \alpha = \frac{\beta}{16} \quad (38)$$

In Table 1, the infrared spectrum^{7,17} shows that the benzene ring skeleton vibration is the basic molecular vibration, and the energy average value is $E_{6460}=0.192$ eV. *C-H* flexural vibration can be regarded as the characteristic of benzene ring resonance that makes the ring expand and shrink. The average value of resonance energy is $E_{3265}=0.380$ eV. $-\beta$ is used to judge the energy corresponding to the wavelength of the ultraviolet spectrum to briefly define and quantitatively explain the ultraviolet spectrum of benzene (see Table 2).

Table 2 Comparison of the energy corresponding to the wavelength of the benzene ultraviolet spectrum and the calculated values of some basic indicators

UV Spectral measurement value		Basic index calculated value (eV)	Error rate (%)
$\lambda(nm)$	E (eV)		
184	6.786	$-8B+E_{3265} = 6.873$	1.282
203	6.151	$-8B- E_{3265} = 6.113$	0.618
212	5.890	$-7B+ E_{6460} = 5.876$	0.238
231	5.429	$-7B- E_{6460} = 5.492$	1.604
270	4.625	$-6B- E_{6460} = 4.680$	1.189

From Table 1, Table 2 and (30), it can be clearly seen that the energy

corresponding to the wavelength of the ultraviolet spectrum of benzene is within the range of the ground state transition energy. Using the transition integral β and the benzene ring skeleton vibration energy E_{6460} and resonance kinetic energy E_{3265} , the energy value was combined by three simple indicators, imitating the energy value corresponding to the absorption peak of the ultraviolet spectrum and exploring the relationship and significance of the ultraviolet spectrum of benzene. The analysis shows that before the transition of the ground state of the benzene molecule, whether the external energy of the system has been absorbed is related to the amount of ultraviolet light energy absorbed during the transition.

It is also found that the energy corresponding to the median wavelength of 212 nm is 5.890 eV. The transition energy of the ground state is 6.493 eV. Their ratio is exactly equal to the ratio of the benzene ring bond length of 0.1397 nm to the ordinary chain hydrocarbon single bond length of 0.154 nm, which is 0.907.

$$\frac{5.890}{6.493} = \frac{0.1397}{0.1540} = 0.907 \quad (39)$$

Therefore, the difference between these two energies of 6.493-5.890=0.603 eV can be regarded as the energy that keeps the structure from the ordinary bond length shortened to the benzene ring bond length of 0.1397 nm. It also guarantees the normality of the planar structure of the benzene molecule.

The median wavelength of UV spectrum and quantitative interpretation of the bond length of the benzene ring

The physical concept of the wave function in quantum mechanics can be understood as follows: it must meet the three so-called reasonable conditions of continuous, single value and finite in all variable regions of variable x . Hence, the equation¹³

$$\frac{d\psi}{dx} - ik\psi = 0 \quad (40)$$

Solutions have to

$$\psi = e^{ikx} = \cos kx + i \sin kx \quad (41)$$

Only when k is not an imaginary number or a complex number can the above three conditions be met. The equation of momentum in quantum mechanics²⁰ is

$$\frac{d\psi}{dx} - \frac{i2\pi p}{h} \psi = 0 \quad (42)$$

The wave function is

$$\psi = e^{i2\pi xp/h} \quad (43)$$

When a free particle moves in a circle along a ring with a radius of r (like an equivalent electron), for the wave function to satisfy the single value condition, the wavelength λ must satisfy¹³

$$\lambda = \frac{h}{p} = \frac{2\pi r}{q}, q = 0, 1, 2L \quad (44)$$

Substitute (44) into (43) to obtain the corresponding wave function,

$$\psi = e^{iqx/r} \quad (45)$$

According to the one-dimensional Schrodinger equation²⁰

$$-\frac{h^2}{8\pi^2 m} \frac{\partial^2}{\partial x^2} e^{iqx/r} = E e^{iqx/r} \quad (46)$$

