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Alternant Molecular Orbital Method The Fragment Molecular Orbital Method The Effective Fragment Molecular Orbital Method **Recent Advances of the Fragment Molecular Orbital Method The Alternant Molecular Orbital Method for Alternant Systems of Non-closed Shell Structure Adaptation of Semiempirical Molecular Orbital Methods for Dynamic Calculations in Ionic Molecules and Non-metallic Solids Complete Guide to the Fragment Molecular Orbital Method in Gamess: From One Atom to a Million, at Your Service Introduction to Elementary Molecular Orbital Theory and to Semiempirical Methods Studies on the Alternant Molecular Orbital Method. Ii. Application to Cyclic Systems Fragmentation: Toward Accurate Calculations on Complex Molecular Systems The DV-Xα Molecular-Orbital Calculation Method** The Indo Method for Approximate Self-consistent Field Molecular Orbital Calculations for Transition Metal Compounds The Orbit Method in Geometry and Physics *The LMTO Method The Orbit Method in Representation Theory* Lectures on the Orbit Method **A Method of Estimating Residuals in Orbital Theory The DV-X Molecular-Orbital Calculation Method** Introduction to Elementary Molecular Orbital Theory and to Semiempirical Methods *New Electron Correlation Methods and their Applications, and Use of Atomic Orbitals with Exponential Asymptotes A Universal Method for Calculating Orbital Conditions in an Inverse Gravitational Field* **A Numerical Evaluation of Preliminary Orbit Determination Methods** A Manual Method for Orbital Rendezvous and an Elliptical Relative Coordinate System for Rendezvous Navigation and Guidance *Spin-Orbital Electronegativity, the X-alpha Method, and Reactivity at Transition-Metal Interfaces Methods of Computing the Orbit of a Comet Or Planet* Valency and Molecular Structure Methods of Computing the Orbit of a Comet Or Planet *Electronic Structure and Physical Properties of Solids* **Orbital Approach to the Electronic Structure of Solids Molecular Orbitals and their Energies, Studied by the Semiempirical HAM Method** *Recent Advances of the Fragment Molecular Orbital Method* Bond Orbital Model and the Properties of Tetrahedrally Coordinated Solids **A Graphical Method for the Determination of the True Orbital Elements of Specified Eclipsing Binaries Notes on Molecular Orbital Calculations** *MOLECULAR STRUCTURE AND BONDING; THE QUALITATIVE MOLECULAR ORBITAL APPROACH.* Dictionary of Values of Molecular Constants **The DV-Xa Molecular-orbital Calculation Method** Different Bands for Different Spins **Computational Methods for Large Molecules and Localized States in Solids The Orbit Method in Geometry and Physics**

This book covers recent advances of the fragment molecular orbital (FMO) method, consisting of 5 parts and a total of 30 chapters written by FMO experts. The FMO method is a promising way to calculate large-scale molecular systems such as proteins in a quantum mechanical framework. The highly efficient parallelism deserves being considered the principal advantage of FMO calculations. Additionally, the FMO method can be employed as an analysis tool by using the inter-fragment (pairwise) interaction energies, among others, and this feature has been utilized well in biophysical and pharmaceutical chemistry. In recent years, the methodological developments of FMO have been remarkable, and both reliability and applicability have been enhanced, in particular,

for non-bio problems. The current trend of the parallel computing facility is of the many-core type, and adaptation to modern computer environments has been explored as well. In this book, a historical review of FMO and comparison to other methods are provided in Part I (two chapters) and major FMO programs (GAMESS-US, ABINIT-MP, PAICS and OpenFMO) are described in Part II (four chapters). dedicated to pharmaceutical activities (twelve chapters). A variety of new applications with methodological breakthroughs are introduced in Part IV (six chapters). Finally, computer and information science-oriented topics including massively parallel computation and machine learning are addressed in Part V (six chapters). Many color figures and illustrations are included. Readers can refer to this book in its entirety as a practical textbook of the FMO method or read only the chapters of greatest interest to them. It is shown that the concept of electronegativity, originally viewed as a virtually constant characteristic of an atom, can be generalized to the individual molecular orbitals of aggregates of atoms, utilizing the self-consistent-field X-alpha density-functional representation of molecular-orbital theory in conjuction with the definition of orbital electrnegativity proposed by Hinze et al. This generalization allows for the dependence of electronegativity on the detailed electronic structure of a group of atoms as a function of its composition, geometry, and local chemical environment. In transition metals and transition-metal coordination complexes, where local magnetic spin polarization of electrons is important, the concept of orbital electronegativity can be further generalized to the individual spin-orbitals. By viewing a transition-metal surface, cluster, or coordination complex as providing orbitall or spin-orbital pathways for electrons to effectively flow between reactants, where such flow directly between reactants in the gas phase is forbidden by orbital-symmetry