

CONTENTS

Preface	ix
Chapter 1 DIELECTRIC THEORY	
1. Polarizability of Isolated Systems	1
2. Atom Versus Bond Polarizabilities	3
3. Local Field Corrections: Classical	7
4. Self-Consistent Quantum Polarizabilities	8
5. Quantum Local-Field Corrections	11
6. Quantum Screening Theory	14
7. Quantum Polarizabilities	24
Chapter 2 DIELECTRIC THEORY OF CRYSTALS	
1. Pseudo Wave Functions	26
2. Cancellation Theorem	30
3. Pseudopotential Form Factors	33
4. Chemical Trends	41
5. Microscopic Dielectric Functions	46
6. Exchange and Correlation	53
7. Linear and Nonlinear Screening	55
8. Bonds and Energy Gaps	60
9. Covalent Hybridization	64
10. Self-Consistent Covalent Form Factors	67
11. Electronic Energy Levels of Semiconductors	74
12. Structural Consequences of Nonlinear Screening	78

Chapter 3	MOLECULAR THEORY	
1.	LCAO Theory: Molecular Orbitals	80
2.	Hückel π -Bonding Theory	83
3.	Electron Densities, Bond Orders, and Free Valence: Coulson Theory	90
4.	Bond Energies and Excited States	97
5.	Kinetic Energy in the Hückel Theory	101
6.	Self-Consistent Field Wave Functions	103
7.	Complete Semiempirical MO Theory	109
8.	Static and Dynamic Charges Densities	113
9.	Atomic and Bonding Charges in MO Theory	117
Chapter 4	CHEMICAL THEORY OF BONDS AND ENERGY GAPS	
1.	Directed Valence	119
2.	Anisotropy of Bond Polarizabilities	121
3.	Dielectric Anisotropy	125
4.	Anisotropic Screening	130
5.	Electronegativity Scales	136
6.	Covalent and Ionic Character	146
7.	Heteropolar Form Factors and Bond Sites	156
8.	Terminal Atoms	161
9.	Mixed Bonds and Hydrocarbon Dipole Moments	165
10.	Dielectric Theory of Conformal Energies	170

11.	Dipole Moments in Crystals and Molecules	173
12.	Cohesive Energies in Crystals and Molecules	176
Chapter 5	CRYSTAL STRUCTURE AND VIBRATION SPECTRA	
1.	General Formulation	178
2.	Electron-Ion Screening	180
3.	Covalent Crystals	185
4.	Partially Ionic Crystals	189
Chapter 6	MOLECULAR STRUCTURE AND MOLECULAR VIBRATIONS	
1.	General Theory	196
2.	Empirical Force Fields	198
3.	Simple Bond Charge Models	205
4.	Distributed Charge Model	209
Chapter 7	RECAPITULATION	215
	APPENDICES	
A.	Superunitarity	218
B.	Phase Shifts and Muffin-Tin Potentials	220
C.	Energy Gaps and Optical Spectra	224
D.	Dielectric Constants	229
E.	Table of Dielectrically Defined Electronegativities	230

F. The Variational Principle in Crystals and in Large Molecules	233
G. Form Factors and Structure Factors . . .	238
H. Nonlinear Damping Off the Energy Shell	241
I. Some Dielectric Polarizabilities	247
REFERENCES	253
AUTHOR INDEX	264
SUBJECT INDEX	266