Solve the energy as

$$E = \frac{q^2 h^2}{8\pi^2 m r^2} \quad (47)$$

In (47), when this free particle is given two states (such as the ground state and the excited state), the relationship between the transition energy between its two energy levels and the corresponding absorption wavelength of ultraviolet light is

$$\Delta E = \frac{hc}{\lambda} = \frac{(2^2 - 1)h^2}{8\pi^2 mr^2} = \frac{3h^2}{8\pi^2 mr^2}$$

$$\lambda = \frac{8\pi^2 cmr^2}{3h} \quad (48)$$

Substituting the constant values of h , m , and c into (48), the relationship between the wavelength of the absorbed light and the radius is obtained:

$$\lambda = \frac{8\pi^2 cmr^2}{3h} = 10.847 \times 10^{12} r^2 \quad (49)$$

Substituting the median of the important peak wavelength of the ultraviolet spectrum of benzene at 212 nm , that is, $\lambda = 2.12 \times 10^{-7}$ into (49), obtains

$$r^2 = \frac{2.12 \times 10^{-7}}{1.0847 \times 10^{13}} = 1.954 \times 10^{-20} m^2$$

$$r = 1.398 \times 10^{-10} = 0.1398 (nm) \quad (50)$$

The r value in (50) is almost identical to the calculated value of 0.1397 nm in the recognized rotational Raman spectrum of the benzene molecular bond length. The accepted value of the bond length of the benzene ring should be an average value.

Design methods of new plane structural forms of benzene molecule

In the design of the planar structural form of the benzene molecule, the dotted line represents the half-valent bond. The simple form of the ground state is a double ring of a regular hexagon. The outer circle is a solid line, and the inner circle is a dashed

line. The outer ring of the excited state is the same as the ground state, and the inner ring is composed of two dashed equilateral triangles that are inverted from each other. The positive triangle represents the positive phase, and the inverted triangle represents the negative phase (see Figure 1).

Figure 1 New plane structural forms of benzene molecules

Plane structure design of other molecules related to benzene

To confirm the universality of the design method for the new structural forms of benzene molecules, the structural forms and chemical reaction formulas of more than 50 benzene homologs and derivatives were demonstrated^{2,7,18,19}.

The structure of PAH^{17,18}, although it is also a planar structure, is complex and changeable. The structural design should pay attention to the fact that it is mainly based on the classic hexagonal fused ring solid line frame, following the concept and law of valence bond theory (especially carbon tetravalence), and then use the dotted line to configure the half-valent bond. Because the structural formula is always unique, it also has regularity and is not arbitrarily configured, so structural design is not difficult.

1 The structural form fully embodies and fully expresses the essence of the new structural theory of benzene molecules.

- 2 The valence bond of the structural form is represented by a short solid line.
- 3 The plane structure form of the benzene molecule is designed in two forms: ground state and excited state.
- 4 The excited state structural form can express the positive and negative phases of the benzene ring.
- 5 First, classify according to the main structure. Then, an equal hexagonal solid line frame was used to splice the basic frame of the molecule.
- 6 Starting from the entire periphery of the molecule, add a dotted line of half-valent bonds between interval carbon atoms of the benzene ring. Extend the dotted line as much as possible, even penetrate several benzene rings, so that the line connects into several large straight dotted line loops. Each carbon atom must be linked to two different carbon atoms with a dashed line to ensure that the carbon is tetravalent.
- 7 The large dotted loop is divided into front and back (positive and negative phases). The large loop of straight dotted loopdotted lines on the front is continuous. The dotted line of the large frame on the reverse side is intermittent (indicating that it is partially covered by the front side). Where the front and back dashed lines intersect, the back dashed line must be broken, indicating that it is covered by the front dashed line: link and negative link. The inverted phase indicates that it has entered a positive phase. The dotted line on the reverse side must also be connected into an intermittent loop.
- 8 In the last remaining central part, if it is impossible to continue to arrange the half-valent bond dashed line, a solid line must be used to form a double bond.

