

Contents

CONTRIBUTORS TO VOLUME 35	vii
PREFACE	ix
SUPPLEMENTS	xi

Electronic Structure from the Point of View of the Local Atomic Environment

VOLKER HEINE

I. Fundamental Ideas	1
II. The Method of Matching the Green Functions	19
III. LCAO: From under a Cloud to Out in the Sun	35
IV. Calculations with Atomic Orbitals, Atomic Vibrations, and Other Localized Basis Sets	69
V. Miscellaneous Properties from the Local Point of View	105
VI. Historical Note	123

The Renaissance and Quantitative Development of the Tight-Binding Method

D. W. BULLETT

I. Molecular Orbitals and the LCAO Representation	129
II. Semiempirical Methods and Model Hamiltonians	143
III. Modern Quantitative Form of Tight-Binding Theory	170
IV. From Resonant Phase Shifts to Tight-Binding Parameters	192
V. Conclusion	213

The Recursive Solution of the Schrödinger Equation

ROGER HAYDOCK

I. Basics	216
II. Green Functions and the Local Density of States	250
III. Perturbation Theories, Energy Differences, and Computing the Density of States	263
IV. Relation to Other Methods and Conclusion	287

Applications of the Recursion Method to the Electronic Structure from an Atomic Point of View

M. J. KELLY

I. Introduction	296
II. The Recursion Method in Practice	299

III. Surface Electronic Structure	320
IV. The Electronic Structure of Random Networks	339
V. Phonon Spectra	356
VI. Problems Involving Small Energy Differences	363
VII. Miscellany	372
VIII. Concluding Remarks	380
Note Added in Proof	382
AUTHOR INDEX	385
SUBJECT INDEX	397