

# Contents

<b>1. Introduction .....</b>	<b>1</b>
<b>2. Theoretical Concepts and Methods .....</b>	<b>4</b>
2.1 The One-Electron Model and Band Structure .....	7
2.2 Properties of $E_n(\mathbf{k})$ .....	11
<b>3. Pseudopotentials .....</b>	<b>16</b>
3.1 The Empirical Pseudopotential Method .....	20
3.2 Self-Consistent and Ab Initio Pseudopotentials .....	25
<b>4. Response Functions and Density of States .....</b>	<b>30</b>
4.1 Charge Density and Bonding .....	38
<b>5. Low Energy Probes of Semiconductors .....</b>	<b>43</b>
5.1 Band Gap Measurements .....	43
5.2 Excitonic Effects Near Band Edges .....	45
5.3 Cyclotron Resonance .....	47
5.4 Doping Effects in Semiconductors .....	49
<b>6. Optical and Electronic Spectra of Semiconductors .....</b>	<b>51</b>
6.1 Modulation Spectroscopy .....	51
6.1.1 Wavelength Modulation .....	53
6.1.2 Temperature Modulation .....	54
6.1.3 Stress Modulation .....	56
6.1.4 Electric Field Modulation .....	57
6.1.5 Other Modulation Methods .....	59
6.2 High Energy Reflectivity Measurements .....	60
6.3 Photoemission Spectra of Semiconductors .....	61
6.3.1 X-Ray Photoemission Spectroscopy (XPS) and Ultraviolet Photoemission Spectroscopy (UPS) .....	64
6.3.2 Constant Final State and Constant Initial State Spectroscopies .....	66
6.3.3 Angle-Resolved Photoemission Spectroscopy .....	67
6.3.4 Photoelectron Yield Spectroscopy .....	69
6.4 Electron Energy Loss Spectroscopy for Semiconductors .....	69
6.4.1 Plasmon Excitations in Solids .....	70
6.4.2 Experimental Measurements and Results .....	71

<b>7. High Energy Probes of Semiconductors: X-Rays .....</b>	<b>73</b>
7.1 Crystal Structure Determinations .....	73
7.2 Charge Density Determinations Using X-Rays .....	74
7.3 Temperature Dependence of X-Ray Reflections .....	76
<b>8. Diamond and Zinc-Blende Structure Semiconductors ..</b>	<b>79</b>
8.1 Crystal Structure .....	79
8.2 The Electronic Structure of Silicon .....	80
8.3 The Electronic Structure of Germanium .....	92
8.4 The Electronic Structure of Gray Tin .....	98
8.5 Zinc-Blende Structure Semiconductors .....	101
8.6 The Electronic Structure of Gallium Arsenide .....	102
8.7 The Electronic Structure of Zinc Selenide .....	112
8.8 The Electronic Structure of Other III-V and II-VI Semiconductors .....	117
<b>9. Wurtzite Structure Semiconductors .....</b>	<b>140</b>
9.1 The Electronic Structure of Hexagonal Zinc Sulfide .....	144
9.2 The Electronic Structure of Hexagonal CdS and CdSe .....	154
9.3 The Electronic Structure of Hexagonal ZnO .....	157
<b>10. Chalcopyrite Structure Semiconductors .....</b>	<b>161</b>
<b>11. IV-VI Semiconductors .....</b>	<b>172</b>
11.1 Electronic Band Structure .....	173
11.2 Applications of the Electronic Band Structure .....	182
<b>12. Triatomic, Layer, Chain, and Amorphous Models .....</b>	<b>189</b>
<b>References .....</b>	<b>205</b>

<b>Bibliography: Electronic Structure and Optical Properties of Semiconductors .....</b>	<b>213</b>
<b>B.1 Properties of Semiconductors .....</b>	<b>213</b>
B.1.1 Charge Densities in Semiconductors .....	213
B.1.2 Chemical Trends and Bonding in Semiconductors .....	213
B.1.3 Compilation of Properties of Semiconductors .....	214
B.1.4 Electronic Structure of Semiconductors .....	215
B.1.5 Lattice Forces and Dynamics .....	216
B.1.6 Optical and Dielectric Properties of Solids .....	217
B.1.7 Photoemission and Electron Spectroscopies .....	220
B.1.8 Temperature and Pressure Effects in Semiconductors ...	221

B.2 General Semiconductor Articles .....	222
B.2.1 II-VI Semiconductors .....	222
B.2.2 III-V Semiconductors .....	223
B.2.3 IV-IV Semiconductors .....	225
B.2.4 IV-VI Semiconductors .....	226
B.3 Chalcopyrite Semiconductors .....	227
B.4 Properties of Specific Semiconductors .....	227
B.4.1 Aluminum Antimonide .....	227
B.4.2 Beryllium Oxide .....	228
B.4.3 Bismuth Triiodide .....	228
B.4.4 Cadmium Germanium Arsenide .....	228
B.4.5 Cadmium Oxide .....	228
B.4.6 Cadmium Selenide .....	228
B.4.7 Cadmium Sulphide .....	229
B.4.8 Cadmium Telluride .....	230
B.4.9 Carbon .....	231
B.4.10 Copper Bromide .....	232
B.4.11 Copper Chloride .....	232
B.4.12 Copper Iodide .....	232
B.4.13 Gallium Antimonide .....	233
B.4.14 Gallium Arsenide .....	234
B.4.15 Gallium Phosphide .....	237
B.4.16 Gallium Selenide .....	239
B.4.17 Gallium Sulphide .....	239
B.4.18 Gallium Telluride .....	240
B.4.19 Germanium .....	240
B.4.20 Germanium Telluride .....	243
B.4.21 Indium Antimonide .....	244
B.4.22 Indium Arsenide .....	245
B.4.23 Indium Phosphide .....	245
B.4.24 Lead Diiodide .....	246
B.4.25 Lead Selenide .....	246
B.4.26 Lead Sulphide .....	247
B.4.27 Lead Telluride .....	247
B.4.28 Magnesium Oxide .....	248
B.4.29 Magnesium Silicide .....	248
B.4.30 Mercury Selenide .....	248
B.4.31 Mercury Sulphide .....	248
B.4.32 Mercury Telluride .....	248
B.4.33 Selenium .....	249
B.4.34 Silicon .....	249
B.4.35 Silver Chloride .....	254
B.4.36 Silver Iodide .....	254
B.4.37 Tellurium .....	254

B.4.38 Tin .....	255
B.4.39 Tin Diselenide .....	255
B.4.40 Tin Disulphide .....	256
B.4.41 Tin Telluride .....	256
B.4.42 Zinc Germanium Phosphide .....	256
B.4.43 Zinc Oxide .....	257
B.4.44 Zinc Selenide .....	257
B.4.45 Zinc Sulphide .....	258
B.4.46 Zinc Telluride .....	259
<b>Subject Index .....</b>	<b>261</b>