Basic structural forms of fused ring aromatics of benzene design example

The new structure of polycyclic aromatic hydrocarbons (PAHs) is not formed by splicing the same Kekule style before. The internal structure of each benzene ring in

the structural form is different. However, these changes are not arbitrary but are determined by the internal structure. The structure is unique. Moreover, each ring conforms to the overall structure. Such a structural form can truly record the chemical reaction process (see Figure 2).

Figure 2 Basic structural forms of benzene: fused ring aromatic design example

The relationship between PAHs structure and carcinogenic mechanism

Some PAHs have strong carcinogenic effects and are related to structure. Designing a new structural formula of PAHs based on the new theory of benzene molecular structure is helpful to the study of carcinogenic mechanisms.

Pullman, a French chemist, studied the relationship between the carcinogenic¹⁹ effects of 37 PAHs and the reaction index. Notably, the main carcinogenic area of PAHs, such as 3,4-benzopyrene, in the *K* area, the *L* area plays an auxiliary role²¹ (see Figure 3).

Figure 3 Schematic diagram of the *K*-zone and median *L*-zone of 3,4-benzopyrene

He used the Huckel molecular orbital method^{2,17} to calculate 37 kinds of unsubstituted PAHs and the β value of the transition integral: the adjacent localized energy (*O*, *L*, *E*), the paralocalized energy (*P*, *L*, *E*) and the adjacent. The three indicators of two types of carbon localization energy (*C*, *L*, *E*) were aligned, and some carcinogenic trends were found¹⁹:

$$\text{Zone } K: (O, L, E) + (C, L, E) \min \leq 3.31\beta$$

$$\text{Zone } L: (P, L, E) + (C, L, E) \min > 5.66\beta$$

Except for 4 exceptions, all are in line with the experimental results¹⁹. In addition, according to these laws, he also predicted dibenzopyrene, which was later confirmed by experiments. People were very pleasantly surprised by the results and quickly accepted the *K*-zone and *L*-zone theories.

For 10 types carcinogenic molecules of the 37 PAHs¹⁹, (see Figure 4) the plane structural forms are designed according to the new theory method too of plane structural forms of PAHs are as follows:

Figure 4 Pullman theory 10 cases of PAH carcinogenic molecular new plane structure

For 37 structural forms of PAHs used in Pullman' s theory, there are 10 cases of PAHs carcinogenic effects. These newly designed structural forms (see Figure 4) found 3 of the strong carcinogenic PAHs all contain one double bond. See Table 3.

Table 3 Comparison of 10 cases of oncogenic PAHs with Pullman theory and the new structural formula

No PAHs	Carcinogenic Contains		<i>K</i> -zone			<i>L</i> -zone	
		intensity double	-----			-----	
				Bonds position O.L.E.+		position P.L.E.+	
				C.L. E _{min}		C.L. E _{min}	
3,4- Benzopyrene	++++	1	6-7	3.23	----	----	
1,2,3,4-Dibenzopyrene	++++	1	6-7	3.24	----	----	
3,4,8,9-Dibenzopyrene	++++	1	6-7	3.17	----	----	
1,2,5,6-Dibenzoanthracene	++	0	3-4	3.30	9-10	5.69	
1,2,3,4- Dibenzoanthrene	+	0	1-2	3.34	----	----	
1,2,3,4- Dibenzoanthracene	+	0	3-4	3.31	9-10	5.66	
3,4,6,7- Dibenzoanthrene	+	1	1-2	3.34	----	----	
1,2,5,6-Triphenylene	+	0	7-8	3.41	----	----	
1,2-Benzoanthracene	+	0	3-4	3.29	9-10	5.53	
3,4-Benzophenanthrene	+	0	1-2	3.41	----	----	

The results in Table 3 show that the newly designed PAH structural formula is helpful for judging the carcinogenicity intensity. Of course, there are many carcinogenic factors, and it is not enough to judge by the molecular structure alone¹⁹.