restrictions or unfavorable electronegativity differences, orbital or spin-orbital electronegativity can be used in conjunction with X-alpha calculations for representative clusters and complexes as an approximate index of heterogeneous or homogeneous reactivity. Recent applications of this concept to a number of problems associated with reactivity at transition-metal interfaces are reviewed, including: the dissociation and reactivity of hydrogen at low-coordination transition-metal sites; the interaction of atomic hydrogen with transition-metal interfaces; and the surface reactivity of iron. (Author). This book covers recent advances of the fragment molecular orbital (FMO) method, consisting of 5 parts and a total of 30 chapters written by FMO experts. The FMO method is a promising way to calculate large-scale molecular systems such as proteins in a quantum mechanical framework. The highly efficient parallelism deserves being considered the principal advantage of FMO calculations. Additionally, the FMO method can be employed as an analysis tool by using the inter-fragment (pairwise) interaction energies, among others, and this feature has been utilized well in biophysical and pharmaceutical chemistry. In recent years, the methodological developments of FMO have been remarkable, and both reliability and applicability have been enhanced, in particular, for non-bio problems. The current trend of the parallel computing facility is of the many-core type, and adaptation to modern computer environments has been explored as well. In this book, a historical review of FMO and comparison to other methods are provided in Part I (two chapters) and major FMO programs (GAMESS-US, ABINIT-MP, PAICS and OpenFMO) are described in Part II (four chapters). dedicated to pharmaceutical activities (twelve chapters). A variety of new applications with methodological breakthroughs are introduced in Part IV (six chapters). Finally, computer and information science-oriented topics including massively parallel computation and machine learning are addressed in Part V (six chapters). Many color figures and illustrations are included. Readers can refer to this book in its entirety as a practical textbook of the FMO method or read only the chapters of greatest interest to them. Historical introduction; The Experimental Foudation of the quantum theory; Elementary quantum theory; The hydrogen atom; Quantum theory and the periodic classification; The molecular orbital method; The valence-bond method; Directed valency; Ionic Hydrogen and metallic bond; The Structures of some simple inorganic compounds; Complex compounds; Electronic spectar of tarnsition-metal complex; Electron-

deficient molecules. A cyclic pi-electron system is treated by the alternant molecular-orbital method using different orbitals for different spins. The energy depression per electron is studied and approaches 0.4 ev for large systems. (Author). These notes summarize in part lectures held regularly at the University of Zurich and, in the Summer of 1974, at the Semi nario Latinoamericano de QUimica Cuantica in Mexico. I am grateful to those who have encouraged me to publish these lec tures or have contributed to them by their suggestions. In particular, I wish to thank Professor J. Keller of the Univer sidad Nacional Autonoma in Mexico, Professor H. Labhart and Professor H. Fischer of the University of Zurich, as well as my former students Dr. J. Kuhn, Dr. W. Hug and Dr. R. Geiger. The aim of these notes is to provtde a summary and concise introduction to elementary molecular orbital theory, with an emphasis on semiempirical methods. Within the last decade the development and refinement of ab initio computations has tended to overshadow the usefulness of semiempirical methods. However, both approaches have their justification. Ab initio methods are designed for accurate predictions, at the expense of greater computational labor. The aim of semiempirical methods mainly lies in a semiquantitative classification of electronic pro perties and in the search for regularities within given classes of larger molecules. The reader is supposed to have had some previous basic instruc tion in quantum mechanics, such as is now offered in many uni versities to chemists in their third or fourth year of study. The bibliography should encourage the reader to consult other texts, in particular also selected publications in scientific journals. This Technical Note presents a general FORTRAN Code and computer program flowcharts for twelve different Preliminary Orbit Determination Methods (PODM). A number of solutions were obtained from each PODM using input data from a predetermined reference orbit. A comparison of these PODMs in their ability to converge, error propogation, computation time, and total computer core requirements is presented. The simplifications of band-structure calculations which are now referred to as linear methods were introduced by Ole K. Andersen almost ten years ago. Since then these ideas have been taken up by several workers in the field and translated into computer programmes that generate the band structure of almost any material. As a result, running times on computers have been cut by orders of magnitude. One of the strong motivations behind the original proposal was a desire to give the conventional methods' a physically meaningful content which could be understood even by the non-specialist. Unfortunately, this aspect