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Computer Simulation and Design of Organic Functional Molecules for New Energy Materials

Muhammand Hamanm*

Uni de Moncton, Canada

**corresponding author*

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Abstract: New energy materials are materials that support the development of new energy, have energy storage and conversion functions, or materials that integrate structure and function. This material can increase the investment and operation of new energy systems. The focus is mainly on the research process of material design through physical research. The proposal of this technology can save the use of non-renewable resources, and its performance exceeds the traditional meaning. New energy is mainly based on new technologies and new materials to make energy renewable, and through utilization and development, limited resources can form a cycle. This article aims to study the use of computer simulations and the design of organic functional molecules for new energy materials, observe the difference between new energy materials and traditional materials through these two technologies, and obtain their characteristics through the analysis of this new energy material. The analysis of these theories is finally applied to practice. In this article, a related introduction to a process and design of computer simulation is proposed, and then combined with the analysis of organic functional molecules, through the derivation of formulas and related data, the motion properties of the relevant molecules of new energy materials are obtained, and the new energy materials are further understood. Energy materials, through quantification and data presentation, it can be concluded from experiments and analysis that the molecular tension of new energy materials is related to various factors.

1. Introduction

Renewable energy replaces fossil energy with limited resources and pollutes the environment. Wang Q believes that in the establishment of emerging engineering education, with the rapid development of global economy and technology, environmental pollution caused by traditional extensive energy sources has become more and more serious, and the practical efficiency of

traditional energy has been low. Therefore, energy and the environment has become two very serious basic issues. Under such a general environment, how to optimize the energy structure and develop efficient, recyclable and low-carbon new energy sources has triggered a wave. New energy materials are an effective collection, use and conversion of clean energy, and alleviate economic conflicts. The analysis of new energy materials through computer simulation and the application of organic functional molecules is conducive to future development and promotes a deeper understanding of new energy.

After the introduction of environmental protection concepts, it triggered the protection of new technological concepts and the use of non-renewable resources. Based on some of the above research interests, Bayneva II analyzed the computer simulation model diagrams and design principles, conducted a detailed analysis of the characteristics and design ideas of new energy materials, linked the two through organic functions, and found the difference between the two the difference [1]. On the basis of computer simulation and understanding, carry out quantitative analysis of the characteristics and functions of organic molecules, and then introduce the structure of some organic functional molecules. Analyzing different organic molecules and discovering the shapes of molecules in different environments; at the same time, Michael predicts that there will be a new allotrope of nitrogen under environmental conditions, in which atoms are connected to form new molecules. Compared with solids, Charge transfer induces ionic properties in intermolecular interactions and leads to the predicted cohesive energy of the crystal to be much higher. Since the energy difference between single and triple bonds is large, the dissociation of the crystal is expected to release a large amount of energy [2], through the analysis of the allotrope of nitrogen, it is found that the tension between the molecules and the ionic properties, the understanding of the molecules is more in-depth. In addition, Dong JX believes that organic functional materials have improved performance or new characteristics in the design and synthesis. In the article, it focuses on the structure of organic functional molecules, and uses quantitative calculations and molecular dynamics to design several methods. Effective organic functional molecules, and apply them to the fields of new energy materials and organic electronics [3]. Terranova Z L has studied the application of organic functional molecules to new energy materials through molecular dynamics simulation, and found that new materials under organic functions are more practical than traditional materials [4]. For the classification of different new energy sources,Zhu W proposed that energy materials mainly include solar cell materials and solid oxide battery materials. New energy and new materials are materials with excellent performance in new development or research and development. Under the background of infinite repetition[5], the teaching of organic chemistry for engineering majors needs innovation. From the selection of teaching materials and teaching content, the reform of teaching methods, and the evaluation system Improve and optimize the organic chemistry experiment course, and strive to improve the teaching effect of organic chemistry [6]. Based on the understanding of new energy, Martinho F proposed that the monolithic series integration of third-generation solar materials on silicon has broad prospects in the field of photoelectrochemistry and photovoltaics. By using very thin (10 nm) TiN-based materials at the interface Diffusion barriers have different compositions and properties. At the device level, he proved that the protection of Si bottom cells depends to a large extent on barrier layer engineering, and its performance is comparable to traditional interface layers based on transparent conductive oxides., And pointed out a promising alternative design in solar energy conversion equipment [7]. In addition, according to an analysis of lithium-ion, Li L lithium-ion batteries have played a key role in portable electronic products and transportation electrification in modern society. However, the limited maximum energy density of lithium-ion batteries is not enough to meet the long-term needs

