DOWNLOAD PDF QUANTUM CHEMISTRY OF ATOMS AND MOLECULES

Chapter 1 : Quantum chemistry - Wikipedia

In this book, Dr Matthews emphasises the fundamental ideas of quantum theory as they relate to mainstream areas of quantum theory such as bonding and spectroscopy; elementary ideas on the use of symmetry are also included.

Experimental quantum chemists rely heavily on spectroscopy , through which information regarding the quantization of energy on a molecular scale can be obtained. Common methods are infra-red IR spectroscopy , nuclear magnetic resonance NMR spectroscopy , and scanning probe microscopy. Theoretical quantum chemistry, the workings of which also tend to fall under the category of computational chemistry , seeks to calculate the predictions of quantum theory as atoms and molecules can only have discrete energies; as this task, when applied to polyatomic species, invokes the many-body problem , these calculations are performed using computers rather than by analytical "back of the envelope" methods. It involves heavy interplay of experimental and theoretical methods. In these ways, quantum chemists investigate chemical phenomena. Quantum chemistry studies the ground state of individual atoms and molecules, and the excited states , and transition states that occur during chemical reactions. On the calculations, quantum chemical studies use also semi-empirical and other methods based on quantum mechanical principles, and deal with time dependent problems. Many quantum chemical studies assume the nuclei are at rest Bornâ€"Oppenheimer approximation. Many calculations involve iterative methods that include self-consistent field methods. Major goals of quantum chemistry include increasing the accuracy of the results for small molecular systems, and increasing the size of large molecules that can be processed, which is limited by scaling considerationsâ€"the computation time increases as a power of the number of atoms. This is the first application of quantum mechanics to the diatomic hydrogen molecule, and thus to the phenomenon of the chemical bond. In the following years much progress was accomplished by Edward Teller , Robert S. Mulliken , Max Born , J. Then, in , to explain the photoelectric effect , i. In the years to follow, this theoretical basis slowly began to be applied to chemical structure, reactivity, and bonding. Probably the greatest contribution to the field was made by Linus Pauling. This is called determining the electronic structure of the molecule. It can be said that the electronic structure of a molecule or crystal implies essentially its chemical properties. Wave model[edit] The foundation of quantum mechanics and quantum chemistry is the wave model, in which the atom is a small, dense, positively charged nucleus surrounded by electrons. Unlike the earlier Bohr model of the atom, however, the wave model describes electrons as " clouds " moving in orbitals , and their positions are represented by probability distributions rather than discrete points. The strength of this model lies in its predictive power. Specifically, it predicts the pattern of chemically similar elements found in the periodic table. The wave model is so named because electrons exhibit properties such as interference traditionally associated with waves. These are n, the principal quantum number, for the energy, l, or secondary quantum number, which correlates to the angular momentum, ml, for the orientation, and ms the spin. This model can explain the new lines that appeared in the spectroscopy of atoms. It focuses on how the atomic orbitals of an atom combine to give individual chemical bonds when a molecule is formed. Molecular orbital theory An alternative approach was developed in by Friedrich Hund and Robert S. Mulliken , in which electrons are described by mathematical functions delocalized over an entire molecule. The Hundâ€"Mulliken approach or molecular orbital MO method is less intuitive to chemists, but has turned out capable of predicting spectroscopic properties better than the VB method. This approach is the conceptional basis of the Hartreeâ€"Fock method and further post Hartreeâ€"Fock methods. Density functional theory[edit] Main article: Density functional theory The Thomasâ€"Fermi model was developed independently by Thomas and Fermi in This was the first attempt to describe many-electron systems on the basis of electronic density instead of wave functions , although it was not very successful in the treatment of entire molecules. The method did provide the basis for what is now known as density functional theory DFT. Modern day DFT uses the Kohn-Sham method , where the density functional is split into four terms; the Kohn-Sham kinetic energy, an external potential, exchange and correlation energies. A large part of the focus on developing DFT is on improving the exchange and correlation terms. Though this method is less developed than post