Structure and reaction design of homologs and derivatives of benzene

The types of homologues and derivatives of benzene are many and complex, which test the universality and practicability of the new design method. Not only can the structural formula be easily designed, but it can also be used to record chemical reaction formulas.

Phenylbenzene structural forms and reaction formula

Phenyl² is a special molecular structure composed entirely of a benzene ring. It is not like the fused ring compound of benzene tightly joined together but the structural forms connected to each other through bonds (see Figure 5).

Biphenyl

(Positive phase) (reversed-phase)

Triphenylboron

(Positive phase) (reversed-phase)

Tetraphenylethylene

Pentaphenylcyclopentane

Tetraphenylcyclopentadienone Diphenylacetylene Hexaphenylbenzene

Figure 5 Cycloaddition of tetraphenylcyclopentadienone and diphenylacetylene to produce hexaphenylbenzene

Hexaphenylbenzene is a very special phenylbenzene compound. It is difficult to obtain. Only under strict conditions can this reaction be realized, and the desired result can be obtained.

Design examples of structural forms of benzene homologs and derivatives

Design examples of the planar structure form of benzene homologs and derivatives (see Figure 6)

1,3,5-Trinitrobenzene

Resveratrol

Basa

Metronidazole

Sudan Red IV

Gallic Acid

Cephalixin

Leonurusine

Ampicillin Sodium

Benzoic Anhydride

Codonopsis

Lidocaine

Serotonin

Figure 6 Design example of the new structural formula of benzene homologous derivatives

Design examples of chemical reaction formulas of homologs and derivatives of benzene.

When a new concept of covalent bonds is proposed based on the nature of chemical bonds, that is, every electron shared between atomic nuclei is recorded as half valence. There are two states of benzene molecule: ground state and excited state. It is deduced that a half-valent bond can be formed between carbon atoms in the excited state of benzene molecule. Regarding the overall behavior of six electron are as an equivalent electron moving in a circular motion around a benzene ring, the wave function of the equivalent electron and its wave equation are established, and the equivalent electronic ground state transition energy calculated by solving the equation can be used to quantitatively explain the *UV* spectrum and Benzene molecular bond length. The excited state transition can quantitatively explain the experimental value of the heat of hydrogenation. It not only verified the reliability of the structural theory. At the same time, it is shown that the half-valent bond is represented by a dotted line. The design method of forming a half-valent bond between the carbon atoms of the benzene ring has a wide range of simplicity and versatility (see Figure 7).

Toluene to benzoic acid reaction

Reaction of salicylic acid to aspirin

The benzene ring participates in the free radical 1,5-rearrangement reaction

Coupling reaction of p-(N,N-dimethyl) aminoazobenzene (yellow)

Reaction of 2,6-dimethylphenol ether to 4-allyl-2,6-dimethylphenol

Enolene Rearrangement

Reaction of Allyl

Phenol Ether

Synthesis of Benzyl Acetate from Benzyl Chloride

Synthesis of jasmonal

Cinnamaldehyde reduction reaction

The reaction of dioxins in the hydrocarbon solution replacing chlorine with hydrogen

Figure 7 Design example of the chemical reaction formula of the benzene homolog

Three layer stacked structure of benzene and its thickness

In the excited state of benzene, the p_z orbitals of the three interval carbon atoms of the benzene ring are perpendicular to the plane. On both positive and negative phases,

they can laterally form three half-valent π bonds and bond rings and form agenerating pulsed ring currents and magnetic fields. Vertical p_z orbitals form three σ bonds longitudinally, forming a two layer three-dimensional molecular structure. This two tier structure may not be stable. This is because another benzene ring in the same phase is stacked and combined longitudinally to form a new compound with a three layer three-dimensional structure. The new compound with a three layer three-dimensional structure has a stable structure and becomes a whole six-carbon ring tube. Its top and bottom are exactly the same as a single layer. The middle layer becomes an amonocyclic structure similar to cyclohexane in the middle. It can be called a three layer unit benzene tube. If it is connected in a horizontal direction such as a fused ring, it can be called honeycomb benzene.

