

CONTENTS

<i>List of Abbreviations</i>	<i>xiii</i>
<i>Preface to Five-Volume Set</i>	<i>xv</i>
<i>About the Author</i>	<i>xxi</i>
<i>Foreword to Volume IV: Quantum Solids and Orderability</i>	<i>xxiii</i>
<i>Preface to Volume IV: Quantum Solids and Orderability</i>	<i>xxvii</i>
Chapter 1. Bondons on Graphenic Nanoribbons with Topological Defects.....	1
Abstract	2
1.1 Introduction	3
1.2 Graphenic Topological Isomorphism	5
1.2.1 Graphenic's Type Ribbons and Their Stone-Wales Defects	5
1.2.2 Stone-Wales Rearrangements' Generation and Propagation	15
1.3 Fourth Order Quantum Conditional Density and Partition Function	19
1.3.1 Path Integral Semiclassical Time Evolution Amplitude	19
1.3.2 Schrödinger's Conditional Probability Density	31
1.3.3 Partition Function Quantum Expansion.....	36
1.4 Topological-Bondonic Algorithm on Extended Nanostructures	39
1.4.1 Second Order Implementation	42
1.4.2 Fourth Order Implementation	45
1.5 Bondons on Nano-Ribbons with Stone-Wales Defects	48
1.5.1 Second Order Effects of Bondons on Graphenic Fragments	48
1.5.2 Fourth Order Effects of Bondons on Honeycomb Fragments	52
1.6 Conclusion.....	69
Keywords	71
References	72
Author's Main References	72
Specific References	73

Chapter 2. Geometrical Crystallography	79
Abstract	80
2.1 Introduction	81
2.2 A Brief History of Crystallography: The Influence in Art and Philosophy	82
2.3 The Symmetry of the Isolated Bodies	87
2.4 The Crystals' Metrics	98
2.4.1 Mathematical Point Networks: Ideal Crystals	98
2.4.2 Crystallographic Systems	104
2.4.3 The Reducing Cell Method.....	108
2.4.4 The Bravais Lattice	114
2.5 Point Groups.....	116
2.5.1 Symmetry Formulas: Symmetry Classes.....	116
2.5.2 Schoenflies Notation.....	120
2.5.3 The International (Hermann-Mauguin) Notation	125
2.5.4 The Crystals Morphology and Its Structural Laws.....	128
2.5.4.1 The Crystalline Habitus.....	128
2.5.4.2 The general Laws of the Crystalline Shape.....	130
2.5.5 The Crystallographic Indexing	137
2.5.5.1 Miller Indices.....	138
2.5.5.2 The Weiss Zone Law of Crystal Faces	140
2.5.5.3 Crystallographic Formulae	145
2.5.5.4 The Miller-Bravais Indices	147
2.5.6 Stereographic Projection. The Wulff Map	150
2.5.7 The Crystallographic Groups.....	156
2.5.7.1 Holohedric and Merihedric Classes.....	156
2.5.7.2 The Crystallographic Forms	158
2.5.7.3 Correlated crystallographic systems and classes.....	163
2.5.8 Group Symmetry Perturbation.....	173
2.5.8.1 The Crystallographic Anisotropy.....	173
2.5.8.2 The Curie Principle of Symmetry.....	183
2.5.8.3 Optical Activity by Crystals	185
2.6 Space Groups.....	188
2.6.1 Introduction to the Space Groups	188
2.6.1.1 Helicals and the Glide Planes	189
2.6.1.2 The Symbolistics for the Space Groups	195
2.6.1.3 The Pearson Classification	213

2.6.2	The Crystallographic Description of the Spatial Groups.....	214
2.6.2.1	The Symmetry Analysis of the Space Groups.....	214
2.6.2.1	Determination of a Space Group Symmetries.....	221
2.6.3	Extensions of the Space Groups	242
2.6.3.1	The Structural Class.....	242
2.6.3.2	The Magnetic/Colored Groups	246
2.7	Conclusion.....	249
	Keywords	251
	References	252
	Author's Main Reference.....	252
	Specific References	252
Chapter 3. Quantum Roots of Crystals and Solids		255
	Abstract	256
3.1	Introduction	256
3.2	Overview on The Quantum Postulates of Matter	260
3.2.1	Postulate of Operators and State Functions [P1]	261
3.2.2	Postulate of the Averaged Measured Values [P2]	263
3.2.3	Postulate of Wave Function Basic Sets and Operators' Commutativity [P3]	264
3.2.4	Postulate of the Schrödinger Equations [P4].....	265
3.3	Bloch' Theorem and the Crystal Orbitals.....	267
3.4	Quantum Models for Crystals	276
3.4.1	Reciprocal Lattice.....	276
3.4.2	Quantum Models of Crystals	286
3.4.2.1	Quantum Model of Free Electrons in Crystal	286
3.4.2.2	Quantum Model of Quasi-Free Electrons in Crystals.....	293
3.4.2.3	Quantum Model of Bonding Electrons in Crystal	299
3.4.3.4	Quantum Model of Tight-Binding Electrons in Crystal	305
3.5	Modeling Quantum Solids	312
3.5.1	Fermi Distribution	312
3.5.2	Semiconductors and Junctions.....	322
3.5.3	Moletronics.....	335
3.6	Conclusion.....	341
	Keywords	343

