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Chemical Informatics in Environmental Chemistry: Towards Sustainable Practices

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Description

In the context of chemistry, the term "models" refers to theoretical frameworks or simplified representations used to describe and understand the behavior of atoms, molecules, and chemical reactions. These models help chemists and scientists visualize and predict the properties and interactions of various chemical systems. Some of the most common models in chemistry include this computational approach uses classical mechanics to model the geometry and energetics of molecules by approximating atoms and bonds as simple spheres and springs.

Molecular Mechanics (MM) is a computational method used to study the structure, energetics, and dynamics of molecules and molecular systems. It is based on classical mechanics principles, where atoms and molecules are treated as simple particles interacting through classical force fields. Molecular mechanics is particularly useful for studying large molecules, such as proteins, nucleic acids, and complex organic molecules, which can be computationally challenging to study using quantum mechanics methods. In molecular mechanics, the interactions between atoms and molecules are described by mathematical functions known as force fields. These force fields define the potential energy of the system as a function of atomic coordinates and include terms for bonded interactions (bonds, angles, dihedrals), non-bonded interactions (van der Waals interactions and electrostatic interactions), and other terms to account for solvent effects or specific interactions. One of the primary applications of molecular mechanics is energy minimization, where the potential energy of the system is minimized by adjusting the atomic coordinates to find the most stable conformation or geometry. Molecular mechanics can also be used for molecular dynamics simulations, where the system's time evolution is followed by numerically solving Newton's equations of motion for each atom. MD simulations provide information about the system's behavior over time and are valuable for studying molecular motion and conformational changes. Molecular mechanics is frequently used to explore the different conformations of a molecule and determine their relative stability. Molecular mechanics is often employed in molecular docking studies to predict the binding mode of a ligand (small molecule) to a receptor or enzyme. Molecular mechanics plays a crucial role in rational drug design by analyzing interactions between drugs and their target molecules, helping to optimize d rug candidates for better binding affinity and selectivity.

Density Functional Theory (DFT)

Density Functional Theory (DFT) is a powerful quantum mechanical method used to study the electronic structure and properties of atoms, molecules, and materials. It is widely employed in various fields of chemistry, physics, materials science, and other related disciplines. DFT was first formulated by Walter Kohn and Pierre Hohenberg in 1964 and later developed by Kohn and Lu Jeu Sham in 1965. In DFT, the central quantity of interest is the electron density, denoted by ρ(r), which represents the distribution of electrons in space. The electron density is a more tractable and physically meaningful quantity compared to the complex wave functions used in traditional quantum mechanics methods. The first Hohenberg-Kohn theorem states that the ground-state electron density uniquely determines the external potential (such as the electrostatic potential due to atomic nuclei) for a given system. The second theorem states that the ground-state energy is a unique functional of the electron density. The Kohn-Sham equations are the central equations of DFT. They are a set of self-consistent equations that involve a set of auxiliary non-interacting electrons moving in an effective potential. These equations mimic the behavior of the interacting electron system while being solvable using standard quantum mechanical techniques. The exchange-correlation functional is a key component of DFT and accounts for the electron-electron interactions that are not explicitly considered in the Kohn-Sham equations. It combines the exchange energy (arising from the Pauli exclusion principle) and the correlation energy (related to electron-electron interactions) into a single functional of the electron density.

Crystal Field Theory (CFT)

Crystal Field Theory (CFT) is a model used in solid-state chemistry and condensed matter physics to explain the electronic structure and properties of transition metal complexes and ions in crystal environments. It provides a qualitative understanding of the interaction between metal ions and the surrounding ligands (ions or molecules) in a crystal lattice. The theory was developed in the 1930’s by physicists Hans Bethe and John Hasbrouck van Vleck.

Crystal field: In a crystal lattice, the metal ion is surrounded by ligands (e.g., water molecules or other ions) that create a crystal field. This crystal field arises due to the electrostatic interactions between the positively charged metal ion and the negatively charged ligands.

Splitting of d orbitals: In free atoms or ions, the five d orbitals (d_{xy}, d_{xz}, d_{yz}, d_{x2-y2}, d_{z2}) are degenerate, meaning they have the same energy. However, when the metal ion is placed in a crystal field, the degeneracy is lifted, and the d orbitals split into different energy levels. The energy difference between these levels determines the absorption of light and influences the magnetic properties of the complex. Ligand Field Ligands approach the central metal ion along the x, y, and z axes, which leads to the repulsion or attraction between the metal ion's d orbitals and the ligand's electrons. Ligands with lone pairs or negative charges tend to cause higher energy repulsion, while ligands with positive charges or no lone pairs lead to weaker repulsion.

Crystal field splitting diagram: The arrangement of the d orbitals' energy levels after the crystal field splits them is represented in a crystal field splitting diagram. Depending on the geometry of the ligand arrangement, different crystal field splitting patterns can arise, such as tetrahedral or octahedral.

Spectrochemical series: The ligands can be ordered in a spectrochemical series based on their strength in causing crystal field splitting. Ligands that cause large energy differences between the d orbitals are called strong-field ligands (e.g., cyanide or ammonia), while those that cause small energy differences are called weak-field ligands (e.g., water or chloride).

Color and magnetism: One of the significant consequences of crystal field theory is the explanation of the color of transition metal complexes. One of the significant consequences of crystal field theory is the explanation of the color of transition metal complexes.