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W. Hergert A. Ernst M. Däne (Eds.)

Computational Materials Science

From Basic Principles to Material Properties

Springer

Editors

Prof. W. Hergert
M. Däne
Martin-Luther-Universität Halle-Wittenberg
Fachbereich Physik, Fachgruppe Theoretische Physik
Von-Seckendorff-Platz 1
06120 Halle, Germany

Dr. A. Ernst
Max Planck Institute for Microstructure Physics
Weinberg 2
06120 Halle, Germany

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Preface

Computational modelling of novel materials is an increasingly powerful tool being used in the development of advanced materials and their device applications. Computational materials science is a relatively new scientific field, in which known concepts and recent advancements in physics, chemistry, mathematics and computer science are combined and applied numerically. The unique advantage of such modelling lies in the possibility to predict macroscopic properties of materials based on calculations of microscopic quantities, i.e., at the atomic level. This has been made possible by the spectacular increase in computational power over recent decades, allowing us to solve numerically and with unprecedented accuracy, fundamental equations at the atomic level. Today, based only on our knowledge of a single atom, we can predict how the material formed by that atom type will look, what properties that material will have and how it will behave under certain conditions. By simply changing the arrangement of constituent atoms, or by adding atoms of a different type, the macroscopic properties of all materials can be modified. It is in this way that one can learn how to improve mechanical, optical and/or electronic properties of known materials, or one can predict properties of new materials, those which are not found in nature but are designed and synthesized in the laboratory. Supercomputers (both vector and parallel) and modern visualization techniques are utilized to generate direct comparisons with experimental conditions, and in some cases experiments may become redundant.

The authors of this book have endeavoured to give an overview of the techniques, which operate at various levels of sophistication to describe microscopic and macroscopic properties of wide range of materials. The most important methods used today in computational physics are addressed and, in general, each topic is illustrated by a number of applications. The book starts with basic aspects of density functional theory and the discussion of modern methods to calculate the electronic structure of materials. A rapidly developing field of scientific interest over the last years is nanophotonics. Two articles discuss how properties of photonic nanostructures can be computed. The main part of the book contains contributions dealing with different aspects of simulation methods. Ab initio calculations of free and supported molecules and clusters are discussed. The application of molecular-dynamics in biology, chemistry and physics is studied. The articles give a representative

cross section of different simulation methods on the one hand and of their application to different materials on the other hand. Essential for the field of the Computational Material Science is the availability of effective algorithms and numerical methods. Therefore multigrid methods and strategies for the implementation of sparse and irregular algorithms are discussed as well.

The editors are grateful to the authors for their valuable contributions to the book. The chapters are based, to some extent, on lectures given at the WE-Heraeus course of the same name as the present book, held from 16th to 27th September 2002 in Halle. We gratefully acknowledge the support of the Wilhelm und Else Heraeus Stiftung.

Halle/Saale,
January 2004

Wolfram Hergert
Arthur Ernst
Markus Däne

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List of Contributors

W.A. Adeagbo
Universität Duisburg-Essen
Institut für Physik,
Theoretische Tieftemperaturphysik
Duisburg Campus, Lotharstraße 1
47048 Duisburg, Germany
adeagbo@thp.uni-duisburg.de

H. Altenbach
Martin-Luther-Universität
Halle-Wittenberg
Fachbereich Ingenieurwissenschaften
06099 Halle, Germany
silvia.runkel@iw.uni-halle.de

J. W. Andzelm
Accelrys Inc.
9685 Scranton Rd
San Diego, CA 92121, USA
jwa@accelrys.com

I.M.L. Billas
Département de Biologie
et de Génomique Structurales,
Institut de Génetique et de Biologie
Moléculaire et Cellulaire,
1 rue Laurent Fries, BP 10142
67404 Illkirch, France
billas@igbmc.u-strasbg.fr

K. Busch
Department of Physics and School
of Optics: CREOL & FPCE,
University of Central Florida,
Orlando, FL 32816, USA
kbusch@physics.ucf.edu

M. Celino
Ente per le Nuove Tecnologie,
l'Energia e l'Ambiente,
C.R. Casaccia, CP 2400
00100 Roma, Italy
and
Istituto Nazionale per la Fisica
della Materia,
Unità di Ricerca Roma1, Italy
Massimo.Celino@casaccia.enea.it

M. Däne
Martin-Luther-Universität
Halle-Wittenberg
Fachbereich Physik,
Fachgruppe Theoretische Physik
Von-Seckendorff-Platz 1
06120 Halle, Germany
daene@physik.uni-halle.de

P. Entel
Universität Duisburg-Essen
Institut für Physik,
Theoretische Tieftemperaturphysik
Duisburg Campus, Lotharstraße 1
47048 Duisburg, Germany
entel@thp.uni-duisburg.de

A. Ernst
Max Planck Institute
of Microstructure Physics
Weinberg 2
06120 Halle, Germany
aernst@mpi-halle.mpg.de

H. Eschrig
Leibniz Institute for Solide State and Materials Research Dresden
PF 27 01 16
01171 Dresden, Germany
h.eschrig@ifw-dresden.de

