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This book addresses the problem of teaching the Electronic Structure and Chemical Bonding of atoms and molecules to high school and university students. It presents the outcomes of thorough investigations of some teaching methods as well as an unconventional didactical approach which were developed during a seminar for further training organized by the University of Bordeaux I for teachers of the physical sciences. The text is the result of a collective effort by eleven scientists and teachers: physicists and chemists doing research at the university or at the CRNS, university professors, and science teachers at high-school or university level. While remaining wide open to the latest discoveries of science, the text also offers a large number of problems along with their solutions and is illustrated by several pedagogic suggestions. It is intended for the use of teachers and students of physics, chemistry, and of the physical sciences in general. Contents:Historical Survey:Main Events in the History of Chemical BondingTheoretical Bases for the Description of Molecular Electronic Structure and Chemical Bonding: Quantum Mechanics and Molecular Symmetry:Quantum Bases of Chemical BondingMolecular Symmetry, Its Description and ConsequencesTwo Complementary Descriptions of Chemical Bonding: Mechanical Aspect of Chemical Bonding:BasicsApplicationsLanguage of Orbitals and Chemical Bonding: Applications and Limits:One-Electron Treatment of Many-Electron ParticlesChemical Bonding in Terms of MO LanguageBeyond the One-Electron DescriptionIndex Readership: Physicists and chemists, graduate and undergraduate students in chemical physics. keywords: with contributions by numerous experts "Steude's book offers a very readable and easy-to-understand presentation of the key concepts of inorganic molecular chemistry. Following an introduction into chemical bonding, the book focuses on the material chemistry of the main group elements." Prof. Dr. Michael Ruck, TU Dresden The bond valence model is a recently developed model of the chemical bond in inorganic chemistry that complements the bond model widely used in organic chemistry. It is simple, quantitative, intuitive, and predictive - no more than a pocket calculator is needed to calculate it. This book focuses on the theory that underlies the model, and shows how it has been used in physics, materials science, chemistry, mineralogy, soil science, and molecular biology. Unlike many other books on

chemical bonding, this introduction to the subject does not adopt the traditional historical treatment in which the two basic theories of valence, molecular orbital and valence bond, are introduced and applied to increasingly complex molecules. Molecular surface science has made enormous progress in the past 30 years. The development can be characterized by a revolution in fundamental knowledge obtained from simple model systems and by an explosion in the number of experimental techniques. The last 10 years has seen an equally rapid development of quantum mechanical modeling of surface processes using Density Functional Theory (DFT). Chemical Bonding at Surfaces and Interfaces focuses on phenomena and concepts rather than on experimental or theoretical techniques. The aim is to provide the common basis for describing the interaction of atoms and molecules with surfaces and this to be used very broadly in science and technology. The book begins with an overview of structural information on surface adsorbates and discusses the structure of a number of important chemisorption systems. Chapter 2 describes in detail the chemical bond between atoms or molecules and a metal surface in the observed surface structures. A detailed description of experimental information on the dynamics of bond-formation and bond-breaking at surfaces make up Chapter 3. Followed by an in-depth analysis of aspects of heterogeneous catalysis based on the d-band model. In Chapter 5 adsorption and chemistry on the enormously important Si and Ge semiconductor surfaces are covered. In the remaining two Chapters the book moves on from solid-gas interfaces and looks at solid-liquid interface processes. In the final chapter an overview is given of the environmentally important chemical processes occurring on mineral and oxide surfaces in contact with water and electrolytes. Gives examples of how modern theoretical DFT techniques can be used to design heterogeneous catalysts This book suits the rapid introduction of methods and concepts from surface science into a broad range of scientific disciplines where the interaction between a solid and the surrounding gas or liquid phase is an essential component Shows how insight into chemical bonding at surfaces can be applied to a range of scientific problems in heterogeneous catalysis, electrochemistry, environmental science and semiconductor processing Provides both the fundamental perspective and an overview of chemical bonding in terms of structure, electronic