

Contents

Preface *IX*

List of Contributors *XI*

Colour Plates *XV (after page 154)*

1	The Electronic Structure of Solids	<i>1</i>
	<i>Uwe Bovensiepen, Silke Biermann, and Luca Perfetti</i>	
1.1	Single-Electron Approximation	<i>2</i>
1.1.1	The Drude Model of the Free Electron Gas	<i>2</i>
1.1.2	The Electronic Band Structure: Metals, Insulators, and Semiconductors	<i>4</i>
1.2	From Bloch Theory to Band Structure Calculations	<i>6</i>
1.2.1	Bloch Theory	<i>6</i>
1.2.2	The Tight Binding Approach to the Solid	<i>7</i>
1.2.3	Band Structure Calculations	<i>8</i>
1.3	Beyond the Band Picture	<i>8</i>
1.3.1	Mott's Hydrogen Solid	<i>9</i>
1.3.2	Mott Insulators in Nature	<i>10</i>
1.4	Electronic Structure of Correlated Materials	<i>14</i>
1.4.1	The Hubbard Model	<i>14</i>
1.4.2	Dynamical Mean Field Theory	<i>16</i>
1.4.3	Electronic Structure Calculations	<i>17</i>
1.4.4	Ordered States	<i>18</i>
1.4.5	Cooperation Between Lattice Instabilities and Electronic Correlations: The Example of Vanadium Dioxide	<i>21</i>
	References	<i>23</i>
2	Quasi-Particles and Collective Excitations	<i>27</i>
	<i>Evgueni V. Chulkov, Irina Sklyadneva, Mackillo Kira, Stephan W. Koch, Jose M. Pitarke, Leonid M. Sandratskii, Paweł Buczek, Kunie Ishioka, Jörg Schäfer, and Martin Weinelt</i>	
2.1	Introduction	<i>27</i>
2.2	Quasi-Particles	<i>30</i>
2.2.1	Electrons and Holes	<i>30</i>

2.2.2	Phonons	31
2.2.2.1	Adiabatic Approximation	31
2.2.2.2	Harmonic Approximation	31
2.2.2.3	Lattice Dynamics	32
2.2.2.4	Phonons at Surfaces	33
2.2.3	Electron–Phonon Coupling in Metals	34
2.2.4	Excitons: Electron–Hole Pairs in Semiconductor Quantum Wells	38
2.2.4.1	Microscopic Theory	39
2.2.4.2	Excitonic Resonances and Populations	41
2.2.4.3	Terahertz Spectroscopy of Exciton Populations	43
2.2.4.4	Excitonic Signatures in the Photoluminescence	44
2.2.5	Polarons: Electron–Phonon Coupling in Polar and Ionic Solids	46
2.3	Collective Excitations	49
2.3.1	Plasmons: Electron Density Oscillations	49
2.3.1.1	Surface Plasmons	51
2.3.1.2	Acoustic Surface Plasmons	52
2.3.2	Magnons: Elementary Excitations in Ferromagnetic Materials	53
2.3.2.1	Spin Waves in the Heisenberg Model	54
2.3.2.2	Itinerant Electrons	57
2.3.2.3	Conclusions	64
2.4	Experimental Access to Quasi-Particle and Collective Excitations	65
2.4.1	Coherent Phonons	65
2.4.1.1	Coherent Optical Phonons	65
2.4.1.2	Coherent Acoustic Phonons	74
2.4.2	High-Resolution Angle-Resolved Photoemission	78
2.4.2.1	Photoemission Spectral Function of Quasi-Particles	78
2.4.2.2	Experimental Considerations for Photoelectron Spectroscopy	80
2.4.2.3	Quasi-Particles from Electron–Phonon Interaction	81
2.4.2.4	Quasi-Particles from Electron–Magnon Interaction	82
2.4.2.5	Conclusions and Implications	88
2.4.3	Time-Resolved Photoelectron Spectroscopy	89
2.4.3.1	Experiment	89
2.4.3.2	Electron Lifetimes	91
2.4.3.3	Electron–Phonon Coupling	94
2.4.3.4	Surface Exciton Formation	97
2.4.3.5	Magnon Emission	101
2.4.3.6	Magnon–Phonon Interaction	103
2.5	Summary	105
	References	106
3	Surface States and Adsorbate-Induced Electronic Structure	115
	<i>Thomas Fauster, Hrvoje Petek, and Martin Wolf</i>	
3.1	Intrinsic Surface States	115
3.1.1	Basic Concepts of Surface States	115
3.1.2	Scattering Model of Surface States	116

