

Table of Contents

List of Symbols	1
I Basic Notions of Solid State Physics	6
I.1 Dark Conductivity: Generalities	6
I.2 Conduction in Metals: Drude and Sommerfeld Models	8
I.3 Band Model of Conduction	10
I.4 Limitations to Band Theory	16
I.5 Hopping and Tunneling Mechanisms of Charge Migration	16
I.6 Charge Carrier Trapping Processes	19
a Molecular Crystals	19
b Polymers	24
II Photoelectric Phenomena in Molecular Semiconductors	28
II.1 Light Absorption	29
II.2 Energy Migration in Molecular Materials	32
a Mechanisms of Energy Migration	32
b Effect of Traps	37
II.3 Photogeneration of Charge Carriers	39
II.4 Semiconductor Junctions	42
a p-n Junctions: Formation and Electrical Properties	42
b Schottky Junctions: Semiconductor-Metal Contacts	51
c Insulator-Metal Contacts	53
II.5 Photovoltaic Effect	59
a Molecular Solar Cells: Classical Formulation	59
b Molecular Solar Cells: Localized States Formulation	63
c Effect of Surface States	66
d Characterization of Junctions by the Capacitance Method	68
III Metallophthalocyanines	73
III.1 Syntheses and Physico-Chemical Properties	74
a Syntheses	74
b Structure and Morphology	80
c Spectroscopic Properties	86
d Photoelectron Spectroscopy	94
e Oxidation-Reduction Properties	98
f Electron Spin Resonance Measurements (ESR)	101

III.2	Dark Electrical Properties	103
a	Energy Band Structures	103
b	Electrical Properties: Intrinsic Case	104
c	Determination of the Trapping Levels	110
d	Doping of PcM by O ₂	112
e	Doping of PcM by other Doping Agents	116
III.3	Photovoltaic Effect and Solar Cells	122
a	Photoelectrical Properties	122
b	Photovoltaic Effect: Generalities	126
c	Junction in the Dark	127
d	Junction Studies under Illumination	137
e	Effect of Doping on the Performances of Molecular Solar Cells	145
f	Solar Energy Conversion Efficiencies of Molecular Solar Cells	147
IV	Polyacetylene	150
IV.1	Synthesis and Physico-Chemical Properties of Polyacetylene	151
a	Synthesis	151
b	Morphology	155
c	Molecular Weight and Length of the Conjugated Sequences	157
d	Stability of Polyacetylene and Effect of O ₂	158
e	Isomers	161
f	Crystalline Structures	164
IV.2	Theoretical Properties	166
a	Origin of the Band Gap	166
b	Band Structure	169
c	Bond Length Alternation Defects in Polyenes: the Solitons	171
IV.3	Properties of Doped Polyacetylene	173
a	Dopants and Doping Processes	173
b	Structural Features	175
c	Optical Properties	176
d	Magnetic Properties	176
IV.4	Transport Properties of Polyacetylene	179
a	Conduction Mechanisms at Low Doping Levels	181
b	Semiconductor-Metal Transition	183
c	Metallic Domain	184
d	Comparison of the Models with the Experimental Results in the Low Dopant Concentration Domain	185
IV.5	Photoelectric Properties and Solar Cells	188
a	Luminescence and Photoconductive Properties of Cis- and Trans- Polyacetylene	188
b	Junctions Properties and Molecular Solar Cells	192
V	The Main Other Molecular Semiconductors	201
V.1	Aromatic Hydrocarbons and Graphite	201
V.2	Metallo-Organic Derivatives	207
V.3	Charge Transfer Systems	212

a	Different Types of Charge-Transfer Systems	215
b	Charge Distribution	218
c	Charge-Transport Properties	220
d	Tetrathiofulvalene-tetracyanoquinodimethane (TTF-TCNQ) and Related Complexes	223
e	(Tetramethyltetraselenofulvalene) ₂ -X and Related Radical-Ion Salts	226
V.4	Polysulfurnitride and Polydiacetylene	230
V.5	Polymethines	236
V.6	Polymeric Conjugated Systems	240
a	Polyphenylene and Related Materials	240
b	Substituted Polyacetylenes, Phenylacetylene	242
c	Pyrolyzed Polyacrylonitrile	244
d	Polypyrroles	245
V.7	Molecular Solar Cells	247
a	Squaric Acid and Merocyanine	247
b	Aromatic Derivatives	251
c	Aromatic Liquid Crystals	252
d	Chlorophylls and Porphyrins	253
e	Polymeric Systems	253
Conclusion		255
References		256
Subject Index		283