Hartreeâ€”Fock methods, its significantly lower computational requirements scaling typically no worse than n3 with respect to n basis functions, for the pure functionals allow it to tackle larger polyatomic molecules and even macromolecules. This computational affordability and often comparable accuracy to MP2 and CCSD T post-Hartreeâ€”Fock methods has made it one of the most popular methods in computational chemistry. Statistical approaches, using for example Monte Carlo methods , are also possible. Adiabatic chemical dynamics[edit] Main article: Adiabatic formalism or Bornâ€—Oppenheimer approximation In adiabatic dynamics, interatomic interactions are represented by single scalar potentials called potential energy surfaces. This is the Bornâ€—Oppenheimer approximation introduced by Born and Oppenheimer in Pioneering applications of this in chemistry were performed by Rice and Ramsperger in and Kassel in , and generalized into the RRKM theory in by Marcus who took the transition state theory developed by Eyring in into account. These methods enable simple estimates of unimolecular reaction rates from a few characteristics of the potential surface. Non-adiabatic chemical dynamics[edit] Main article: Vibronic coupling Non-adiabatic dynamics consists of taking the interaction between several coupled potential energy surface corresponding to different electronic quantum states of the molecule. The coupling terms are called vibronic couplings. The pioneering work in this field was done by Stueckelberg , Landau , and Zener in the s, in their work on what is now known as the Landauâ€—Zener transition. Their formula allows the transition probability between two diabatic potential curves in the neighborhood of an avoided crossing to be calculated. Spin-forbidden reactions are one type of non-adiabatic reactions where at least one change in spin state occurs when progressing from reactant to product.

Chapter 2 : Scientists Create a Molecule by Combining Just Two Atoms

Molecules, small structures composed of atoms, are essential substances for lives. However, we didn't have the clear answer to the following questions until the s: why molecules can exist in stable as rigid networks between atoms, and why molecules can change into different types of molecules.