3.2	Crystal-Induced Surface States	119
3.2.1	Tamm and Shockley Surface States	119
3.2.2	Dangling Bond States	120
3.3	Barrier-Induced Surface States	121
3.3.1	Image Potential States	121
3.3.2	Quantum Well States	124
3.4	Experimental Methods	125
3.4.1	Photoemission	125
3.4.2	Two-Photon Photoemission	128
3.4.3	Scanning Tunneling Methods	133
3.5	Adsorbate-Induced Electronic Structure	135
3.5.1	Bonding at Surfaces	135
3.5.2	Energy-Level Alignment: Alkali–Metal Interfaces as a Model System	138
3.5.3	Electronic Band Structure: Chemisorbed and Physisorbed Adsorbates	147
	References	151
4	Basic Theory of Heterogeneous Electron Transfer	155
	<i>Daniel Sanchez-Portal, Julia Stähler, and Xiaoyang Zhu</i>	
4.1	Resonant Charge Transfer in Chemisorbed Systems	155
4.1.1	Anderson–Grimley–Newns Hamiltonian	156
4.1.2	Main Factors that Determine RCT Decay Rates	158
4.1.3	Theoretical Approaches to Calculate RCT Rates in Realistic Systems	161
4.1.4	Effect of the Adsorbate Motion	163
4.2	Electron Transfer in the Presence of Polar/Polarizable Media	166
4.2.1	Nonadiabatic (Outer Sphere) Electron Transfer	167
4.2.1.1	Continuum of Accepting States	169
4.2.2	Adiabicity and the Effect of Strong Electronic Coupling	170
4.2.3	Intermediate Coupling and the Impact of Solvent Relaxation	171
4.2.3.1	Classical Description and a Wide Band Acceptor	174
4.3	Transient Electronic Coupling: Crossover between Limiting Cases	174
4.4	Conclusions	177
	References	178
5	Electromagnetic Interactions with Solids	181
	<i>Ricardo Díez Muñoz, Eugene E. Krasovskii, Wolfgang Schattke, Christoph Lienau, and Hrvoje Petek</i>	
5.1	Dielectric Function of Metals	182
5.1.1	Calculations of Dielectric Functions	183
5.2	Band Mapping of Solids by Photoemission Spectroscopy	186
5.2.1	Nonlinear Photoemission as a Band Mapping Tool for Unoccupied States	189
5.3	Optical Excitations in Metals	191

5.3.1	Optical Response of Noble Metals	193
5.3.2	Interband Absorption	195
5.3.3	Intraband Absorption	197
5.3.4	Extended Drude Model	199
5.3.5	Frequency-Dependent Scattering Rate	201
5.3.6	Surface Absorption	204
5.3.7	Summary	206
5.4	Plasmonic Excitations at Surfaces and Nanostructures	206
5.4.1	Drude Model for Optical Conductivity	207
5.4.2	Interaction of Light with a Planar Metallic Surface	208
5.4.3	Surface Plasmon Polariton Fields	210
5.4.3.1	Planar Interfaces	210
5.4.4	Surface Plasmons in Nanostructured Metal Films	215
5.4.4.1	Spherical Nanoparticles	215
5.4.4.2	Elliptical Nanoparticles	219
5.4.4.3	Diffraction Gratings	220
5.4.4.4	Adiabatic Metallic Tapers	224
5.4.5	Exciton–Plasmon Coupling	227
5.4.6	Summary	230
	References	231

Index 239