

---

# Contents

---

## Part I Formalisms

---

<b>1</b>	<b>Introductory Information</b> . . . . .	3
1.1	Objectives and What You Will Learn from Reading This Book	3
1.2	On Units . . . . .	4
1.3	Obtaining RSPt and the RSPt Web Site . . . . .	4
1.4	A Short Comment on the History of Linear Muffin-Tin Orbitals and RSPt . . . . .	4
<b>2</b>	<b>Density Functional Theory and the Kohn–Sham Equation</b> .	7
2.1	The Many-Particle Problem . . . . .	8
2.2	Early Attempts to Solve the Many-Particle Problem . . . . .	10
2.2.1	Free Electron Model . . . . .	10
2.2.2	The Hartree and Hartree–Fock Approaches . . . . .	10
2.2.3	Thomas–Fermi Theory . . . . .	11
2.3	Density Functional Theory . . . . .	12
2.3.1	Hohenberg–Kohn Theory . . . . .	12
2.3.2	The Kohn–Sham Equation . . . . .	14
2.3.3	Approximations to $E_{xc}[n]$ . . . . .	16
<b>3</b>	<b>Consequences of Infinite Crystals and Symmetries</b> . . . . .	21
<b>4</b>	<b>Introduction to Electronic Structure Theory</b> . . . . .	25
4.1	Born–Oppenheimer Approximation and One-Electron Theory .	25
4.2	Born–von Karman Boundary Condition and Bloch Waves . . . .	25
4.3	Energy Bands and the Fermi Level . . . . .	26
4.4	Different Types of k-Space Integration . . . . .	27
4.5	Self-Consistent Fields . . . . .	31
4.6	Rayleigh–Ritz Variational Procedure . . . . .	33

<b>5</b>	<b>Linear Muffin-Tin Orbital Method in the Atomic Sphere Approximation</b>	35
5.1	Muffin-Tin Methods	35
5.1.1	The Korringa, Kohn, and Rostoker (KKR) Method	36
5.1.2	The KKR-ASA Method	39
5.1.3	The LMTO-ASA Method	40
5.1.4	Matrix Elements of the Hamiltonian	42
5.1.5	Logarithmic Derivatives and Choice of the Linearization Energies	44
5.1.6	Advantages of LMTO-ASA Method	45
<b>6</b>	<b>The Full-Potential Electronic Structure Problem and RSPt</b>	47
6.1	General Aspects	47
6.1.1	Notation	47
6.1.2	Dividing Space: The Muffin-Tin Geometry	49
6.1.3	A Note on the Language of FPLMTO Methods	49
6.2	Symmetric Functions in RSPt	50
6.2.1	The Fourier Grid for Symmetric Functions in RSPt	52
6.3	Basis Functions	52
6.3.1	Muffin-Tin Orbitals	52
6.3.2	FP-LMTO Basis Functions	53
6.3.3	Choosing a Basis Set	58
6.3.4	Choosing Basis Parameters	58
6.4	Matrix Elements	62
6.4.1	Muffin-Tin Matrix Elements	62
6.4.2	Interstitial Matrix Elements	63
6.5	Charge Density	66
6.6	Core States	67
6.7	Potential	67
6.7.1	Coulomb Potential	67
6.7.2	Density Gradients	69
6.8	All-Electron Force Calculations	69
6.8.1	Symmetry	69
6.8.2	Hellmann–Feynman and Incomplete Basis Set Contributions	70
<b>7</b>	<b>Dynamical Mean Field Theory</b>	75
7.1	Strong Correlations	75
7.2	LDA/GGA+DMFT Method	76
7.2.1	LDA/GGA+U Hamiltonian	77
7.2.2	LDA/GGA+DMFT Equations	78
7.3	Implementation	80
7.3.1	Using the LMTO Basis Set	81
7.3.2	Correlated Orbitals	82
7.3.3	Other Technical Details	82

