

Hugues Dreyssé (Ed.)

Electronic Structure and Physical Properties of Solids

The Uses of the LMTO Method

Lectures of a Workshop Held at Mont Saint Odile,
France, October 2–5, 1998



Springer

Contents

Part I Ground and Excited-State Formalisms	
--	--

Developing the MTO Formalism	
<i>O. K. Andersen, T. Saha-Dasgupta, R. W. Tank, C. Arcangeli, O. Jepsen, G. Krier</i>	3
From ASA Towards the Full Potential	
<i>J. Kollár, L. Vitos, H. L. Skriver</i>	85
A Full-Potential LMTO Method	
Based on Smooth Hankel Functions	
<i>M. Methfessel, M. van Schilfgaarde, R. A. Casali</i>	114
Full-Potential LMTO	
Total Energy and Force Calculations	
<i>J. M. Wills, O. Eriksson, M. Alouani, D. L. Price</i>	148
Excited States Calculated by Means of the LMTO Method	
<i>M. Alouani, J. M. Wills</i>	168

Part II Magnetic Properties	
---------------------------------------	--

Fully Relativistic Band Structure Calculations	
for Magnetic Solids – Formalism and Application	
<i>H. Ebert</i>	191
First Principles Theory of Magneto–Crystalline Anisotropy	
<i>O. Eriksson, J. Wills</i>	247
On the Implementation of the Self-Interaction Corrected Local	
Spin Density Approximation for d- and f-Electron Systems	
<i>W. M. Temmerman, A. Svane, Z. Szotek, H. Winter, S. V. Beiden</i>	286
Ab Initio Theory of the Interlayer Exchange Coupling	
<i>J. Kudrnovský, V. Drchal, I. Turek, P. Bruno, P. Dederichs, P. Weinberger</i>	313

Part III Disordered Alloys

Disordered Alloys and Their Surfaces:

The Coherent Potential Approximation

I. Turek, J. Kudrnovský, V. Drchal 349

Locally Self-Consistent Green's Function

Method and Its Application in Theory of Random Alloys

I. A. Abrikosov, P. A. Korzhavyi, B. Johansson 379

Part IV Large-Scale Real-Space Calculations

Sparse Direct Methods: An Introduction

J. A. Scott 401

Real-Space Tight-Binding Approach to Magnetic Anisotropy:

Application to Nickel Films on Copper

D. Spišák and J. Hafner 416

Combining Real Space and Tight Binding

Methods for Studying Large Metallic Systems

C. Cornea and D. Stoeffler 434