Molecular And Electronic Geometry

The field is often termed simply as "molecular electronics", but this term is also used to refer to the distantly related field of conductive polymers and organic electronics, which uses the properties of molecules to affect the bulk properties of a material. A nomenclature distinction has been suggested so that molecular materials for electronics refers to this latter field of bulk applications, while molecular-scale electronics refers to the nanoscale single-molecule applications treated here. 78d2f35301

Molecular symmetry This involves classifying the states of the molecule using the irreducible representations from the character table of the symmetry group of the molecule. Many university level textbooks on physical chemistry, quantum chemistry, spectroscopy and inorganic chemistry discuss symmetry. Another framework on a larger scale is the use of crystal systems to describe crystallographic symmetry in bulk materials. Molecular symmetry is a fundamental concept in chemistry, as it can be used to predict or explain many of a molecule's chemical properties, such as whether or not it has a dipole moment, as well as its allowed spectroscopic transitions. Molecular symmetry In chemistry, molecular symmetry describes the symmetry present in molecules and the classification of these molecules according to their symmetry. To do this it is necessary to use group theory. chemistry, molecular symmetry describes the symmetry present in molecules and the classification of these molecules according to their symmetry. Symmetry is useful in the study of molecular orbitals, with applications to the Hückel method, to ligand field theory, and to the Woodward–Hoffmann rules 78d2f35301

There are many techniques for determining the symmetry of a given molecule, including X-ray crystallography and various forms of spectroscopy. Spectroscopic notation is based on symmetry considerations.... 78d2f35301 Colour molecular graphics are often used on chemistry journal covers artistically. 78d2f35301

Chemical bonding model structure, molecular geometry, properties, and reactivity of physical matter. This can refer to: VSEPR theory, a model of molecular geometry. Valence bond A chemical bonding model is a theoretical model used to explain atomic bonding structure, molecular geometry, properties, and reactivity of physical matter. This can refer to: 78d2f35301

Molecular Hamiltonian This operator and the associated Schrödinger equation play a central role in computational chemistry and physics for computing properties of molecules and aggregates of molecules, such as thermal conductivity, specific heat,

electrical conductivity, optical, and magnetic properties, and reactivity. In atomic, molecular, and optical physics and quantum chemistry, the molecular Hamiltonian is the Hamiltonian operator representing the energy of the In atomic, molecular, and optical physics and quantum chemistry, the molecular Hamiltonian is the Hamiltonian operator representing the energy of the electrons and nuclei in a molecule 78d2f35301

== Early life and family == 78d2f35301 == History == 78d2f35301 Molecular orbital theory revolutionized the study of chemical bonding by approximating the states of bonded electrons – the molecular orbitals – as linear combinations of atomic orbitals (LCAO). These approximations are made by applying the density functional theory (DFT) or Hartree–Fock (HF) models to the Schrödinger equation. 78d2f35301 Ligand field theory, the application of molecular orbital theory to transition metal complexes. 78d2f35301

Molecular-scale electronics nature of the molecular junction can be ignored, and the current–voltage traits of the device can be calculated using the equilibrium electronic structure Molecular-scale electronics, also called single-molecule electronics, is a branch of nanotechnology that uses single molecules, or nanoscale collections of single molecules, as electronic components. Because single molecules constitute the smallest stable structures imaginable, this miniaturization is the ultimate goal for shrinking electrical circuits 78d2f35301

In the LCAO method, each molecule has... 78d2f35301 Conventional electronics have conventionally been made from bulk materials. Ever since their invention in 1958, the performance and complexity of integrated circuits has undergone exponential growth, a trend named Moore’s law, as feature sizes of the embedded components have shrunk accordingly. As the structures shrink... 78d2f35301

Electronic effect The term polar effect is sometimes used to refer to electronic effects An electronic effect influences the structure, reactivity, or properties of a molecule but is neither a traditional bond nor a steric effect. between the electronic structure and the geometry (stereochemistry) of a molecule. In organic chemistry, the term stereoelectronic effect is also used to emphasize the relation between the electronic structure and the geometry (stereochemistry) of a molecule 78d2f35301

Molecular orbital theory and valence bond theory are the foundational theories of quantum chemistry. 78d2f35301 == Fundamental concepts == 78d2f35301

Molecular orbital theory It was proposed early in the 20th century. The MOT explains the paramagnetic nature of O2, which

valence bond theory cannot explain. It In chemistry, molecular orbital theory (MO theory or MOT) is a method for describing the electronic structure of molecules using quantum mechanics. In chemistry, molecular orbital theory (MO theory or MOT) is a method for describing the electronic structure of molecules using quantum mechanics 78d2f35301

