SOLID-STATE SCIENCES

R. A. Evarestov

Quantum Chemistry of Solids

The LCAO First Principles Treatment of Crystals

固体量子化学

Springer

世界图书出版公司
www.wpcbj.com.cn

Robert A. Evarestov

Quantum Chemistry of Solids

The LCAO First Principles Treatment of Crystals

With 78 Figures and 126 Tables

Springer

图书在版编目(CIP)数据

固体量子化学:晶体的原子轨道线性组合第一性原理计算方法 = Quantum Chemistry of Solids:The LCAO First Princip:英文/(俄罗斯)叶瓦列斯托夫著. —影印本. —北京:世界图书出版公司北京公司,2012.1

ISBN 978-7-5100-4284-3

Ⅰ.①固… Ⅱ.①叶… Ⅲ.①固体—量子化学—研究 Ⅳ.①O641.12

中国版本图书馆 CIP 数据核字(2011)第 267579 号

书　　名:	Quantum Chemistry of Solids:The LCAO First Principles Treatment of Crysals
作　　者:	R. A. Evarestov
中 译 名:	固体量子化学
责任编辑:	高蓉　刘慧
出 版 者:	世界图书出版公司北京公司
印 刷 者:	三河市国英印务有限公司
发　　行:	世界图书出版公司北京公司(北京朝内大街 137 号　100010)
联系电话:	010-64021602,010-64015659
电子信箱:	kjb@wpcbj.com.cn
开　　本:	24 开
印　　张:	24
版　　次:	2012 年 03 月
版权登记:	图字:01-2011-2562
书　　号:	978-7-5100-4284-3/O·924　　定　　价: 65.00 元

Springer Series in

SOLID-STATE SCIENCES 153

Springer Series in

SOLID-STATE SCIENCES

The Springer Series in Solid-State Sciences consists of fundamental scientific books prepared by leading researchers in the field. They strive to communicate, in a systematic and comprehensive way, the basic principles as well as new developments in theoretical and experimental solid-state physics.

138 **Phase Separation in Soft Matter Physics**
Micellar Solutions, Microemulsions, Critical Phenomena
By P.K. Khabibullaev and A.A. Saidov

139 **Optical Response of Nanostructures**
Microscopic Nonlocal Theory
By K. Cho

140 **Fractal Concepts in Condensed Matter Physics**
By T. Nakayama and K. Yakubo

141 **Excitons in Low-Dimensional Semiconductors**
Theory, Numerical Methods, Applications By S. Glutsch

142 **Two-Dimensional Coulomb Liquids and Solids**
By Y. Monarkha and K. Kono

143 **X-Ray Multiple-Wave Diffraction**
Theory and Application
By S.-L. Chang

144 **Physics of Transition Metal Oxides**
By S. Maekawa, T. Tohyama, S.E. Barnes, S. Ishihara, W. Koshibae, and G. Khaliullin

145 **Point-Contact Spectroscopy**
By Y.G. Naidyuk and I.K. Yanson

146 **Optics of Semiconductors and Their Nanostructures**
Editors: H. Kalt and M. Hetterich

147 **Electron Scattering in Solid Matter**
A Theoretical and Computational Treatise
By J. Zabloudil, R. Hammerling, L. Szunyogh, and P. Weinberger

148 **Physical Acoustics in the Solid State**
By B. Lüthi

149 **Solitary Waves in Complex Dispersive Media**
Theory · Simulation · Applications
By V.Yu. Belashov and S.V. Vladimirov

150 **Topology in Condensed Matter**
Editor: M.I. Monastyrsky

151 **Particle Penetration and Radiation Effects**
By P. Sigmund

152 **Magnetism**
From Fundamentals to Nanoscale Dynamics
By H.C. Siegmann and J. Stöhr

153 **Quantum Chemistry of Solids**
The LCAO First Principles Treatment of Crystals
By R.A. Evarestov

154 **Low-Dimensional Molecular Metals**
By N. Toyota, M. Lang and J. Müller

Volumes 91–137 are listed at the end of the book.

Professor Dr. Robert A. Evarestov
St. Petersburg State University
Chemistry Department
Stary Peterghof University Prospect 26
198504 St. Petersburg, Russia
E-mail: evarest@hm.csa.ru

Library of Congress Control Number: 2006936622

ISBN 978-3-540-48746-3 Springer Berlin Heidelberg New York

This book is dedicated to my teacher and friend
Professor Marija I. Petrashen

Preface

Nobel Prize Winner Prof. Roald Hoffmann forewarding a recently published book by Dronskowski [1] on computational chemistry of solid-state materials wrote that one is unlikely to understand new materials with novel properties if one is wearing purely chemical or physical blinkers. He prefers a coupled approach – a chemical understanding of bonding merged with a deep physical description. The quantum chemistry of solids can be considered as a realization of such a coupled approach.

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 [2] or the theory of the chemical bond in tetrahedral semiconductors [3]. 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 [4].

During the last 10 years this gap between molecular quantum chemistry and the theory of the crystalline electronic structure has become smaller. The concepts of standard solid-state theory are now compatible with an atomic-scale description of crystals. There are now a number of general-purpose computer codes allowing prediction from the first-principles LCAO calculations of the properties of crystals. These codes are listed in Appendix C. Nowadays, the quantum chemistry of solids can be considered as the original field of solid-state theory that uses the methods of molecular quantum chemistry and molecular models to describe the different properties of solid materials including surface and point-defect modeling.

In this book we have made an attempt to describe the basic theory and practical methods of modern quantum chemistry of solids.

This book would not have appeared without the help of Prof. M. Cardona who supported the idea of its writing and gave me useful advice.

I am grateful to Prof. C. Pisani and members of the Torino group of Theoretical Chemistry, Prof. R. Dovesi, Prof. C. Roetti, for many years of fruitful cooperation. Being a physicist-theoretician by education, I would never have correctly estimated of the role of quantum chemistry approaches to the solids without this cooperation. I am grateful to all my colleagues who took part in our common research (Prof. V. Smirnov, Prof. K. Jug, Prof. T. Bredow, Prof. J. Maier, Prof. E. Kotomin, Prof. Ju. Zhukovskii, Prof. J. Choisnet, Prof. G. Borstel, Prof. F. Illas, Dr. A. Dobrotvorsky, Dr. V. Lovchikov, Dr. V. Veryazov, Dr. I. Tupitsyn, Dr. A. Panin, Dr. A. Bandura, Dr. D. Usvyat, Dr. D. Gryaznov, V. Alexandrov) or sent me the recent results of their research (Prof. C. Pisani, Prof. R. Dovesi, Prof. C. Roetti, Prof. P. Deak, Prof. P. Fulde, Prof. G. Stoll, Prof. M. Schütz, Prof. A. Schluger, Prof. L. Kantorovich, Prof. C. Minot, Prof. G. Scuseria, Prof. R. Dronskowski, Prof. A. Titov). I am grateful to Prof. I. Abarenkov, head of the Prof. M.I. Petrashen named seminar for helpful discussions and friendly support. I would like to express my thanks to the members of the Quantum Chemistry Department of St. Petersburg State University, Dr. A. Panin and Dr. A. Bandura, for help in preparing the manuscript – without their help this book would not be here.

I am especially indebted to Dr. C. Ascheron, Mrs. A. Lahee and Dr. P. Capper of Springer-Verlag for encouragement and cooperation.

St. Petersburg,

Robert Evarestov
August, 2006

Contents

Part I Theory

Part I

Theory