It is characteristic and unique for each element. The atomic mass also referred to as the atomic weight is the number of protons and neutrons in an atom. Atoms of an element that have differing numbers of neutrons but a constant atomic number are termed isotopes. Isotopes, shown in Figure 1 and Figure 2, can be used to determine the diet of ancient peoples by determining proportions of isotopes in mummified or fossilized human tissues. Biochemical pathways can be deciphered by using isotopic tracers. The age of fossils and artifacts can be determined by using radioactive isotopes, either directly on the fossil if it is young enough or on the rocks that surround the fossil for older fossils like dinosaurs. Isotopes are also the source of radiation used in medical diagnostic and treatment procedures. Note that each of these isotopes of hydrogen has only one proton. Isotopes differ from each other in the number of neutrons, not in the number of protons. Image from Purves et al. Some isotopes are radioisotopes, which spontaneously decay, releasing radioactivity. Other isotopes are stable. Examples of radioisotopes are Carbon symbol 14C , and deuterium also known as Hydrogen-2; 2H. Stable isotopes are 12C and 1H. Carbon has three isotopes, of which carbon and carbon are the most well known. The Periodic Table of the Elements, a version of which is shown in Figure 3, provides a great deal of information about various elements. An on-line Periodic Table is available by clicking here , Figure 3. The Periodic Table of the Elements. Each Roman numeraled column on the label at least the ones ending in A tells us how many electrons are in the outer shell of the atom. Each numbered row on the table tells us how many electron shells an atom has. Thus, Hydrogen, in column IA, row 1 has one electron in one shell. Phosphorous in column VA, row 3 has 5 electrons in its outer shell, and has three shells in total. Image from James K. Electrons and energy Back to Top Electrons, because they move so fast approximately at the speed of light , seem to straddle the fence separating energy from matter. Because of his and others work, we think of electrons both as particles of matter having mass is a property of matter and as units or quanta of energy. When subjected to energy, electrons will acquire some of that energy, as shown in Figure 4. Excitation of an electron by energy, causing the electron to "jump" to another electron energy level known as the excited state. Orbitals have a variety of shapes. Each orbital has a characteristic energy state and a characteristic shape. The s orbital is spherical. Since each orbital can hold a maximum of two electrons, atomic numbers above 2 must fill the other orbitals. The px, py, and pz orbitals are dumbbell shaped, along the x, y, and z axes respectively. These orbital shapes are shown in Figure 5. Energy levels also referred to as electron shells are located a certain "distance" from the nucleus. The major energy levels into which electrons fit, are from the nucleus outward K, L, M, and N. Sometimes these are numbered, with electron configurations being: This nomenclature tells us that for the atom mentioned in this paragraph, the first energy level shell has two electrons in its s orbital the only orbital it can have , and second energy level has a maximum of two electrons in its s orbital, plus one electron in its p orbital. S-orbitals are spherical, p-orbitals are shaped like a dumbbell or figure 8. Chemical Bonding Back to Top During the nineteenth century, chemists arranged the then-known elements according to chemical bonding, recognizing that one group the furthermost right column on the Periodic Table, referred to as the Inert Gases or Noble Gases tended to occur in elemental form in other words, not in a molecule with other elements. It was later determined that this group had outer electron shells containing two as in the case of Helium or eight Neon, Xenon, Radon, Krypton, etc. As a general rule, for the atoms we are likely to encounter in biological systems, atoms tend to gain or lose their outer electrons to achieve a Noble Gas outer electron shell configuration of two or eight electrons. The number of electrons that are gained or lost is characteristic for each element, and ultimately determines the number and types of chemical bonds atoms of that element can form. Atomic diagrams for several atoms are shown in Figure 6. Atomic diagrams illustrating the filling of the outer electron shells. Images from Purves et al. Ionic bonds are formed when atoms become ions by gaining or losing electrons. Chlorine is in a group of elements having seven electrons in their outer shells see Figure 6. Members of this group tend to gain one electron, acquiring a charge of Sodium is in another group with elements having one electron in their outer shells. Ionic bonds generally form between elements in Group I having one electron in their outer shell and Group VIIa having seven electrons in their outer shell. Such bonds are relatively weak, and tend to disassociate in water, producing solutions that have both Na and Cl ions. Formation of a crystal of sodium chloride. Each positively charged sodium ion is surropunded by six negatively charged chloride ions; likewise each negatively charged chloride ion is surrounded by six positively charged sodium ions. The overall effect is electrical neutrality. This image is copyright Dennis Kunkel at www. Covalent bonds form when atoms share electrons. Since electrons move very fast they can be shared, effectively filling or emptying the outer shells of the atoms involved in the bond. Such bonds are referred to as electron-sharing bonds. An analogy can be made to child custody: In a covalent bond, the electron clouds surrounding the atomic nuclei overlap, as shown in Figure 8. Formation of a covalent bond between two Hydrogen atoims. Carbon C is in Group IVa, meaning it has four electrons in its outer shell. Thus to become a "happy atom", Carbon can either gain or lose four electrons. By sharing the electrons with other atoms, Carbon can become a happy atom,. Formation of covalent bonds in methane. Carbon needs to share four electrons, in effect it has four slots. Each hydrogen provides an electron to each of these slots. At the same time each hydrogen needs to fill one slot, which is done by sharing an electron with the carbon. The molecule methane chemical formula CH4 has four covalent bonds, one between Carbon and each of the four Hydrogens. Carbon contributes an electron, and Hydrogen contributes an electron. The sharing of a single electron pair is termed a single bond. When two pairs of electrons are shared, a double bond results, as in carbon dioxide. Triple bonds are known, wherein three pairs six electrons total are shared as in acetylene gas or nitrogen gas. The types of covalent bonds are shown in Figure Ways of representing covalent bonds. Sometimes electrons tend to spend more time with one atom in the bond than with the other. In such cases a polar covalent bond develops. Water H2O is an example. Since the electrons spend so much time with the oxygen oxygen having a greater electronegativity, or electron affinity that end of the molecule acquires a slightly negative charge. Conversely, the loss of the electrons from the hydrogen end leaves a slightly positive charge. The water molecule is thus polar, having positive and negative sides. Hydrogen bonds , as shown in Figure 11, result from the weak electrical attraction between the positive end of one molecule and the negative end of another. Individually these bonds are very weak, although taken in a large enough quantity, the result is strong enough to hold molecules together or in a three-dimensional shape. Formation of a hydrogen bond between the hydrogen side of one water molecule and the oxygen side of another water molecule. Chemical reactions and molecules Back to Top Molecules are compounds in which the elements are in definite, fixed ratios, as seen in Figure Those atoms are held together usually by one of the three types of chemical bonds discussed above. Molecular formulas are an expression in the simplest whole-number terms of the composition of a substance. For example, the sugar glucose has 6 Carbons, 12 hydrogens, and 6 oxygens per repeating structural unit. The formula is written C6H12O6. Determination of molecular weights by addition of the weights of the atoms that make up the molecule. Chemical reactions occur in nature, and some also can be performed in a laboratory setting. One such reaction is diagrammed in Figure Chemical equations are linear representations of how these reactions occur. Combination reactions occur when two separate reactants are bonded together, e. Disassociation reactions occur when a compound is broken into two products, e. Diagram of a chemical reaction: This chemical reaction takes place in a camping stove as well as in certain welding torches. Biological systems, while unique to each species, are based on the chemical bonding properties of carbon. Major organic chemicals those associated with or formed by the actions of living things usually include some ratios of the following elements:

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Chapter 3 : Quantum LEGOâ€"building ultracold molecules

Quantum chemistry studies the ground state of individual atoms and molecules, and the excited states, and transition states that occur during chemical reactions. On the calculations, quantum chemical studies use also semi-empirical and other methods based on quantum mechanical principles, and deal with time dependent problems.