structure and dynamics of bond rearrangements at surfaces The series Structure and Bonding publishes critical reviews on topics of research concerned with chemical structure and bonding. The scope of the series spans the entire Periodic Table and addresses structure and bonding issues associated with all of the elements. It also focuses attention on new and developing areas of modern structural and theoretical chemistry such as nanostructures, molecular electronics, designed molecular solids, surfaces, metal clusters and supramolecular structures. Physical and spectroscopic techniques used to determine, examine and model structures fall within the purview of Structure and Bonding to the extent that the focus is on the scientific results obtained and not on specialist information concerning the techniques themselves. Issues associated with the development of bonding models and generalizations that illuminate the reactivity pathways and rates of chemical processes are also relevant. The individual volumes in the series are thematic. The goal of each volume is to give the reader, whether at a university or in industry, a comprehensive overview of an area where new insights are emerging that are of interest to a larger scientific audience. Thus each review within the volume critically surveys one aspect of that topic and places it within the context of the volume as a whole. The most significant developments of the last 5 to 10 years should be presented using selected examples to illustrate the principles discussed. A description of the physical basis of the experimental techniques that have been used to provide the primary data may also be appropriate, if it has not been covered in detail elsewhere. The coverage need not be exhaustive in data, but should rather be conceptual, concentrating on the new principles being developed that will allow the reader, who is not a specialist in the area covered, to understand the data presented. Discussion of possible future research directions in the area is welcomed. Review articles for the individual volumes are invited by the volume editors This is the perfect complement to "Chemical Bonding - Across the Periodic Table" by the same editors, who are two of the top scientists working on this topic, each with extensive experience and important connections within the community. The resulting book is a unique overview of the different approaches used for

describing a chemical bond, including molecular-orbital based, valence-bond based, ELF, AIM and density-functional based methods. It takes into account the many developments that have taken place in the field over the past few decades due to the rapid advances in quantum chemical models and faster computers. T. Koritsanszky, A. Volkov, M. Chodkiewicz: New Directions in Pseudoatom-Based X-Ray Charge Density Analysis.- B. Dittrich, D. Jayatilaka: Reliable Measurements of Dipole Moments from Single-Crystal Diffraction Data and Assessment of an In-Crystal Enhancement.- B. Engels, Th. C. Schmidt, C. Gatti, T. Schirmeister, R.F. Fink: Challenging Problems in Charge Density Determination: Polar Bonds and Influence of the Environment.- S. Fux, M. Reiher: Electron Density in Quantum Theory.- K. Meindl, J.Henn: Residual Density Analysis.- C. Gatti: The Source Function Descriptor as a Tool to Extract Chemical Information from Theoretical and Experimental Electron Densities. The state-of-the-art in contemporary theoretical chemistry is presented in this 4-volume set with numerous contributions from the most highly regarded experts in their field. It provides a concise introduction and critical evaluation of theoretical approaches in relation to experimental evidence. D. Stalke, U. Flierler: More than Just Distances from Electron Density Studies.- A.O. Madsen: Modeling and Analysis of Hydrogen Atoms.- B.B. Iversen/J. Overgaard: Charge Density Methods in Hydrogen Bond Studies.- U. Flierler, D. Stalke: Some Main Group Chemical Perceptions in the Light of Experimental Charge Density Investigations.- D. Leusser: Electronic Structure and Chemical Properties of Lithium Organics Seen Through the Glasses of Charge Density.- L. J. Farrugia, P. Macchi: Bond Orders in Metal–Metal Interactions Through Electron Density Analysis.- W. Scherer, V. Herz, Ch. Hauf: On the Nature of β-Agostic Interactions: A Comparison Between the Molecular Orbital and Charge Density Picture. Absorption Spectra and Chemical Bonding in Complexes focuses on chemical bonding in transition group complexes and molecules, including molecular orbitals, absorption bands, and energy levels. The book first outlines the history of chemical bonding, giving emphasis to different theories that paved the way for further studies in this field. The text then examines the energy levels of a configuration and molecular orbitals and microsymmetry. The publication takes a look at the interelectronic repulsion in M.O. configurations, the characteristics of absorption bands, and spectrochemical series. Electron transfer spectra, energy levels