In molecular orbital theory, electrons in a molecule are not assigned to individual chemical bonds between atoms, but are treated as moving under the influence of the atomic nuclei in the whole molecule. Quantum mechanics describes the spatial and energetic properties of electrons as molecular orbitals that surround two or more atoms in a molecule and contain valence electrons between atoms. 78d2f35301

Molecular orbital This function can be used to calculate chemical and physical properties such as the probability of finding an electron in any specific region. Mulliken in 1932 to mean one-electron orbital wave functions. The terms atomic orbital and molecular orbital were introduced by Robert S. Molecular orbitals In chemistry, a molecular orbital is a mathematical function describing the location and wave-like behavior of an electron in a molecule. At an elementary level, they are used to describe the region of space in which a function has a significant amplitude. approximation, and highly accurate descriptions of the molecular electronic wave function do not have orbitals (see configuration interaction) 78d2f35301

Crystal field theory, an electrostatic model for transition metal complexes. 78d2f35301 In an isolated atom, the orbital electrons' location is determined by functions called atomic orbitals. When multiple atoms combine chemically into a molecule by forming a valence chemical bond, the electrons' locations are determined by the molecule as a whole, so the atomic orbitals combine to form molecular orbitals. The electrons from the constituent atoms occupy the molecular orbitals. Mathematically, molecular orbitals are an approximate solution to the Schrödinger equation for the electrons in the field of the molecule's atomic nuclei. They are usually constructed by combining atomic orbitals or hybrid orbitals from each atom of the molecule, or other... 78d2f35301 The term polar effect is sometimes used to refer to electronic effects, but also may have the more narrow definition of effects resulting from non-conjugated substituents. 78d2f35301 Molecular orbital theory, which describes molecular electronic structure with delocalized molecular orbitals. 78d2f35301 == Molecular scale electronics == 78d2f35301

Gerhard Herzberg physicist and physical chemist, who won the Nobel Prize for Chemistry in 1971, "for his contributions to the knowledge of electronic structure and geometry of Gerhard Heinrich Friedrich Otto Julius Herzberg, (German: [ˈgeːɐ̯. haʁt ˈhɛʁt͡sˌbɛʁk] ; December 25, 1904 – March 3, 1999) was a German-Canadian pioneering physicist and physical chemist, who won the Nobel Prize for Chemistry in 1971, "for his contributions to the knowledge of electronic structure and geometry of molecules, particularly free radicals". Herzberg served as Chancellor of Carleton University in Ottawa, Canada from 1973 to

1980. He is well known for using these techniques that determine the structures of diatomic and polyatomic molecules, including free radicals which are difficult to investigate in any other way, and for the chemical analysis of astronomical objects. Herzberg's main work concerned atomic and molecular spectroscopy 78d2f35301

Valence bond theory, which describes molecular electronic structure with localized bonds and lone pairs. 78d2f35301

Molecular graphics model – Type of 3D molecular model Molecular modelling – Discovering chemical properties by physical simulations Molecular geometry – Study of the 3D shapes Molecular graphics is the discipline and philosophy of studying molecules and their properties through graphical representation. Ever since Dalton's atoms and Kekulé's benzene, there has been a rich history of hand-drawn atoms and molecules, and these representations have had an important influence on modern molecular graphics. IUPAC limits the definition to representations on a "graphical display device" 78d2f35301

Molecular electronics It is an interdisciplinary Molecular electronics is the study and application of molecular building blocks for the fabrication of electronic components. It provides a potential means to extend Moore's Law beyond the foreseen limits of small-scale conventional silicon integrated circuits. Molecular electronics is the study and application of molecular building blocks for the fabrication of electronic components. It is an interdisciplinary area that spans physics, chemistry, and materials science 78d2f35301

== Types == 78d2f35301 VSEPR theory, a model of molecular geometry. 78d2f35301 == Linear combination of atomic orbitals (LCAO) method == 78d2f35301 The elementary parts of a molecule are the nuclei, characterized by their atomic numbers, Z, and the electrons, which have negative elementary charge, −e. Their interaction gives a nuclear charge of Z + q, where q = −eN, with N equal to the number of electrons. Electrons and nuclei are, to a very good approximation, point charges and point masses. The molecular Hamiltonian is a sum of several terms: its major terms are the kinetic energies of the electrons and the Coulomb (electrostatic) interactions between the two kinds of charged particles. The Hamiltonian that contains only the kinetic energies of electrons and nuclei, and the Coulomb interactions between them, is known as the Coulomb Hamiltonian.... 78d2f35301

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