In the study of the three-dimensional structure of benzene, it was found that the thickness of the three-layer unit benzene tube was almost equal to the thickness of the graphene data^{2,20}. Calculation method

This total thickness of the three-layer benzene tube is easy to calculate. The three layers are connected by two σ bonds, the top and bottom p_z orbitals are in the same direction, and only one p_z orbital length is counted, that is, the 0.5 σ bond length. The total thickness of the three-layer structure is 2.5 times the σ bond length (see Figure 8). The length of this σ bond, calculated according to the effect of the relevant bond force, will not exceed the bond length of the benzene ring. With a benzene ring bond length of 0.1397 nm, the total thickness of the three-layer structure is 2.5 times the σ bond length, that is, 0.349 nm. .The thickness of graphene is 0.334-0.335 nm, which is very close.

Figure 8 Model of the structure and thickness of the three-layer benzene tube

Generally, the chain hydrocarbon sigma bond length is 0.154 nm , while the double bond can shrink to 0.134 nm . If there are 3 bonds with the same force acting direction, the sigma bond length here may not be longer than the general double bond. Therefore, the total thickness of the three layer unit benzene tube will not exceed 0.349 nm .

The energy required to synthesize a multilayer benzene tube can be calculated. Except for each half of the benzene ring structure in the top and bottom layers, the others are all cyclohexane-type single ring laminated benzene tubes, which release $(n-1)$ times the heat of hydrogenation, that is, $(n-1) B_H$. At the same time, $3(n-1)$ times the energy for C-C bond synthesis must be obtained from outside the system. According to the general C-C bond energy of 3.590 eV (346 kJ/mol)¹¹, the total energy required to form an n layer benzene tube is

$$\begin{aligned}
 E_N &= (3E_{C-C} - B_H) (n-1) = (3.590 \times 3 - 2.165) (n-1) \\
 &= 8.605 (n-1) \text{ eV}
 \end{aligned}
 \tag{5-1}$$

When $n=2$, the total energy of the 3 C-C σ bonds between the two layers is only 8.605 eV , which is much weaker than the total energy of 6 σ bonds in each ring. Therefore,

the interlayer structural energy is much smaller than the structural energy of the layer itself. It is the foundation that tends to be twisted, tilted or broken. It is conceivable that honeycomb benzene, which is composed of a fused ring compound of benzene, can be torn into a single layer with tape such as graphene^{20,21}.

The study of the real structure of benzene molecules has greatly broadened the thinking on the structure of benzene and graphene. Imagine that if graphene is truly a single layer structure, the p_z orbitals of the carbon atoms spaced on the six-carbon ring²¹ are vertical. Single-layer graphene with the same phase is stacked on a flip surface so that the p_z orbitals are completely symmetrical. Under certain conditions (high temperature, high pressure, catalyst), it will be linked by bonds to form a double layer three-dimensional structure. The relatively stable three-layer structure has many characteristics similar to the one-layer structure. In addition, stable, like the honeycomb benzene mentioned above.

Many data indicate that the thickness of single-layer graphene²⁰ is 0.334-0.335 *nm*. There are more estimated to be 0.34-0.35 *nm* or thicker. However, to date, there is no conclusive evidence that graphene must be a single layer structure. What is puzzling is that the thickness of these single-layer graphene data is equivalent to the thickness of a three-layer benzene tube. The benzene ring bond length is 0.1397 *nm*, and the calculated three-layer similar structure thickness is 2.5 times the benzene ring bond length, which is 0.349 *nm*. When the graphene superlattice constant²² of benzene is 0.246 *nm*, the calculated side length of the hexagonal carbon ring (or the vertical σ bond length between two layers) is 0.142 *nm*. It is recognized that the bond length of the C-C bond in the graphite crystal is also 0.142 *nm*. Its 2.5 times is 0.355 *nm*. All these calculations are basically consistent with the recognized thickness of graphene.

