

<<固体量子化学>>

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## &lt;&lt;固体量子化学&gt;&gt;

## 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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## &lt;&lt;固体量子化学&gt;&gt;

## 书籍目录

part i theory

1 introduction

2 space groups and crystalline structures

2.1 translation and point symmetry of crystal&lz

2.1.1 symmetry of molecules and crystals: similarities and differences

2.1.2 translation symmetry of crystals. point symmetry of bravais lattices. crystal class

2.2 space groups

2.2.1 space groups of bravais lattices. symmorphic and nonsymmorphic space groups

2.2.2 three-periodic space groups

2.2.3 site symmetry in crystals. wyckoff positions

2.3 crystalline structures

2.3.1 crystal-structure types. structure information for computer codes

2.3.2 cubic structures: diamond, rocksalt, fluorite, zincblende, cesium chloride, cubic perovskite

2.3.3 tetragonal structures: rutile, anatase and  $\text{LaCuO}_4$

2.3.4 orthorhombic structures:  $\text{LaMnO}_3$  and  $\text{YBa}_2\text{Cu}_3\text{O}_7$

2.3.5 hexagonal and trigonal structures: graphite, wurtzite, corundum and  $\text{ScMnO}_3$

3 symmetry and localization of crystalline orbitals

3.1 translation and space symmetry of crystalline orbitals. bloch functions

3.1.1 symmetry of molecular and crystalline orbitals

3.1.2 irreducible representations of translation group. brillouin zone

3.1.3 stars of wavevectors. little groups. full representations of space groups

3.1.4 small representations of a little group. projective representations of point groups

3.2 site symmetry and induced representations of space groups

3.2.1 induced representations of point groups. localized molecular orbitals

3.2.2 induced representations of space groups in q-basis

3.2.3 induced representations of space groups in k-basis. band representations

3.2.4 simple and composite induced representations

3.2.5 simple induced representations for cubic space groups  $O_h$ , and

3.2.6 symmetry of atomic and crystalline orbitals in  $\text{MgO}$ ,  $\text{Si}$  and  $\text{SrZrO}_3$  crystals

3.3 symmetry of localized crystalline orbitals. wannier functions

## &lt;&lt;固体量子化学&gt;&gt;

- 3.3.1 symmetry of localized orbitals and band representations of space groups
- 3.3.2 localization criteria in wannier-function generation
- 3.3.3 localized orbitals for valence bands: lcao approximation
- 3.3.4 variational method of localized wannier-function generation on the base of bloch functions
- 4 hartree-fock lcao method for periodic systems
- 4.1 one-electron approximation for crystals
  - 4.1.1 one-electron and one-determinant approximations for molecules and crystals
  - 4.1.2 symmetry of the one-electron approximation hamiltonian
  - 4.1.3 restricted and unrestricted hartree-fock lcao methods for molecules
  - 4.1.4 specific features of the hartree-fock method for a cyclic model of a crystal
  - 4.1.5 restricted hartree-fock lcao method for crystals
  - 4.1.6 unrestricted and restricted open-shell hartree-fock methods for crystals
- 4.2 special points of brillouin zone
  - 4.2.1 supercell of three-dimensional bravais lattices
  - 4.2.2 special points of brillouin-zone generating
  - 4.2.3 modification of the monkhorst-pack special-points meshes
- 4.3 density matrix of crystals in the hartree-fock method
  - 4.3.1 properties of the one-electron density matrix of a crystal
  - 4.3.2 the one-electron density matrix of the crystal in the lcao approximation
  - 4.3.3 interpolation procedure for constructing an approximate density matrix for periodic systems
- 5 electron correlations in molecules and crystals
- 5.1 electron correlations in molecules: post-hartree-fock methods
  - 5.1.1 what is the electron correlation ?
  - 5.1.2 configuration interaction and multi-configuration self-consistent field methods
  - 5.1.3 coupled-cluster methods
  - 5.1.4 many-electron perturbation theory
  - 5.1.5 local electron-correlation methods
- 5.2 incremental scheme for local correlation in periodic systems
  - 5.2.1 weak and strong electron-correlation
  - 5.2.2 method of increments: ground state
  - 5.2.3 method of increments: valence-band structure and bandgap
- 5.3 atomic orbital laplace-transformed mp2 theory for periodic

systems

5.3.1 laplace mp2 for periodic systems: unit-cell correlation energy

5.3.2 laplace mp2 for periodic systems: bandgap

5.4 local mp2 electron-correlation method for nonconducting crystals

5.4.1 local mp2 equations for periodic systems

5.4.2 fitted wannier functions for periodic local correlation methods

5.4.3 symmetry exploitation in local mp2 method for periodic systems

6 semiempirical lcao methods for molecules and periodic systems

6.1 extended h/ickel and mulliken-r/idenberg approximations

6.1.1 nonself-consistent extended h/ickel-tight-binding method

6.1.2 iterative mulliken-r/idenberg method for crystals

6.2 zero-differential overlap approximations for molecules and crystals

6.2.1 zero-differential overlap approximations for molecules

6.2.2 complete and intermediate neglect of differential overlap for crystals

6.3 zero-differential overlap approximation in cyclic-cluster model

6.3.1 symmetry of cyclic-cluster model of perfect crystal

6.3.2 semiempirical lcao methods in cyclic-cluster model

6.3.3 implementation of the cyclic-cluster model in msindo and hartree-fock lcao methods