G. Fitzgerald
Accelrys Inc.
9685 Scranton Rd
San Diego, CA 92121, USA
gxf@accelrys.com

G. Goldbeck-Wood
Accelrys Inc
334 Science Park
Cambridge CB4 0WN, UK
Goldbeck-Wood@accelrys.com

N. Govind
Accelrys Inc.
9685 Scranton Rd
San Diego, CA 92121, USA
nxg@accelrys.com

M.E. Grillo
Accelrys, GmbH
Inselkammerstr. 1
82008 Unterhaching, Germany
mariag@accelrys.com

F. Hagmann
Institut für Theorie der Kondensierten Materie,
Universität Karlsruhe
76128 Karlsruhe, Germany
hagmann@
tkm.physik.uni-karlsruhe.de

J. Hamm
Advanced Technology Institute
School of Electronics
and Physical Sciences
University of Surrey
GU2 7XH, UK
j.hamm@surrey.ac.uk

W. Hergert
Martin-Luther-Universität
Halle-Wittenberg
Fachbereich Physik, Fachgruppe
Theoretische Physik
Von-Seckendorff-Platz 1
06120 Halle, Germany
hergert@physik.uni-halle.de

D. Hermann
Institut für Theorie
der Kondensierten Materie,
Universität Karlsruhe
76128 Karlsruhe, Germany
hermann@
tkm.physik.uni-karlsruhe.de

O. Hess
Advanced Technology Institute
School of Electronics and Physical Sciences
University of Surrey
GU2 7XH, UK
o.hess@surrey.ac.uk

K. Kadau
Universität Duisburg-Essen
Institut für Physik,
Theoretische Tieftemperaturphysik
Duisburg Campus, Lotharstraße 1
47048 Duisburg, Germany
kadau@comphys.uni-duisburg.de

A. Klaedtke
Advanced Technology Institute
School of Electronics
and Physical Sciences
University of Surrey
GU2 7XH, UK
a.klaedtke@surrey.ac.uk

D. Ködderitzsch
Martin-Luther-Universität
Halle-Wittenberg
Fachbereich Physik, Fachgruppe
Theoretische Physik
Von-Seckendorff-Platz 1
06120 Halle, Germany
d.koedderitzsch@
physik.uni-halle.de

M. Kreth
Universität Duisburg-Essen
Institut für Physik,
Theoretische Tieftemperaturphysik
Duisburg Campus, Lotharstraße 1
47048 Duisburg, Germany
magnus@thp.uni-duisburg.de

M. Lüders
Daresbury Laboratory,
Daresbury, Warrington,
Cheshire, WA4 4AD, UK
m.lueders@dl.ac.uk

C. Massobrio
Institut de Physique et Chimie
des Matériaux de Strasbourg
23 Rue du Loess BP 43
67034 Strasbourg Cedex 2, France
Carlo.Massobrio@
ipcms.u-strasbg.fr

S. McGrother
Accelrys Inc.
9685 Scranton Rd
San Diego, CA 92121, USA
smcgrother@accelrys.com

S.F. Mingaleev
Institut für Theorie
der Kondensierten Materie,
Universität Karlsruhe
76128 Karlsruhe, Germany
smino@
tkm.physik.uni-karlsruhe.de

Y. Pouillon
Ente per le Nuove Tecnologie,
l'Energia e l'Ambiente,
C.R. Casaccia, CP 2400
00100 Roma, Italy
and
Istituto Nazionale per la Fisica
della Materia,
Unità di Ricerca Roma1, Italy
pouillon@pcpm.ucl.ac.be

T. Rauber
Universität Bayreuth
Fakultät für Mathematik und Physik
95440 Bayreuth, Germany
rauber@uni-bayreuth.de

G. Rollmann
Universität Duisburg-Essen
Institut für Physik,
Theoretische Tieftemperaturphysik
Duisburg Campus, Lotharstraße 1
47048 Duisburg, Germany
georg@thp.uni-duisburg.de

G. Rünger
Technische Universität Chemnitz
Fakultät für Informatik
Professur Praktische Informatik
Straße der Nationen 62
09107 Chemnitz, Germany
ruenger@
informatik.tu-chemnitz.de

M. Schillinger
Institut für Theorie
der Kondensierten Materie,
Universität Karlsruhe
76128 Karlsruhe, Germany
matthias@
tkm.physik.uni-karlsruhe.de

K.B. Stark
Accelrys Inc.
9685 Scranton Rd
San Diego, CA 92121, USA
kstark@accelrys.com

V. Stepanyuk
Max Planck Institute
of Microstructure Physics
Weinberg 2
06120 Halle, Germany
stepanyu@mpi-halle.de

M. Sugihara
Universität Duisburg-Essen
Institut für Physik,
Theoretische Tieftemperaturphysik
Duisburg Campus, Lotharstraße 1
47048 Duisburg, Germany
minoru@thp.uni-duisburg.de

G. Wittum
Interdisziplinäres Zentrum für
Wissenschaftliches Rechnen (IWR)
Simulation in Technology Center
Im Neuenheimer Feld 368
69120 Heidelberg, Germany
wittum@iwr.uni-Heidelberg.de

A.T. Zayak
Universität Duisburg-Essen
Institut für Physik,
Theoretische Tieftemperaturphysik
Duisburg Campus, Lotharstraße 1
47048 Duisburg, Germany
alexei@thp.uni-duisburg.de