However, The thickness of graphene is questionable. According to the graphene superlattice constant of 0.246 *nm*, the diameter of the six carbon rings is also less than 0.3 *nm*, and the thickness of a single layer is the thickness of carbon atoms of 0.334 *nm*. It is impossible for the thickness of one carbon atom to be larger than the

diameter of a ring formed by 6 carbon atoms.

At present, it is generally recognized that graphene is a two-dimensional structure. When two layers of graphene are stacked together, the interaction between them is regarded as a van der Waals heterostructure. This may be related to the opposite of the top and bottom magnetic fields.

In addition to the inconsistencies with these calculated thicknesses, graphene also exhibits highly stable chemical properties, physical properties, solid structure, good electrical conductivity and thermal conductivity, high hardness and toughness, etc., which are similar to metal lattices²². Therefore, it also shows that graphene is not a single-layer structure, so graphene is more like a three-dimensional structure.

If a three-dimensional benzene tube and honeycomb graphene exist, their crystal lattice can hold a large number of electrons and can conduct electricity. A large number of regular hexagonal carbon rings form the line at the center of the tube. If there is no deflection or distortion²², it is likely to become an undisturbed channel for superconducting electrons and is an ideal superconducting structural material.

Results

Represents the excited state transition energy of the equivalent electron of the benzene ring of the benzene molecule, which is only a coefficient b that is 0.231% different from the experimental value of the hydrogenation heat of benzene. When this coefficient is neglected, the heat of hydrogenation is a constant composed of basic physical constants. Li Debao's constant is proportional.

The energy corresponding to the wavelength peak of the ultraviolet spectrum of benzene is in the transition energy range of the equivalent electronic ground state. The transition energy is 8 times the integral of Huckel's theory. From the median wavelength peak of benzene ultraviolet spectrum, the calculated benzene ring bond length is almost equal to the benzene molecular bond length measured by Raman

spectroscopy.

The half-valent bond is represented by the dashed line, and the planar structure design method that can form a half-valent bond between the carbon atoms of the benzene ring has a wide range of simplicity and versatility. In this way, more than 50 structural formulas and chemical reaction examples of benzene homologs and derivatives have been easily designed. And found that the strong carcinogenic polycyclic aromatic hydrocarbon molecules all contain double bonds.

Benzene molecules are stacked on a plane, and it is possible to form a multilayer benzene tube. The calculated energy required is $8.605(n-1)$ eV. The thickness of the three-layer benzene tube is 0.349nm, which is consistent with the thickness of graphene.

Discussion

When a new concept of covalent bonds is proposed based on the nature of chemical bonds, that is, every electron shared between atomic nuclei is recorded as half valence. There are two states of benzene molecule: ground state and excited state. It is deduced that a half-valent bond can be formed between carbon atoms in the excited state of benzene molecule. Regarding the overall behavior of six p_z electrons are like an equivalent electron moving in a circular motion around a benzene ring, the wave function of the equivalent electron and its wave equation are established, and the equivalent electronic ground state transition energy calculated by solving the equation can be used to quantitatively explain the UV spectrum and Benzene ring bond length. The excited state transition can quantitatively explain the experimental value of the heat of hydrogenation. It not only verified the reliability of the structural theory. The use of half-valent bonds breaks the concept that only integer valence bonds exist in valence bond theory. The benzene ring can form a half-valent bond between carbon atoms, laying the foundation for the mechanism that the multi-substitution reaction of

benzene often occurs in the meta or ortho-para position. At the same time, it is shown that the half-valent bond is represented by a dotted line. The design method of forming a half-valent bond between the carbon atoms of the benzene ring has a wide range of simplicity and versatility.