of society. It is found that the research on new energy materials is more practical and can be recycled, although the molecules can be observed in the model and quantitative methods. However, due to the existence of errors in organic molecules in reality, it is still necessary to collect a large amount of experimental data for general research [8].

The innovation of this article is (1) The application of computer simulation is added to the analysis of different molecules. By analyzing the structure of different molecules, the influence of the molecular structure in the Raman spectrum is guaranteed to ensure accuracy. Under the circumstances, the calculation of this method is simplified (2) In the analysis of molecular structure, through the combination of theory and reality, new energy materials are quantified and modeled, and empirical knowledge is used to explain the theory of experimental phenomena.

2. Application of Computer Simulation and Organic Functional Molecules to New Energy Materials

2.1. New Energy Materials

New energy materials refer to the conversion and utilization of new energy, and the main materials needed to realize the development of new energy technologies. New energy materials are an important foundation for realizing the production and utilization of new energy. The main classification can be divided into solar energy, biomass energy materials, etc. according to the application of new energy fields.

(1)Routine Characterization of New Energy Materials

The structure of new energy materials is mainly divided into two phases, one is the method of electron diffraction, and the other is mainly the method of X-ray diffraction. Both of the basic principles of diffraction follow the Bragg equation, which can reflect the long-range order structure information of crystalline materials [9-10]. X-ray diffraction can accurately determine the unit cell parameters. The current electron diffraction is generally carried out in an electron microscope, which can be combined with "aperture selected area diffraction" for micro-area analysis, and at the same time the topography can be obtained. In terms of morphological characterization, there are currently the following methods, such as scanning electron microscopy and transmission electron microscopy. Among them, transmission electron microscopy mainly collects the information of transmission electrons generated by the interaction between electrons and materials, which usually carry materials. Internal information, while the scanning electron microscope mainly collects secondary electron information to observe the surface morphology of the sample. It is a very important analysis method. The principle of operation is to use the van der Waals force between atoms to generate the electron tunneling effect and give Draw a three-dimensional surface map. As shown in Figure 1:

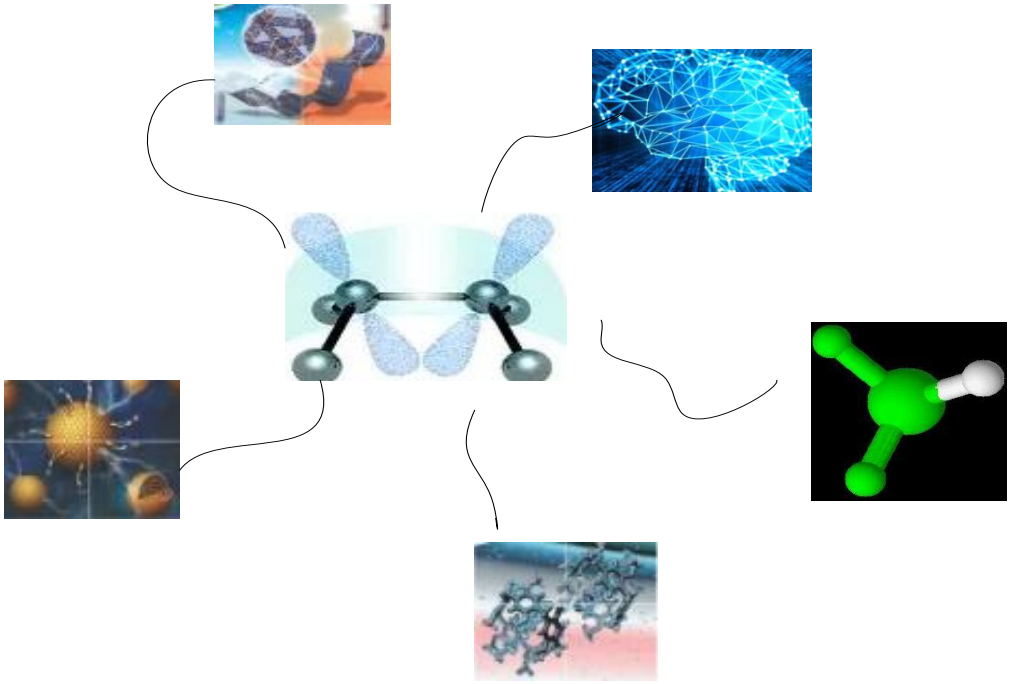

Figure 1. Three-dimensional surface map of new energy materials

(2) Key Applications of New Energy Materials

The invention of new energy materials promotes the birth of new energy systems and is applied to improve the efficiency of new energy systems. The application directly affects the investment and operating costs of new energy systems. According to the density of different organic molecules, there are discrepancies and multi-particles. The basic exchange correlation function of the system [11] is solved. The total energy of a multi-molecular system can be expressed as a functional function of molecular strength:

$$\mathrm{E}(\lambda)=\mathrm{P}(\lambda)+\mathrm{T}(\lambda)+\oint \mathrm{d}rV(\lambda) \tag{1}$$

In the above formula, $\mathrm{P}(\lambda)$ refers to the kinetic energy term of organic molecules, and $\mathrm{T}(\lambda)$ refers to the interaction energy between different molecules. However, because of the ignorance of the molecular kinetic energy term, it needs to be under the image of a single molecule. Describe the orbital wave function to construct the interaction of the molecular system:

$$\mathrm{T}_s(\zeta)=\frac{\Delta}{3r}\sum_{r=1}^{occ} dr\phi^2(r)\left(-\mathrm{O}^2\right)\lambda \tag{2}$$

In,

$$\phi(r)=\int_{r=1}^{occ}\left|E(r)^2\right| \tag{3}$$

According to the above formula, the potential energy of organic molecules without interaction can be obtained to calculate the correlation function.

2.2. Computer Simulation Method Design and Organic Functional Molecules

Computer simulation refers to the method of experimenting and researching by establishing models instead of physical objects. Computer simulation can provide a convenient and flexible "live mathematical model" for many experiments [12], so computer simulation technology can be used in the research process of spacecraft, missiles, aircraft, atomic energy industry, chemical industry, petroleum and coal energy resources, etc., To simulate various experiments, select the best parameters and design the most reasonable system plan. Real-time simulation can also be realized by connecting the computer system with the physical object. The use of computer simulation technology can speed up the progress of engineering design and development and save a lot of model experiment costs.

(1) Computer Simulation Process

Computer organic simulation is an experimental research method that uses computers to build models instead of physical objects. It can be either macroscopic or onlookers. It can calculate the results of data through logical relations and mathematical expressions, and can provide a variety of The output parameters of the intuitive form are used to perform partial structure of the system model, and then recalculate. Since the organic molecular system will change or be random with the change of the data, the experimental results of the real system data and the model will often be changed. Using sequence analysis method, as shown in Figure 2:

