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Lecture Notes in Chemistry

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One-Dimensional Organometallic Materials

An Analysis of Electronic Structure Effects



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Foreword

This lecture note gives an analysis of electronic structure effects for a new class of molecular solids, i.e. one-dimensional organometallic systems formed by transition-metal atoms that are embedded in a matrix of macrocyclic organic ligands. These systems as well as organic metals have focused considerable interest due to the potential formation of high-mobility charge carriers. For the present author it is difficult to participate in this restriction on a single physical property (i.e. high electronic conductivities, technical applications, etc.). The lecture note is hopefully a small contribution to enhance the general understanding of certain electronic properties in organometallic polymers. Those problems have been considered in the first place that seem to form a theoretical deficit in one specific field of solid-state chemistry. For the reader it will become evident that this contribution is a compromise always guided and limited by boundaries:

- i) An attempt to present problems to a 'chemical' audience which have their roots in solid-state physics.
- ii) The model calculations are limited by the currently available computational facilities. This 'boundary' implies that the computational data are subject to severe theoretical approximations.
- iii) Theorists have often a strong tendency to identify their numerical results and models with physical effects. Also this lecture note is not free of this almost universal trend. Nevertheless the author hopes that this text leads to some insight into a rather modern research field.