in complexes with almost spherical symmetry, molecular orbitals lacking spherical symmetry, and chemical bonding are also discussed. The book examines the determination of complex species in solution and their formation constants; survey of the chemistry of heavy, metallic elements; and tables of absorption spectra. The manuscript is a dependable source of data for physicists and group theorists interested in absorption spectra and chemical bonding. Modern life is made up of a mind-boggling array of materials. A simple drinking cup, for example, might be made of Styrofoam, paper, or glass, depending on the drinkers needs at the moment. Home storage cabinets can be made of metal, wood, or plastic. Space shuttles are assembled from silicon, steel, and hundreds of other materials. All of these items owe their properties to the chemical bonds between the atoms that make up the substance. "Chemical Bonds" examines the nature of the chemical bonds, answering fundamental questions about how they form, how they are broken, and how they help define life as we know it. The renowned Oxford Chemistry Primers series, which provides focused introductions to a range of important topics in chemistry, has been refreshed and updated to suit the needs of today's students, lecturers, and postgraduate researchers. The rigorous, yet accessible, treatment of each subject area is ideal for those wanting a primer in a given topic to prepare them for more advanced study or research. The learning features provided, including questions at the end of every chapter and online multiple-choice questions, encourage active learning and promote understanding. Furthermore, frequent diagrams, margin notes, and glossary definitions all help to enhance a student's understanding of these essential areas of chemistry. Chemical Bonding gives a clear and succinct explanation of this fundamental topic, which underlies the structure and reactivity of all molecules, and therefore the subject of chemistry itself. Little prior knowledge or mathematical ability is assumed, making this the perfect text to introduce students to the subject. The result of decades of research by a pioneer in the field, this is the first book to deal exclusively with achieving high-performance metal-polymer composites by chemical bonding. Covering both the

academic and practical aspects, the author focuses on the chemistry of interfaces between metals and polymers with a particular emphasis on the chemical bonding between the different materials. He elucidates the various approaches to obtaining a stable interface, including, but not limited to, thermodynamically driven redox reactions, bond protection to prevent hydrolysis, the introduction of barrier layers, and stabilization by spacer molecules. Throughout, chemical bonding is promoted as a simple and economically viable alternative to adhesion based on reversible weak physical interaction. Consequently, the text equips readers with the practical tools necessary for designing high-strength metal-polymer composites with such desired properties as resilience, flexibility, rigidity or degradation resistance. MOLECULES and the Chemical Bond is about understanding Schrödinger's equation, for chemical systems. In his famous Lectures on Physics, Richard Feynman quotes Paul Dirac on what it means to understand an equation. "I understand what an equation means," said Dirac, "if I have a way of figuring out the characteristics of its solutions without actually solving it." That hits the nail on the head! It's precisely what Conceptual Valence Bond Theory does for Schrödinger's equation. A "physical understanding" of an equation, adds Feynman, "is a completely unmathematical, imprecise, and inexact thing, but absolutely necessary for a physicist." It unfolds in MCB in two stages, described by Newton as a stage of "Analysis" (a union of observations and inductions) and a stage of "Synthesis" (use of inductions, accepted as first principles, to explain observations). The book's chief vehicle for creating an intuitive understanding of solutions of Schrödinger's equation is the world's largest - and to the author's knowledge, virtually only - library of line drawings of exclusive orbital models of chemical species' electron density profiles. By focussing attention on fundamental physical principles and by avoiding use of atomic orbitals and, thereby, mathematical complexities associated with Schrödinger's equation (the only source of atomic orbitals), the book's essays provide a scientifically sound, student-friendly introduction to modern valence theory. Repetition of fundamental ideas, here and there, is intended to make individual essays understandable and interesting, each by itself, so that readers may examine them in any order, in leisurely walks, so to speak, in the big garden that is valence theory, picking bouquets to their liking. This profusely illustrated book, by a world-renowned chemist and award-winning chemistry teacher, provides science students with an introduction