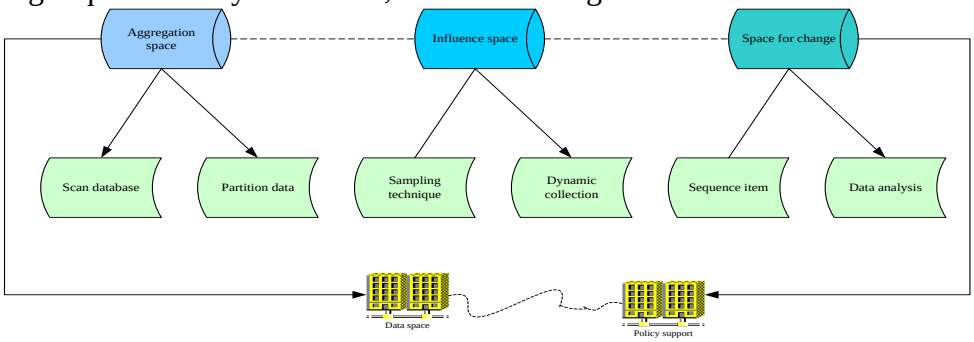

Figure 2. Computer data sequence analysis method

(2)Ab Initio Algorithm of Computer Simulation Method

The computer simulation method is to conduct simulation experiments on the computer for the research object. Computer model

The basic steps of the quasi-method are: first, analyze the relevant properties of the research object, and construct a mathematical model; then,

Calculate the mathematical model according to the simulation method, and get the relevant data; finally, the calculated data calculate the final result to analyze the relevant properties of the research object.

The ab initio calculation method is to build a model of the research object through a computer [13-14]. Through the electronic structure and electronic behavior of different atoms in the established model, the Schrodinger equation is analyzed for the atoms and molecules in the model, and some approximations are used. Method, calculate the microscopic properties of the model

constructed by the smallest atoms and molecules, such as predicting the properties of the research object in the mechanical properties. The ab initio calculation method can be divided into two main methods, molecular orbital method and bond valence theory method in the early stage of development. Among the two methods, the molecular orbital method is more widely used. The main idea of the molecular orbital method is that the electrons outside the nucleus do not actually move alone, but move extremely fast in the entire molecule. However, this processing ignores the influence of the exchange correlation between electrons and electrons in the entire molecular motion, which greatly reduces the calculation accuracy. It has been widely used in the field of materials science. According to the initially given charge density and wave function, the calculation of potential energy and exchange-related energy uses the calculated electric energy and exchange-related energy to construct the Hamiltonian [15]. Mainly calculate the interaction between particles, analyze the valence bond interaction and valence structure between atoms or molecules; calculate the structural parameters of solid crystals, such as crystal structure, lattice constants; calculate the mechanical properties and electromagnetic properties of materials, such as mechanics related Modulus.

Born-Oppenheimer functional molecular approximation

A method based on quantum mechanics to analyze organic functional molecules, and then use this method to analyze new energy materials. By studying the structure of molecules, for a molecular system, a quantitative equation is carried out according to a non-relativistic algorithm:

$$\tilde{\mathrm{P}}_{\mathrm{rat}} = \hat{R}_V + \hat{R}_{Ve} + \hat{T}_e + \hat{T}_{ne} \tag{4}$$

In the formula, V and e represent the nucleus and electrons, where $\hat{\mathrm{R}}_{\mathrm{v}}$ is the kinetic energy symbol of the nucleus, $\hat{\mathrm{T}}_e$ is the kinetic energy operator of the electron, $\hat{\mathrm{R}}_{\mathrm{Ve}}$ is the interaction energy operator between the nucleus and the electron, and $\hat{\mathrm{T}}_{\mathrm{ne}}$ is the electron cluster. The interaction energy operator, in the non-relativistic kinetic energy T and the potential energy R, can observe the movement of organic molecules. Therefore, the Schrödinger equation of the multi-electron system can be expressed as:

$$\tilde{\mathrm{K}}_{\mathrm{rat}}\upsilon(p,P) = E\upsilon(p,P) \tag{5}$$

Among them, $\upsilon(\mathrm{p},P)$ refers to the wave function of the functional molecular system, E refers to the total energy, and p and P refer to the coordinates of the electron and atomic nucleus, respectively.