Apr 15 , Apr 16 , Lee Liu and Yu Liu The dipolar molecule holds great promise for quantum computing Researchers from Harvard University have just made a major scientific breakthrough. For the first time, they have created a molecule by combining just two atoms. The result represents a level of precision that has never been achieved before. A molecule is the smallest particle in an element or compound. Usually, molecules are made up of many atoms that are held together by chemical bonds. In the latest work, researchers have used laser and optical tweezers to capture two atoms and merged them to form a single molecule. The new dipolar molecule holds implications for quantum computing as it consists of a new type of qubit, the smallest unit of quantum information and could lead to more efficient devices. We need molecules for all different applications in our daily lives. Researchers used a laser to cool those atoms to over absolute zero, which is an extremely low temperature where new quantum phases beyond liquid, solid and gas emerge. The chemical reaction created a molecule. What we have done differently is to create more control over it. We grabbed two different species of individual atoms with optical tweezers and shine a pulse of the laser to bind them. The whole process is happening in an ultra-high vacuum, with very low air density. These kinds of experiments provide more insight into how molecules interact and how we can control their chemical reaction. The latest experiment is also part of this effort. It created a molecule with just two atoms, though it did not last long. We wanted to take the simplest case, the laws of quantum mechanics, which are the underlying laws of nature. Our quantum pieces will then build up to something more complex; that was the initial motivation. Certainly, the work is not finished, but this is one breakthrough step. Find rare products online! Get the free Tracker App now.

Chapter 4 : Operators, Eigenfunctions, Eigenvalues, and Eigenstates - Chemistry LibreTexts

As a result, the classification based upon the concept of atoms in molecules is freed from its empirical constraints and the full predictive power of quantum mechanics can be incorporated into the resulting theory--a theory of atoms in molecules.

ATOMS The world around you seems to consist of solid material, but if you could look closely enough you would find that "solid" is an illusion. Matter is made up of atoms, tiny little objects made up mostly of space and separated by a lot more space. When atoms were first conceived, they were imagined as tiny versions of our solar system, with an important but relatively tiny star in the middle and a number of even tinier planets circling at set distances. Atoms dont really behave like little solar systems, but the image is good for getting across just how little material and how much space an atom is made up of. Where the image fails is in showing movement: What makes materials solid, liquid, or gas is the freedom of the atoms there: When atoms actually interact, its less like the bumping of balls and more a matter of attraction and repulsion; at atomic levels, mass is much less an important consideration than charges , which are electrical: Much of what atoms and molecules do is based upon their charged particle parts: Most of the terms associated with atoms: Dont confuse this with the nucleus found in the middle of advanced cells - both nuclei are in the middle of something, but there is no comparison beyond that. There are usually two types of particles "glued" together in an atomic nucleus, protons and neutrons. A nucleus with 6 protons would have 6 positive charges. With several same-charged particles jammed into a small space, they really do need to be "glued" there, but how that works is beyond the detail we want to cover here. The number of protons in an atom is also the deciding factor for which element that atom belongs to. Every atom must be a particular element, with an atomic number corresponding to its particular number of protons. The number can change due to certain types of radioactivity, which is one reason why some radioactive elements can change into other elements. It is also the attraction of protons to negatively-charged electrons that hold the electrons in place near the atom. For convenience sake, a proton is given a mass of one Atomic Unit AU. They also are given a mass of 1 AU each, and since electrons are so tiny as to be considered zero AU, the atomic weight of an atom is the total weight of protons plus neutrons. Neutrons provide stability to a nucleus, so there is usually one particular number of neutrons present in stable atoms. However , for most elements, variants can be found with more or fewer neutrons than the most stable form - these would have the same atomic number based on the protons present but different atomic weights protons plus neutrons. These variants are called isotopes, and they can vary greatly in their stability. Unstable nuclei may release radiation in the form of particles, or energy, or both to get more stable - this release is radioactivity. Each has a single negative charge. These orbit distances may be called orbitals where pairs of electrons move or shells where several electrons whiz around a nucleus at roughly the same distance to acknowledge that they really arent like planet orbits. Each electron shell has a particular capacity for electrons: Whether shells are full or not affects another type of atomic stability: An atom that has stabilized by altering its outer shell, that has filled it by adding or emptied it by dumping off electrons, will have an unequal number of negative electrons and positive protons and will carry a charge - these atoms are called ions. Ions can also be produced other ways, and molecules with unbalanced charges can be ions as well. An uncharged number of electrons equals the number of protons atom may have balanced charges, but if its outer shell isnt full it will be chemically unstable. This type of uncharged atom is a radical - in human, free oxygen radicals are released from many processes of cell chemistry and are thought to damage our other molecules over time, producing some aging effects. Only Helium is an exception, in Column 8 where outer shells are full with only 2 valence electrons, the "full" number of the smallest electron shell. This arrangement means that elements in the same column will show similar chemical properties. The rows in the table represent each new orbital, so lower elements have larger atoms than upper ones. This will have some effects on their properties. As size grows, the potential for nuclear instability grows too - some elements way down the table are only found in nature in various radioactive forms, and the very last elements are so unstable that they have only been seen fleetingly in artificial forms generated in laboratories. And in larger atoms, electron shells become more complex, with suborbitals within the main orbitals, producing the "bridge" of the Periodic Table - but that complexity is also beyond the scope of this book. Not a lot of the "main players" in biological chemistry are on the bridge.