to atomic and molecular structure and bonding. (This is a reprint of a book first published by Benjamin/Cummings, 1973.) Axel Christian Klixbüll Jørgensen was a “Polyhistor”,one of the very few in the highly specialized science of our time.His interests and contributions in ch- istry covered the whole Periodic Table.This statement demonstrates the breadth of his interests,however,it also sheds light on the constraints of chemistry which deals with a large, yet limited number of elements. It is not surprising that Jørgensen went beyond these limits,exploring the probable or plausible ch- istry of yet unknown elements and elementary particles such as quarks. Even chemistry itself did not place rigid limits on his mind,he was able to transfer his chemical concepts to scientific problems far beyond the normal such as in astrophysics. “Structure and Bonding” is intimately associated with the name C.K. J- gensen both as initiator and author over several decades.The appearance of a special edition in memory of this great scientist is a self-evident prolongation of his many contributions to the success of this series. Contents: Chemical Bonding-I : Basic Concepts, Chemical Bonding-II : Additional Aspects, Intermolecular Force and Crystal Structures. Provides an introduction to models and theories of chemical bonding and geometry as applied to the molecules of the main group elements. This text also elucidates the relationships between these various models and theories. It is useful for courses on chemical bonding in chemistry departments at the senior/first year graduate level. The Special Edition 'Compounds with Polar Metallic Bonding' is a collection of eight original research reports presenting a broad variety of chemical systems, analytical methods, preparative pathways and theoretical descriptions of bonding situations, with the common aim of understanding the complex interplay of conduction electrons in intermetallic compounds that possess different types of dipoles. Coulombic dipoles introduced by electronegativity differences, electric or magnetic dipoles, polarity induced by symmetry reduction—all the possible facets of the term 'polarity'—can be observed in polar intermetallic phases and have their own and, in most cases, unique consequences on the

physical and chemical behaviour. Elucidation of the structure–property relationships in compounds with polar metallic bonding is a modern and growing scientific field which combines solid state physics, preparative chemistry, metallurgy, modern analytic methods, crystallography, theoretical calculations of the electronic state and many more disciplines. MOLECULES AND THE CHEMICAL BOND Chemistry Simplified This highly original book by a famous chemistry teacher about general chemistry in a new key may change how teachers teach - - Atomic Theory - The Mole Concept and Avogadro's Constant - The Gas Laws - Solving Problems in Chemical Stoichiometry - The Saturation and Directional Character of Chemical Affinity - The Pauli Exclusion Principle - Linnett's Double Spin Set Theory - Pauling's Rules of Crystal Chemistry - The Octet Rule - Lewis Structures for O2, NO, CO, SO2 and SO3 - Construction of Bond Diagrams - VSEPR Theory - Dative Bonding - Multicenter Bonding - Bonding in Metals - pH Calculations - The Periodic Table - The Energy Function and the First Law of Thermodynamics - The Entropy Function and the Second Law of Thermodynamics - How an Inductive Science Advances This book explains in non-mathematical terms where possible, the factors that govern covalent bond formation, the lengths and strengths of bonds and molecular shapes. The present four volumes, published under the collective title of "Chemical Bonds in Solids," are the translation of the two Russian books "Chemical Bonds in Crystals" and "Chemical Bonds in Semiconductors." These contain the papers presented at the Conference on Chemical Bonds held in Minsk between May 28 and June 3, 1967, together with a few other papers (denoted by an asterisk) which have been specially incorporated. Earlier collections (also published by the Nauka i Tekhnika Press of the Belorussian Academy of Sciences) were entitled "Chemical Bonds in Semiconductors and Solids" (1965) and "Chemical Bonds in Semiconductors and Thermody namics" (1966) and are available in English editions from Consultants Bureau, New York (pub lished in 1967 and 1968, respectively). The subject of chemical bonds in crystals, including semiconductors, has recently become highly topical and has attracted the interest of a wide circle of physicists, chemists, and engineers. Until recently, the most successful description of the properties of solids (including semi conductors) has been provided by the band theory, which still dominates the physics of solids. Nevertheless, it is clear that the most universal approach is that based on the general theory of chemical bonds in crystals, in which details of the electron distributions between atoms and of the wave functions appear quite explicitly.