In the relative movement of the nucleus and electrons, the potential energy between molecules can be seen [16]. According to this special electrical movement, the special properties of functional molecular materials can be analyzed.

(3)Raman Spectroscopy Theory

Raman spectroscopy is an inelastic scattering phenomenon, one of the main spectra used to study molecular vibration, mainly to distinguish a certain substance from a variety of spectra and then to quantitatively determine a certain substance in the sample Therefore, the spectrum can also be said to be a fingerprint-like feature of molecular structure, which can detect the surface structure of microscopic particles or bulk substances according to the state of all substances [17]. Each molecule

has a series of electronic states. When the molecules vibrate between them, the energy obtained by quantization is observed according to a typical Morse curve, as shown in Figure 3:

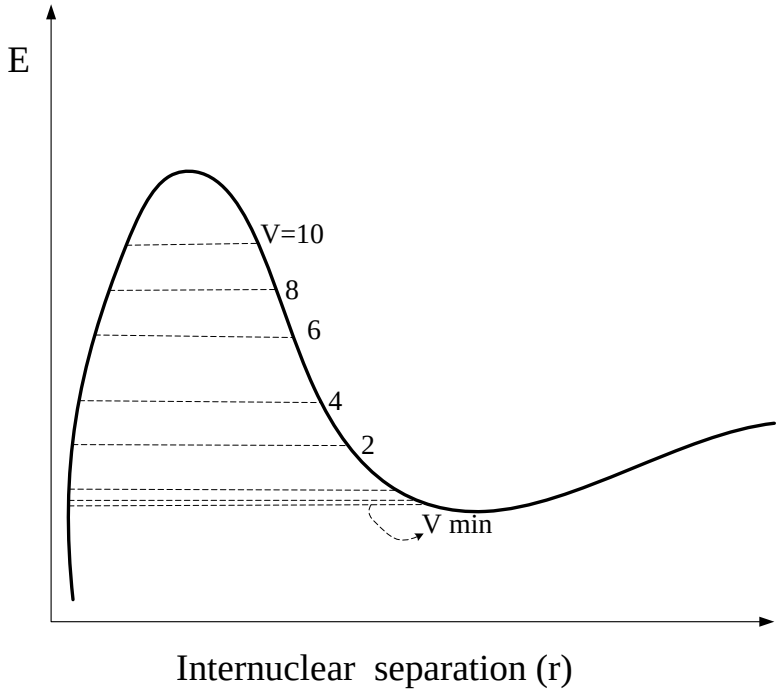

Figure 3. Typical Morse curve of electronic state

In the Morse curve in the above figure, the molecular vibration can be generally simplified to a simple harmonic approximation for research. In this approximation, a parabola is used to replace the Morse curve to study the vibration mode of the atoms in the molecule.

2.3. Application of Organic Molecular Methods and Design to New Energy Materials

(1) Classical Molecular Dynamics

Classical molecular dynamics simulation is a system for studying the physical motion of atomic nuclei and molecules, because molecular dynamics will be applied in a larger size range. Normally, because the system described by molecular dynamics contains a huge number of molecules, molecular dynamics simulation is used to study the adsorption mechanism of different organic functional molecules on the surface. Observe the contact area between different ionic liquids. Under the binding energy of the matrix between different ionic liquids, it is concluded that the increase in chain length will also affect the binding energy between molecules. The relationship between the two shows a positive correlation. As the chain length increases, the binding energy between molecules will also become larger [18-19]. For different binding energies, there will be different adsorption capacities and different gripping performances. The stable adsorption of the surface is different, and the configuration between the molecules is also different. What follows is the dynamics between the molecules. Different, and with the different covalent bonds between various organic molecules, different new energy materials will be formed. From the computer simulations analyzed above, different new energy materials will produce different Performance, for different

performances to form different new energy, showing a good electrochemical effect.