Chapter 5 : Online Introduction to Biology - Chemistry - Atoms & Molecules

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June 12, , University of Amsterdam Cooling matter is not easy. Atoms and molecules have the tendency to jump around, to rotate and to vibrate. Freezing these particles by slowing them down is a complicated process. For individual atoms, physicists have figured out over the years how to carry out this cooling process, using techniques like laser cooling, where finely tuned lasers remove energy from the particles. Molecules, on the other hand, are much harder to cool down so that they stand still. These particles consist of two or more atoms that are bound together, and as compound particles they are able to jiggle around in many more ways. First cool, then build Still, physicists would like to have a dense gas of ultracold molecules at their disposal. Since it is not yet possible to directly cool the molecules themselves into this regime, physicists first cool down atoms â€” a process which is much easier â€" and then attempt to build molecules. The answer to this question is a process that exploits a phenomenon known as Feshbach resonance. By applying a magnetic field, the energy of an unbound atom pair can be tuned to exactly the energy of a specific molecular level. Florian Schreck, the research group leader, explains: The group of experimental physicists at the University of Amsterdam, together with theoretical physicists from Nicolaus Copernicus University in Torun, Poland and from Durham University in the UK, have now made an important step towards the creation of a second type of ultracold molecule. These resonances are suitable to construct ultracold rubidium-strontium molecules, particles with very different properties from the ultracold molecules that have been constructed so far. The main challenge in this work was that the usual strong coupling mechanisms that exist between alkali atoms do not exist for alkaline-earth atoms. Eight years ago, theorists Piotr Zuchowski and Jeremy Hutson predicted very weak and unusual coupling mechanisms that would still lead to Feshbach resonances. However, the theory was unable to predict the value of the magnetic fields at which these resonances would occur. Employing precise molecular spectroscopy, the experimental team was now able to find the magnetic field values and to experimentally confirm the existence of the sought-for Feshbach resonances. Interesting applications There are several reasons why physicists are interested in creating different types of ultracold molecules. First of all, a very low temperature allows researchers to study the properties of the molecules themselves better: Precision studies of molecules could uncover fundamental physics going beyond the current standard model of fundamental particle interactions. Secondly, cold molecules can be prepared in very precise states that can then be used for quantum-controlled chemistry: Finally, there are applications to the many-body physics of quantum particles. When molecules are very cold, their quantum fuzziness becomes apparent. Molecules can be at several locations or in several internal states at the same time and the locations or states of several molecules may depend on each other in intricate ways. New quantum phenomena can emerge, which are hard or impossible to describe using even the best supercomputers. By controlling the interactions between the molecules or the potential landscape through which they are moving, physicists hope to learn about these emergent phenomena. Given the number of potential applications that such a gas has, we are very excited about these new possibilities.

Chapter 6 : Quantum chemistry structures and properties of kilo molecules

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Chapter 7 : The SchrÃ¶dinger Equation For Multi-Electron Atoms - Chemistry LibreTexts

So far, only gases of molecules that consist of two alkali atoms, atoms with a single electron that can form chemical bonds, have been created with the desired high density and ultracold temperature.

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Chapter 8 : CHEMISTRY I: ATOMS AND MOLECULES

3 QUANTUM CHEMISTRY â€¢ In principle, solve SchrÃ¶dinger Equation â€¢ Not possible for many-electron atoms or molecules due to many-body problem â€¢ Requires two levels of approximation.

Chapter 9 : Atoms in molecules - Wikipedia

techniques of quantum control to position single atoms and molecules with nanometer control while, at the same time, manipulating their internal quantum states is a novel area of research that can be used to investigate novel techniques of nano-manufacturing at the.