

<<固体量子化学>>

图书基本信息

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内容概要

It is traditional for quantum theory of molecular systems (molecular quantum chemistry) to describe the properties of a many-atom system on the grounds of interatomic interactions applying the linear combination of atomic orbitals (LCAO) approximation in the electronic-structure calculations. The basis of the theory of the electronic structure of solids is the periodicity of the crystalline potential and Bloch-type one-electron states , in the majority of cases approximated by a linear combination of plane waves (LCPW) . In a quantum chemistry of solids the LCAO approach is extended to periodic systems and modified in such a way that the periodicity of the potential is correctly taken into account , but the language traditional for chemistry is used when the interatomic interaction is analyzed to explain the properties of the crystalline solids. At first , the quantum chemistry of solids was considered simply as the energy-band theory or the theory of the chemical bond in tetrahedral semi-conductors . From the beginning of the 1970s the use of powerful computer codes has become a common practice in molecular quantum chemistry to predict many properties of molecules in the first-principles LCAO calculations. In the condensed-matter studies the accurate description of the system at an atomic scale was much less advanced .

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Molecules consist of positively charged nuclei and negatively charged electrons moving around them. If the translations and rotations of a molecule as a whole are excluded, then the motion of the nuclei, except for some special cases, consists of small vibrations about their equilibrium positions. Orthogonal operations (rotations through symmetry axes, reflections in symmetry planes and their combinations) that transform the equilibrium configuration of the nuclei of a molecule into itself are called the symmetry operations of the molecule. They form a group F of molecular symmetry. Molecules represent systems from finite (sometimes very large) numbers of atoms, and their symmetry is described by so-called point groups of symmetry. In a molecule it is always possible to so choose the origin of coordinates that it remains fixed under all operations of symmetry. All the symmetry elements (axes, planes, inversion center) are supposed to intersect in the origin chosen. The point symmetry of a molecule is defined by the symmetry of an arrangement of atoms forming it but the origin of coordinates chosen is not necessarily occupied by an atom. In modern computer codes for quantum-chemical calculations of molecules the point group of symmetry is found automatically when the atomic coordinates are given. In this case, the point group of symmetry is only used for the classification of electronic states of a molecule, particularly for knowledge of the degeneracy of the one-electron energy levels. To make this classification one needs to use tables of irreducible representations of point groups. The latter are given both in books [13-15] and on an Internet site [16].

Calculation of the electronic structure of a crystal (for which a macroscopic sample contains 10^{23} atoms) is practically impossible without the knowledge of at least the translation symmetry group. The latter allows the smallest possible set of atoms included in the so-called primitive unit cell to be considered. However, the classification of the crystalline electron and phonon states requires knowledge of the full symmetry group of a crystal (space group). The structure of their irreducible representations of the space groups is essentially more complicated and use of existing tables [17] or the site [16] requires knowledge of at least the basics of space-group theory.

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