(2)First-principles Calculation

First-principles calculations are based on quantum mechanics theory, by solving Schleddinger's equations, theoretically predicting various properties of materials, and explaining methods for analyzing the properties of organic molecules. For the understanding of new energy materials, the equation needs to be solved according to the rational simplification and approximation:

$$H_{\gamma} = H_{\psi} \tag{6}$$

In the above formula, H represents the Hamiltonian, and $\gamma and \psi$ represents the energy eigenvalue and the corresponding eigenwave function. In general, any material can be described by the Schrodinger equation, and then for a simple single new energy material, the Schrodinger equation can be used to accurately solve it, but for a system formed by a variety of new energy materials, H will It becomes very complicated, and then it is more difficult to achieve by solving the equation.

According to theoretical methods, solving certain properties of organic functional molecules can generally directly correspond to the expected value of the operator. For example, for a general position operator [20], the value between organic molecules of opposite sex can be calculated as:

$$\mu_{e} = \left\langle \psi \left| \sum_{u} - er_{u} \right| \psi \right\rangle \tag{7}$$

Among them, u is the quantification of the tension between specific molecules, and the same can also be calculated by the derivative of energy, such as:

$$\mu_{i} = \frac{\partial E}{\partial E_{1}} \tag{8}$$

Among them, i represents the direction of a component of a molecule, and E represents the magnitude of the force in that direction. In practical applications, the practicability of the derivative method will be higher.

3. Experimental Design and Result Analysis

3.1. Computer Simulation Method and Application

By changing the lattice constants to observe the convergence of the total energy [21], we have optimized their most reasonable lattice constants. And the energy values of seven crystal structures with different molecular axes and the energy values corrected by the zero-point energy are given. The calculated data are shown in Table 1:

Table 1. Crystal lattice constants and average binding energy of different hydrogen molecules

	[100]	[200]	[300]	[400]	[500]
a	5.43	6.31	6.66	7.02	7.07
E	0.054	0.033	0.653	0.075	0.546
R(ARE)	0.036	0.054	0.352	0.555	0.553

As the above-mentioned experimental data shows, in the case of different molecular lattice

numbers, the performance of different molecules is different. For example, hydrogen molecule is the most commonly used in a variety of new energy sources. The binding energy is compared under the premise, the energy value after the zero point correction changes, and the data is quantified through the application of computer simulation, and the axial value of the different binding energy is used to verify the stability on the incompatible scale. Size, and then calculate the mechanical properties of different structures.

Because the van der Waals force between molecules is different, the shape of the lattice between different molecules is also different, so according to different convergence conditions, it is judged whether the van der Waals force correction method used is suitable for the lattice model [22 -23] calculation research, through the calculation of the above formula, the best cubic structure and the elastic constant of molecular crystals can be tested, and then the mechanical stability between different molecules can be analyzed. Finally, the various structures can be obtained. Under the mechanical constants, and then carry out the stability between different crystal structures, in order to understand the composition of new energy materials. As shown in table 2:

Table 2. Average binding energy of centered cubic molecular crystal lattice constants under different van der Waals correction methods

	PEB	D3(BJ)-rePEB	DF-rePEB	DF2	DF-optB6b	D4(BJ)-rePEB
fcc	5.03	4.47	4.82	4.93	4.79	4.58
	0.020	0.035	0.046	0.066	0.048	0.043

3.2. New Energy Materials under Organic Functional Molecules

We set the cut-off energy reasonably [24], because although the introduction of cut-off energy can simplify the calculation, the calculation results of the total energy of the simulated system will also be biased. The choice of cut-off energy should be determined according to the convergence of the total energy of the system with respect to changes in different cut-off energies. Too large truncation energy will greatly increase the amount of calculation. Too small truncation energy will increase the calculation error. Use discrete and different plane waves to expand any function, select different plane wave coefficients to complete a cutoff value, use different kinetic energy basis sets of plane waves to expand the wave function, if you use continuous plane wave basis sets, then no matter what How to choose the kinetic energy truncation can not make the plane wave basis composition a finite number. So we use a discontinuous plane wave basis set and set the cut-off energy so that the plane wave basis set becomes finite.

