ELECTRONIC STRUCTURE AND ELECTRONIC TRANSITIONS IN
LAYERED MATERIALS

PHYSICS AND CHEMISTRY OF MATERIALS WITH LOW-DIMENSIONAL STRUCTURES

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ELECTRONIC STRUCTURE AND ELECTRONIC TRANSITIONS IN LAYERED MATERIALS

Edited by

VINCENZO GRASSO

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PREFACE

This new volume in the series *Physics and Chemistry of Materials with Layered Structures* satisfies the need for a comprehensive review of the progress made in the decade 1972–1982 in the field of the electronic properties of layer compounds. Some recent theoretical and experimental developments are highlighted by authoritative physicists active in current research. The previous books of this series covering similar topics are volumes 3 and 4. The present review is mainly intended to fulfill the gap up to 1982 and part of 1983.

I am indebted to all the authors for their friendly co-operation and continuous effort in preparing the contributions in their own fields of competence. I am sure that both the expertise scientists and the beginners in the field of the electronic properties of layered materials will find this book a valuable tool for their research work.

Warm thanks are due to Prof. E. Mooser, General Editor of the series, for his constant and authoritative advice.

* * *

This book has been conceived as a tribute to Prof. Franco Bassani to whom the Italian tradition in the field of layer compounds, as well as in other fields of solid-state physics, owes much. The authors of this review have all benefited at some time of their professional life from close cooperation with him.

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FOREWORD

The growing interest in the physical properties of layer materials and the restless expansion of this active area of research are the basic motivations of this new volume. The rapid accumulation of experimental and theoretical results has made necessary this review, which offers a guide-line within the maze of recent achievements, and provides future perspectives in the field.

From the theoretical side, the novelties encountered in the last few years in the physics of layer compounds are numerous; they concern not only the classic subject of band structure calculations, but also several other fascinating topics, such as the study of charge density waves, plasmons, superlattice formation, the analysis of small gap semiconductors or semimetals, the effects of different coordination environments and polytypes. The reasons for recent progress can be traced back to a number of concomitant facts, such as a critical reexamination of the standard methods of band theory, the development of a new generation of pseudopotentials, the surprising success of the local density functional formalism, the interchange of concepts with the primarily related field of surface phenomena, and the availability of the auxiliary integration techniques on the unit cell and on the Brillouin zone.

In the midst of approaches and developments, a nice aspect of this book is that a particular emphasis is steadily given to a few elementary models, which even in relatively complicated crystals can provide the gross features of the physical phenomena. The concepts of bonding and antibonding states, ionic or covalent bonds, population analysis, charge transfer, and Fermi surface nesting often give a simple guideline by which sophisticated calculations or apparently anomalous effects can be interpreted.

From an experimental side, the last years have also been particularly fruitful. The investigations in the layer compounds have not only supplemented new important data in the traditional optical region, but have also provided an almost completely new phenomenology in the far ultraviolet and higher energy region spectroscopy. The systematic use of synchrotron radiation has made available a new wealth of information, which is, to a large extent, still open to the theoretical analysis.

The review of photoemission experiments in layer compounds is timely indeed. These compounds are the natural candidates for angular resolved photoemission investigations, because of the peculiar projected information implied by this technique. Despite this, little systematics on photoemission of layer compounds was until now available in the literature, and this volume has also the merit of covering this lack.

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