

<<分子和固体中的电子关联>>

图书基本信息

书名：<<分子和固体中的电子关联>>

13位ISBN编号：9787510033049

10位ISBN编号：7510033047

出版时间：2011-4

出版时间：世界图书出版公司

作者：福尔德

页数：480

版权说明：本站所提供下载的PDF图书仅提供预览和简介，请支持正版图书。

更多资源请访问：<http://www.tushu007.com>

<<分子和固体中的电子关联>>

内容概要

《分子和固体中的电子关联(英文版)》用独特的方法讲述分子和固体中的电子关联。分子和固体中的电子关联性为量子化学和固态物理学架起了一座桥梁，书中前半部分新概念的讲述为了很好的处理多体和关联效应，结合标准量子化学方法的映射技巧，格林函数方法和monte-carlo技巧；后半部分讲述了在分子、半导体、过渡金属、重费米体系和高- T_c 超导材料中的应用。

目次：导论；独立电子逼近；密度函数理论；电子相关的量子化学方法；累积量，划分和映射；兴奋状态；有限温度技巧；原子和分子相关；半导体和绝缘体；同质金属系统；过渡金属；强关联电子；重费米体系；超导和高- T_c 材料。

读者对象：物理专业的研究生，教师和材料科学相关的专业人士。

<<分子和固体中的电子关联>>

作者简介

作者：（德国）福尔德（P.Fulde）

<<分子和固体中的电子关联>>

书籍目录

- 1.introduction
- 2.the independent-electron approximation
 - 2.1 starting hamiltonian
 - 2.2 basis functions and basis sets
 - 2.3 self-consistent field approximation
 - 2.4 simplified scf calculational schemes
 - 2.4.1 semi-empirical scf methods
 - 2.4.2 pseudopotentials
 - 2.5 koopmans' theorem
 - 2.6 homogeneous electron gas
 - 2.7 local exchange potential - the xa method
 - 2.8 shortcomings of the independent-electron approximation
 - 2.9 unrestricted scf approximation
- 3.density functional theory
 - 3.1 thomas-fermi method
 - 3.2 hohenberg-kohn-sham theory
 - 3.3 local-density approximation
 - 3.4 results for atoms, molecules, and solids
 - 3.5 extensions and limitations
- 4.quantum-chemical approach to electron correlations
 - 4.1 configuration interactions
 - 4.1.1 local and localized orbitals
 - 4.1.2 selection of double substitutions
 - 4.1.3 multireference ci
 - 4.2 many-body perturbation theory
- 5.cumulants, partitioning, and projections
 - 5.1 cumulant representation
 - 5.1.1 ground-state energy
 - 5.1.2 perturbation expansion
 - 5.2 projection and partitioning techniques
 - 5.2.1 coupled-electron-pair approximations
 - 5.2.2 projections based on local operators
 - 5.2.3 method of increments
 - 5.3 coupled-cluster method
 - 5.4 comparison with various trial wavefunctions
 - 5.5 simplified correlation calculations
- 6.excited states
 - 6.1 ci calculations and basis set requirements
 - 6.2 excitation energies in terms of cumulants
 - 6.3 green's function method
 - 6.3.1 perturbation expansions
 - 6.3.2 the projection method
 - 6.4 local operators
- 7.finite-temperature techniques
 - 7.1 approximations for thermodynamic quantities