Table 3. Calculation results of elastic constants and mechanical moduli of hydrogen molecular crystals with hexagonal close-packed structure

E	K-points	C1	C2	C4	C5	C6
400	8*8*7	7.61	3.45	1.87	6.53	2.18
400	6*6*4	7.76	3.34	1.66	5.55	2.23
600	6*6*8	7.46	3.21	1.65	4.51	2.9

It can be seen from Table 3 that in our simulation calculations, when the cut-off energy changes,

there is only a slight difference between the elastic constants and the three mechanical moduli we calculated, and the largest difference is less than what we can find After obtaining the crystal elastic constants of the hexagonal close-packed hydrogen molecule, according to the strain energy theory [25-26], the first condition to prove the stability of the crystal structure is to judge whether the elastic constant matrix is positive or not.

3.3. Computer Simulation and Design of Organic Functional Molecules for New Energy Materials

When a molecule and a molecule are close to each other, the atomic core in the molecule and the electrons outside the core vibrate to produce a dipole moment. The dipole moments generated by the atoms close to each other interact to produce a dispersion force, and the dispersion force generates a binding potential energy between particles Attenuates as the distance between particles increases, as shown in Figure 4 below:

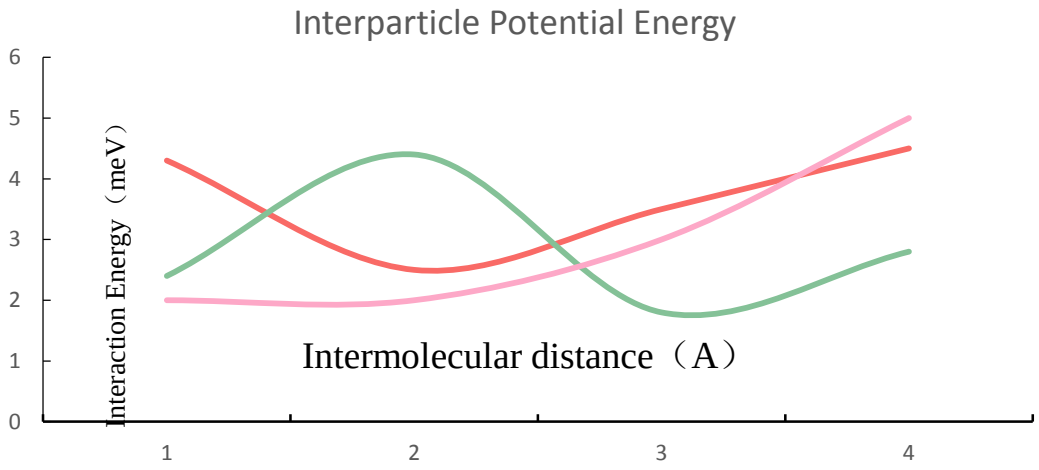

Figure 4. Potential energy between different particles

The calculation results of the independent elastic constants of the hexagonal close-packed hydrogen molecular crystals in Figure 4 are quantified, and it is found that the independent elastic constants calculated by us all meet the requirements of the inequality in the formula, which shows that the hexagonal close-packed hydrogen molecules we have established The crystal model meets the requirements of the strain energy theory for the stability of the hexagonal system.

