

Lecture Notes in Chemistry

Edited by G. Berthier M.J.S. Dewar H. Fischer
K. Fukui G.G. Hall J. Hinze H.H. Jaffé J. Jortner
W. Kutzelnigg K. Ruedenberg J. Tomasi

45

M.C. Böhm



Lec 3
45

One-Dimensional Organometallic Materials

An Analysis of Electronic Structure Effects



Springer-Verlag

Berlin Heidelberg New York London Paris Tokyo

Inventar Nr. 11329 / PC

<u>Contents</u>	Page
I. Introduction and Historical Review.	1
References (Introduction).	10
II. Experimental Results and Global Band Structure Properties.	
II.1 One-Dimensional Building Principles in Organometallic Solids and General Band (Electronic) Structure Properties.	12
II.2 Electric Conductivities of Partially Oxidized Organometallic 1D Systems.	24
II.3 Electron Paramagnetic Resonance (EPR) Data of Organometallic Solids of Class I.	33
References (Section II).	38
III. Theoretical Methods; Crystal Orbital (CO) Approaches.	
III.1 A (Semiempirical) Crystal Orbital Formalism. Appendix III.1.	40 63
III.2 Nonlocal Hartree-Fock Exchange in Narrow-Band Materials.	67
III.3 Electronic Correlations and Relaxations in One-Dimensional (Organometallic) Polymers.	83
III.4 A Simple Electrostatic Model for Interchain Interactions in Quasi 1D Solids.	98
References (Section III).	103

	Page	<u>Foreword</u>
IV. Model Calculations in the Framework of a (Semiempirical) Crystal Orbital Approach.		This le
IV.1 Neighborstrand Interactions in One-Dimensional Tight-Binding Models. The (Tetrathiosquarato)nickel(II) System.	108	for a n lic sys matrix c
IV.2 Band Structure Properties of One-Dimensional Polydecker Sandwich Systems.	119	nic meta formatio
IV.3 Partially Oxidized Transition-Metal Polymers; Stabili- zation of Mixed Valence States.	131	is diffi property
IV.4 The Band Structure of One-Dimensional (Tetrazaporphyrinato)Cobalt(II).	142	etc.). T the gene
IV.5 The Band Structure of the One-Dimensional (Bisglyoximato)Ni(II) System.	148	metallic place th
IV.6 Band Structures of (Porphyrinato)Ni(II) Systems.	156	Solid-sta Contribut
IV.7 The 1D Band Structure of Tetrathiotetracene.	164	(1) An a
IV.8 The Band Structure of Polyferrocenylene;	168	have
References (Section IV).	172	(1) The
V. Outlook.	176	comp
Appendix (Abbreviations)	179	tati