Under the guidance of the new theory, the stacked three-dimensional structure of benzene was explored. Equivalent to the thickness of a layer of graphene. Graphene, a fully carbonized structure of fused ring aromatic hydrocarbons similar to benzene, in addition to the thickness equivalent to the three layer unit benzene tube, also has chemical stability, harder and stronger toughness than steel, and good thermal and electrical conductivity. These properties are more similar to the characteristics of a three-dimensional structure, and their properties are more similar to the characteristics of a three-dimensional structure. If graphene is determined to have a three layer structure, in which a large number of regular hexagonal carbon tubes are connected at the center, without deflection and distortion it is likely to become an undisturbed channel for superconducting electrons.

References

- 1 Kauffman, G. B. Essays on the history of organic chemistry (Traynham, James G.) *Journal of Chemical Education* **65**, 7, A188 (1988).
- 2 Wade, L. G. Wade. *Organic Chemistry*. (Prentice Hall, 2009).
- 3 Carey, F. A. & Sundberg, R. J. *Advanced Organic Chemistry: Structure and Mechanisms Part A*. (Springer, 2008).
- 4 Katsnelson, M. I. *Graphene*. (Cambridge University Press, 2012).
- 5 Klein, D. J. & Trinajstić N. *Valence Bond Theory and Chemical Structure*. (Elsevier, 1990).
- 6 Levine, I. N. *Quantum Chemistry*. (Pearson Education, 2013).
- 7 Rae, A. I. M. & Napolitano, J. *Quantum Mechanics*. (CRC Press, 2015).
- 8 Lowe, J. P. & Peterson, K. *Quantum Chemistry*. (Academic Press, 2005).

- 9 Pauling, L. The Modern Theory of Valence. *Journal of the Chemical Society* **76**, 1461-1467 (1948).
- 10 Bent, H. A. *Molecules and The Chemical Bond: An Introduction to Conceptual Valence Bond Theory*. (Trafford Publishing, 2013).
- 11 Sanderson, R.T. *Chemical Bond and Bond Energy*. (Academic Press, 1977).
- 12 Corry, S. *Symmetry and Quantum Mechanics*. (Chapman and Hall/CRC, 2016).
- 13 Zeidler, E. *Nonlinear Functional Analysis and its Application III: Variational Methods and Optimization*. (Springer, 1985).
- 14 Simon, B. Quantum Mechanics for Hamiltonians Defined as Quadratic Forms. (Princeton University Press, 2016).
- 15 Chandra, S. *Molecular Spectroscopy*. (Alpha Science International Ltd, 2009).
- 16 Huber, K.P. and Herzberg, G. *Molecular Spectra Molecular Structure IV. Constants of Diatomic Molecules*. (Van Nostrand Reinhold Company, New York, 1979).
- 17 Putz, M. V., Cimpoesu, F. & Ferbinteanu, M. *Structural Chemistry*. (Springer International Publishing, 2017).
- 18 Hoard, J. L., Geller, S. & Cashin, W. M. Structures of Molecular Addition Compounds. III. Ammonium-Boron Trifluoride, $\text{H}_3\text{N-BF}_3$. *Acta Crystallographica* **4**, 396-398 (1951).
- 19 Pullman, A. et al: *Adu. Cancer Reseach*, Vol 3 Acadmic Press (1955), 117
- 20 Novoselov, K. S., Geim A. K., Morzov S., Jiang, D., Zhang, Y., Dubonos, S.V., Grigorieva, I.V. & Firsov, A. A. Electric field effect in atomically thin carbon films. *Science*, **306**(5696), 666-669 (2004).
- 21 Lai, D., Chen, W. & Jiang G. Research Progress of Graphene-based Composite Materials. *Current Physical Chemistry* **3**, 269-282 (2013).
- 22 Cao, Y., Fatemi, V., Fang, S., Watanabe, K., Taniguchi, T., Kaxiras, E. & Jarillo-Herrero, P. Unconventional superconductivity in magic-angle graphene superlattices. *Nature* **556**, 43–50 (2018).

Completing Interests

Every issue in this research is completed through mutual negotiation, and there are no disputes over contributions and interests.