7 kohn-sham lcao method for periodic systems

7.1 foundations of the density-functional theory

7.1.1 the basic formulation of the density-functional theory

7.1.2 the kohn-sham single-particle equations

7.1.3 exchange and correlation functionals in the local density approximation

7.1.4 beyond the local density approximation

7.1.5 the pair density. orbital-dependent exchange-correlation functionals

7.2 density-functional lcao methods for solids

7.2.1 implementation of kohn-sham lcao method in crystals calculations

7.2.2 linear-scaling dft lcao methods for solids

7.2.3 heyd-scnseria-ernzerhof screened coulomb hybrid functional

7.2.4 are molecular exchange-correlation functionals transferable to crystals?

7.2.5 density-functional methods for strongly correlated systems: sic dft and dft+u approaches part ii applications

## &lt;&lt;固体量子化学&gt;&gt;

basis sets and pseudopotentials in periodic lcao calculations

8.1 basis sets in the electron-structure calculations of crystals

8.1.1 plane waves and atomic-like basis sets. slater-type functions

8.1.2 molecular basis sets of gaussian-type functions

8.1.3 molecular basis sets adaptation for periodic systems

8.2 nonrelativistic effective core potentials and valence basis sets

8.2.1 effective core potentials: theoretical grounds

8.2.2 gaussian form of effective core potentials and valence basis sets in periodic lcao calculations

8.2.3 separable embedding potential

8.3 relativistic effective core potentials and valence basis sets

8.3.1 relativistic electronic structure theory: dirac-hartree-fock and dirac-kohn-sham methods for molecules

8.3.2 relativistic effective core potentials

8.3.3 one-center restoration of electronic structure in the core region

8.3.4 basis sets for relativistic calculations of molecules

8.3.5 relativistic lcao methods for periodic systems lcao calculations of perfect-crystal properties

9.1 theoretical analysis of chemical bonding in crystals

9.1.1 local properties of electronic structure in lcao hf and dft methods for crystals and post-hf methods for molecules

9.1.2 chemical bonding in cyclic-cluster model: local properties of composite crystalline oxides

9.1.3 chemical bonding in titanium oxides: periodic and molecular-crystalline approaches

9.1.4 wannier-type atomic functions and chemical bonding in crystals

9.1.5 the localized wannier functions for valence bands: chemical bonding in crystalline oxides

9.1.6 projection technique for population analysis of atomic orbitals. comparison of different methods of the chemical-bonding description in crystals

9.2 electron properties of crystals in lcao methods

9.2.1 one-electron properties: band structure, density of states, electron momentum density

9.2.2 magnetic structure of metal oxides in lcao methods: magnetic phases of lamnos and scmno<sub>3</sub> crystals

9.3 total energy and related observables in lcao methods for solids

9.3.1 equilibrium structure and cohesive energy

9.3.2 bulk modulus, elastic constants and phase stability of solids: lcao ab-initio calculations

## &lt;&lt;固体量子化学&gt;&gt;

9.3.3 lattice dynamics and lcao calculations of vibrational frequencies

10 modeling and lcao calculations of point defects in crystals

10.1 symmetry and models of defective crystals

10.1.1 point defects in solids and their models

10.1.2 symmetry of supercell model of defective crystals

10.1.3 supercell and cyclic-cluster models of neutral and charged point defects

10.1.4 molecular-cluster models of defective solids

10.2 point defects in binary oxides

10.2.1 oxygen interstitials in magnesium oxide: supercell lcao calculations

10.2.2 neutral and charged oxygen vacancy in a1203 crystal: supercell and cyclic-cluster calculations

10.2.3 supercell modeling of metal-doped rutile tio2

10.3 point defects in perovskites

10.3.1 oxygen vacancy in sratio3

10.3.2 supercell model of fe-doped sratio3

10.3.3 modeling of solid solutions of lacsr1-cmno3

11 surface modeling in lcao calculations of metal oxides

11.1 diperiodic space groups and slab models of surfaces

11.1.1 diperiodic ( layer ) space groups

11.1.2 oxide-surface types and stability

11.1.3 single- and periodic-slab models of mgo and tio2 surfaces

11.2 surface lcao calculations on tio2 and sno2

11.2.1 cluster models of ( 110 ) tio2

11.2.2 adsorption of water on the tio2 ( rutile ) ( 110 ) surface: comparison of periodic lcao-pw and embedded-cluster lcao calculations

11.2.3 single-slab lcao calculations of bare and hydroxylated sno2 surfaces

11.3 slab models of sratio3, sratio3 and lamno3 surfaces

11.3.1 hybrid hf-dft comparative study of sratio3 and sratio3 ( 001 ) surface properties

11.3.2 f center on the sratio3 ( 001 ) surface

11.3.3 slab models of lamno3 surfaces

a matrices of the symmetrical supercell transformations of 14 three-dimensional bravais lattices

breciprocal matrices of the symmetric supercell transformations of the three cubic bravais lattices

c computer programs for periodic calculations in basis of localized orbitals

references

index



## 章节摘录

版权页：插图： 2.1 Translation and Point Symmetry of Crystals 2.1.1 Symmetry of Molecules and Crystals: Similarities and Differences

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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