Table 4. Theoretical calculation values of elastic constants and bulk modulus of hydrogen molecular crystals with hexagonal close-packed structure

	C1	C2	C3	C4	C5	B
Goldman's.	7.16	3.38	1.94	8.6	1.88	4.17
Exp. b	3.62	1.19	0.41	4.4	0.83	1.74
Exp.c	4.2	1.8	0.5	5.1	1.1	2.1

In Table 4, in addition to the calculated values, there is a big difference in the temperature under the temperature calculation conditions in the test conditions, and the final elastic constant and bulk modulus are also quite different. We believe that it is the difference in the external environment of the crystal that causes the theoretical calculation or our simulation calculation to be quite different from the experimental value. The mechanical properties of hydrogen molecular crystals are particularly sensitive to the external environment, which leads to the incomparability of calculated and experimental values in different external environments. The elastic constants of hydrogen molecular crystals under the same environment as the experimental environment are calculated [27], and they are found to be comparable to those in the experimental environment. The experimental values are in good agreement.

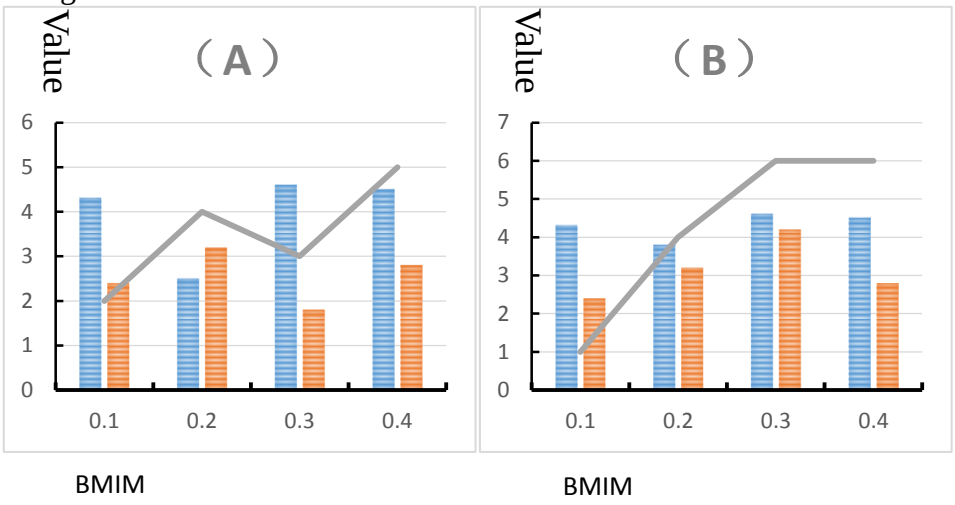

Figure 5. Radial distribution function between different atoms in the system

In Figure 5, the radial distribution function of the tension between molecules between different atoms indicates that during the process of changing the Raman spectrum, the detected target molecules need to be adsorbed on the surface of the substrate. The molecules in the solution act as cationic In addition, the detection molecule is in a solution state [28-29], and the solvent effect of the solvent molecule will also have an unavoidable influence.

4. Discuss

Through the understanding of new energy materials, we realize that new energy and new materials are the future development direction. Through the observation and analysis of organic molecules of different materials, we can see the synthesis process of different molecules, and then add the application of computer simulation technology., You can observe the microscopic part of organic molecules more intuitively and you can grasp the macroscopic and microscopic parts of the new material as a whole [30]. Now, the most widely studied is the self-organized monomolecular membrane of alkyl macaptan adsorbed on the gold surface. Polymonolayer alkyl macaptan has a wide range of applications in molecular equipment applications, sensor equipment, metal corrosion protection and molecular biology. The application of new energy and new materials for different organic functional molecules needs more In-depth exploration.

5. Conclusion

Through the quantitative analysis of computer simulations, we know the van der Waals forces between different organic molecules and the forces between different crystal lattices. New energy materials are obtained through the methods of classical molecular dynamics and Raman relationship theory. In this paper, the main work is to theoretically study the X of three different organic functional molecular materials.

Ray spectrum and Raman spectrum. The ray spectra of the acceptor materials based on organic polymer solar cells are studied; the influence of solvents on the charge states of the Raman spectra of rhodamine series molecules is studied.

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Data Availability

Data sharing is not applicable to this article as no new data were created or analysed in this study.

Conflict of Interest

The author states that this article has no conflict of interest.

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