7.4	Examples . . . . .	83
7.4.1	Body-Centered Cubic Iron . . . . .	83
7.4.2	Systems Close to Localization, the Hubbard-I Approximation . . . . .	85
<b>8</b>	<b>Implementation . . . . .</b>	<b>89</b>
8.1	Fortran-C Interface . . . . .	89
8.2	Diagonalization . . . . .	90
8.3	Fast Fourier Transforms . . . . .	91
8.4	Parallelization . . . . .	92
<b>9</b>	<b>Obtaining RSPt from the Web . . . . .</b>	<b>95</b>
9.1	Installing RSPt . . . . .	95
9.2	Running RSPt . . . . .	96

---

## Part II Applications

---

<b>10</b>	<b>Total Energy and Forces: Some Numerical Examples . . . . .</b>	<b>101</b>
10.1	Equation of State . . . . .	101
10.1.1	Convergence . . . . .	105
10.2	Phonon Calculations . . . . .	106
<b>11</b>	<b>Chemical Bonding of Solids . . . . .</b>	<b>111</b>
11.1	Electron Densities . . . . .	112
11.2	Crystal Orbital Overlap Population (COOP) . . . . .	112
11.3	Equilibrium Volumes of Materials . . . . .	115
11.3.1	Transition Metals . . . . .	116
11.3.2	Lanthanides and Actinides . . . . .	117
11.3.3	Compounds . . . . .	120
11.4	Cohesive Energy . . . . .	121
11.5	Structural Stability and Pressure-Induced Phase Transitions . . . . .	122
11.5.1	An sp-Bonded Material, Ca . . . . .	122
11.5.2	Transition Metals . . . . .	124
11.5.3	Systems with f-Electrons . . . . .	125
11.6	Valence Configuration of f-Elements . . . . .	126
11.7	Elastic Constants . . . . .	128
<b>12</b>	<b>Magnetism . . . . .</b>	<b>133</b>
12.1	Spin and Orbital Moments of Itinerant Electron Systems . . . . .	134
12.1.1	Symmetry Aspects of Relativistic Spin-Polarized Calculations . . . . .	136
12.1.2	Elements and Compounds . . . . .	136
12.1.3	Surfaces . . . . .	138
12.2	Magnetic Anisotropy Energy . . . . .	139

12.2.1	k-Space Convergence	140
12.2.2	MAE of hcp Gd	141
12.3	Magnetism of Nano-objects	142
<b>13</b>	<b>Excited State Properties</b>	<b>145</b>
13.1	Phenomenology	145
13.1.1	Index of Refraction and Attenuation Coefficient	148
13.1.2	Reflectivity	148
13.1.3	Absorption Coefficient	149
13.1.4	Energy Loss	149
13.1.5	Faraday Effect	149
13.1.6	Magneto-optical Kerr Effect	150
13.2	Excited States with DFT: A Contradiction in Terms?	151
13.3	Quasiparticle Theory versus the Local Density Approximation	152
13.4	Calculation of the Dielectric Function	154
13.4.1	Dynamical Dielectric Function	154
13.4.2	Momentum Matrix Elements	156
13.4.3	Velocity Operator and Sum Rules	158
13.5	Optical Properties of Semiconductors	159
13.6	Optical Properties of Metals	162
13.7	Magneto-optical Properties	164
13.8	X-Ray Absorption and X-Ray Magnetic Circular Dichroism	166
13.8.1	The XMCD Formalism	167
13.8.2	The XMCD Sum Rules	170
<b>14</b>	<b>A Database of Electronic Structures</b>	<b>179</b>
14.1	Database Generation	179
14.2	Data-Mining: An Example from Scintillating Materials	180
<b>15</b>	<b>Future Developments and Outlook</b>	<b>183</b>
	<b>References</b>	<b>187</b>
	<b>Index</b>	<b>195</b>



<http://www.springer.com/978-3-642-15143-9>

Full-Potential Electronic Structure Method  
Energy and Force Calculations with Density Functional  
and Dynamical Mean Field Theory

Wills, J.M.; Alouani, M.; Andersson, P.; Delin, A.;

Eriksson, O.; Grechnev, O.

2010, XII, 200 p., Hardcover

ISBN: 978-3-642-15143-9