<<分子和固体中的电子关联>>

- 7.1.1 temperature green's function
- 7.1.2 the projection method for $t \ll \tau_0$
- 7.2 functional-integral method
 - 7.2.1 static approximation
- 7.3 monte carlo methods
 - 7.3.1 sampling techniques
 - 7.3.2 ground-state energy
- 8.correlations in atoms and molecules
 - 8.1 atoms
 - 8.2 hydrocarbon molecules
 - 8.2.1 analytic expressions for correlation-energy contributions
 - 8.2.2 simplified correlation calculations
 - 8.3 molecules consisting of first-row atoms
 - 8.4 strength of correlations in different bonds
 - 8.5 polymers
 - 8.5.1 polyethylene
 - 8.5.2 polyacetylene
 - 8.6 photoionization spectra
- 9.semiconductors and insulators
 - 9.1 ground-state correlations
 - 9.1.1 semi-empirical correlation calculations
 - 9.1.2 ab initio calculations
 - 9.2 excited states
 - 9.2.1 role of nonlocal exchange
 - 9.2.2 the energy gap problem
 - 9.2.3 hedin's gw approximation
- 10.homogeneous metallic systems
 - 10.1 fermi-liquid approach
 - 10.2 charge screening and the random-phase approximation
 - 10.3 spin fluctuations
- 11.transition metals
 - 11.1 correlated ground state
 - 11.2 excited states
 - 11.3 finite temperatures
 - 11.3.1 single-site approximation
 - 11.3.2 two-sites approximation
 - 11.3.3 beyond the static approximation
- 12.strongly correlated electrons
 - 12.1 molecules
 - 12.2 anderson hamiltonian
 - 12.2.1 calculation of the ground-state energy
 - 12.2.2 excited states
 - 12.2.3 noncrossing approximation
 - 12.3 effective exchange hamiltonian
 - 12.3.1 schrieffer-wolff transformation
 - 12.3.2 kondo divergency

<<分子和固体中的电子关联>>

- 12.3.3 fermi-liquid description
- 12.4 magnetic impurity in a lattice of strongly correlated electrons
- 12.5 hubbard hamiltonian
 - 12.5.1 ground-state: gutzwiller's wavefunction and spin-density wave state
 - 12.5.2 excitation spectrum
 - 12.5.3 the limits of one dimension and infinite dimensions
- 12.6 the t - j model
- 12.7 slave bosons in the mean-field approximation
- 12.8 kanamori's t-matrix approach
- 13.heavy-fermion systems
 - 13.1 the fermi surface and quasiparticle excitations
 - 13.1.1 large versus small fermi surface
 - 13.2 model hamiltonian and slave bosons
 - 13.3 application of the noncrossing approximation
 - 13.4 variational wavefunctions
 - 13.5 quasiparticle interactions
 - 13.6 quasiparticle-phonon interactions based on strong correlations
- 14.superconductivity and the high-te materials
 - 14.1 the superconducting state
 - 14.1.1 pair states
 - 14.1.2 bcs ground state
 - 14.1.3 pair breaking
 - 14.2 electronic properties of the high-tc materials
 - 14.2.1 electronic excitations in the cu-o planes
 - 14.2.2 calculation of the spectral weight by projection techniques
 - 14.2.3 size of the fermi surface
 - 14.3 other properties of the cuprates
 - 14.3.1 loss of antiferromagnetic order
 - 14.3.2 optical conductivity
 - 14.3.3 magnetic response
 - 14.4 heavy fermions in $\text{Nd}_2\text{CeCuO}_4$
- appendix
 - a.relation between $\chi_c(p)$ and the pair distribution function
 - b.derivation of several relations involving cumulants
 - c.projection method of mori and zwanzig
 - d.cross:over from weak to strong correlations
 - e.derivation of a general form for $\chi_c(p)$
 - f.hund's rule correlations
 - g.cumulant representation of expectation values and correlation functions
 - h.diagrammatic representation of certain expectation values
 - i.derivation of the quasiparticle equation
 - j.coherent-potential approximation

<<分子和固体中的电子关联>>

k.derivation of the nca equations

l.ground-state energy of a heisenberg antiferromagnet on a square lattice

m.the lanczos method

references

subject index

<<分子和固体中的电子关联>>

章节摘录

版权页：插图：

<<分子和固体中的电子关联>>

编辑推荐

《分子和固体中的电子关联(英文版)》是由世界图书出版公司出版的。

<<分子和固体中的电子关联>>

版权说明

本站所提供下载的PDF图书仅提供预览和简介，请支持正版图书。

更多资源请访问:<http://www.tushu007.com>