References	343
Author's Main References	343
Specific References	344
Further Readings.....	344
Chapter 4. Chemical Crystallography	349
Abstract	351
4.1 Introduction	351
4.2 The Crystal Model of Rigid Spheres	353
4.2.1 Spatial Ordering of Identical Spheres.....	353
4.2.2 Spatial Crystal Stability by the Model of Identical Spheres.....	365
4.2.3 The Crystalline Constitutive Particles' Dimension.....	368
4.2.4 The Crystalline Paradigm for the Genetic Code.....	369
4.3 Crystalline Substances: Typical Networks	375
4.3.1 Systematics of Crystalline Structure.....	375
4.3.2 Crystals' Stoichiometry.....	386
4.3.3 Unary Crystalline Substances	388
4.3.4 Crystalline Compounds with AB Stoichiometry	392
4.3.4.1 CsCl Crystalline Structure	394
4.3.4.2 NaCl Crystalline Structure	395
4.3.4.3 ZnS (Sphalerite/Blende) Cubic Structure Type ...	397
4.3.5 Type Structures of the AB ₂ Stoichiometric Compounds	399
4.3.5.1 CaF ₂ (Fluorite) Type Structure	400
4.3.5.2 TiO ₂ (Rutile) Type Structure.....	401
4.3.5.3 Cu ₂ O (Cuprite) Type Structure	403
4.3.5.4 SiO ₂ (β-Cristo-balite) Structural Type.....	405
4.3.6 Crystalline Structures with AB ₃ Stoichiometry	406
4.3.6.1 ReO ₃ Type Structure	406
4.3.6.2 BiLi ₃ Type Crystalline Structure.....	407
4.3.7 Polyatomic Complex Ions' Structures	408
4.3.7.1 The Perovskit Type	409
4.3.7.2 The Spinel Type.....	412
4.3.8 Silicates Crystalline Structures	414
4.3.8.1 Silicates' Classification.....	414
4.3.8.2 Nesosilicates and Sorosilicates.....	416

4.3.8.3	Cyclosilicates.....	417
4.3.8.4	Inosilicates.....	417
4.3.8.5	Phyllosilicates.....	418
4.3.8.6	Tectosilicates.....	421
4.3.8.7	Borates.....	424
4.4	The Solid and Crystal Structure by Chemical Bonding.....	425
4.4.1	The Chemical Bond in Solids.....	425
4.4.1.1	The Ionic Compounds. The Formal Ions' Paradigm.....	425
4.4.1.2	The Atomic Solid Compounds.....	433
4.4.1.3	The Metallic Compounds.....	436
4.4.1.4	Molecular Solids' Compounds.....	439
4.4.1.5	Relations between Chemical Bonds: The Heterodesmic Lattices.....	443
4.4.2	Pauling Rationalization for the Complex Ions' Bonding.....	452
4.4.3	The Potential Functions' Paradigm of the Chemical Bonding.....	461
4.4.4	Polarization in Crystals.....	476
4.5	Conclusion.....	484
	Keywords.....	486
	References.....	487
	Author's Main References.....	487
	Specific References.....	487
	Chapter 5. X-Ray Crystallography.....	489
	Abstract.....	490
5.1	Introduction.....	491
5.2	X-Ray Diffraction Applied To Crystalline Systems.....	493
5.2.1	X-Ray and Diffraction on Crystals.....	493
5.2.2	X-ray and the Electronic Density.....	503
5.2.3	The Ewald X-Rays Diffraction Rationalization.....	511
5.2.4	X-Ray and Structure Determination.....	521
5.3	Fields and Intensities in Dynamical Theory of X-Ray Diffraction.....	533
5.3.1	Fundamental Equations.....	533
5.3.2	Dynamical Diffraction in Two Waves Approximation.....	538

5.3.3	The Case of Zero Absorption.....	544
5.3.3.1	The Thick Crystal Case	547
5.3.3.2	The Thin Crystal Case	549
5.3.3.3	The Case of Intermediate Thickness Crystal	550
5.3.4	The Case of the Crystals with Absorption	554
5.4	Pendellösung Phenomena: The Plane Waves Approximations	561
5.4.1	The Phenomenology of Ewald's Pendellösung	561
5.4.2	Analytical Ewald's Pendellösung	564
5.4.2.1	The Coupling of Poynting Vectors	565
5.4.2.2	Direction of Propagation of Poynting Vectors.....	570
5.4.3	Integrated Intensities over the Pendellösung Period: The Laue's Case.....	574
5.4.4	Electronic Density by Structure Factor for Deformed Crystals	581
5.4.4.1	Pendellösung and the Electronic Ordered Structure	581
5.4.4.2	Modeling of Elastic Deformation of the Crystalline Structure.....	582
5.4.4.3	Pendellösung and the Amplitude of the Structure Factor	584
5.4.4.4	Application to the Electronic Maps of Contour.....	589
5.5	Total Self-Consistency in X-Ray Diffraction	596
5.5.1	Bormann Phenomenology	596
5.5.2	Quantum Modeling of Dynamical Bormann Effect	599
5.5.2.1	Formulation of Quantum State Vectors	599
5.5.2.2	Quantum Dynamic Localization.....	601
5.5.2.3	The Quantum Diffracted Energies.....	606
5.5.2.4	The Quantum Dynamic Jump.....	610
5.6	Conclusion.....	615
	Keywords	617
	References	617
	Author's Main References	617
	Specific References	618
	Further Readings.....	621
	<i>Index</i>	623