of lin ear methods seems to have been less well appreciated, and most workers are content to use the latter as efficient computational schemes. The present book is intended to give a reasonably complete description of one particular linear method, the Linear Muffin-Tin Orbital (LMTO) method, without losing sight of the physical content of the technique. It is also meant as a guide to the non-specialist who wants to perform band-structure calculations of his own, for example, to interpret experimental results. For this purpose the book contains a set of computer programmes which allow the user to perform full-scale self-consistent band-structure calculations by means of the LMTO method. In addition, it contains a listing of self-con sistent potential parameters which, for instance, may be used to generate the energy bands of metallic elements. The orbit method influenced the development of several areas of mathematics in the second half of the 20th century and remains a useful and powerful tool in such areas as Lie theory, representation theory, integrable systems, complex geometry, and mathematical physics. Among the distinguished names associated with the orbit method is that of A.A. Kirillov, whose pioneering paper on nilpotent orbits (1962), places him as the founder of orbit theory. The original research papers in this volume are written by prominent mathematicians and reflect recent achievements in orbit theory and other closely related areas such as harmonic analysis, classical representation theory, Lie superalgebras, Poisson geometry, and quantization. Contributors: A. Alekseev, J. Alev, V. Baranovksy, R. Brylinski, J. Dixmier, S. Evens, D.R. Farkas, V. Ginzburg, V. Gorbounov, P. Grozman, E. Gutkin, A. Joseph, D. Kazhdan, A.A. Kirillov, B. Kostant, D. Leites, F. Malikov, A. Melnikov, P.W. Michor, Y.A. Neretin, A. Okounkov, G. Olshanski, F. Petrov, A. Polishchuk, W. Rossmann, A. Sergeev, V. Schechtman, I. Shchepochkina. The work will be an

invaluable reference for researchers in the above mentioned fields, as well as a useful text for graduate seminars and courses. Advances in Quantum Chemistry presents surveys of current topics in this rapidly developing field one that has emerged at the cross section of the historically established areas of mathematics, physics, chemistry, and biology. It features detailed reviews written by leading international researchers. In this volume the readers are presented with an exciting combination of themes. Presents surveys of current topics in this rapidly-developing field that has emerged at the cross section of the historically established areas of mathematics, physics, chemistry and biology Features detailed reviews written by leading international researchers The degree of approximation used in determining the orbits of earth satellites is reflected in the residuals (differences between calculated and observed positions). The least-squares procedure generally used to fit theory to observation tends to obscure the significance of theoretical parameters, so that the physical sources of residuals cease to be apparent. A method is outlined herein for estimating the magnitude of the residuals to be expected from an approximate theory presumed to have one missing or incorrect term. This treatment of molecular and atomic physics is primarily meant as a textbook. It is intended for both chemists and physicists. ·It can be read without much knowledge of quantum mechanics or mathematics, since all such details are explained-. It has developed through a series of lectures at the Royal Institute of Technology. The content is to about 50 % theoretical and to 50 % experimental. The reason why the authors, who are experimentalists, went into theory is the following. When we during the beginning of the 1970's measured photo electron spectra of organic molecules, it appeared to be impossible to understand them by use of available theoretical calculations. To handle hydrocarbons we (together with C. Fridh) constructed in 1972 a purely empirical procedure, SPINDO [1] which has proved to be useful, but the extension to molecules with hetero atoms appeared to be difficult. One of us (L.A.) proposed then another purely ~~E!E!~~! EE2~~~~E~ (Hydrogenic Atoms in Molecules, HAM/1, unpublished), in which the Fock matrix elements f5..y were parametrized using Slater's shielding concept. The self-repulsion was compensated by a term "-1". The §~~2~~_~ff2E~, HAM/2 [2] , started from the total energy E:. of the molecule. The atomic parts of L used the Slater shielding constants, and the bond parts of E. were taken from SPINDO. The Fock matrix elements Fpv were then obtained from E in a conventional way. The fragment molecular orbital (FMO) method is a fast linear-scaling quantum-mechanical method employed by chemists and physicists all over the world. It provides a wealth of properties of fragments from quantum-chemical calculations, a bottomless treasure pit for data mining and machine learning. However, there is no user-friendly description of its usage in the widely employed quantum-chemical open-source software GAMESS, nor is there any book covering the usage of GAMESS in general. This leaves very many interested users to their own devices to get through a variety of problems with very cryptic descriptions of keywords in the program manual and no guide whatsoever as to what options should be set for particular scientific tasks. This book is the panacea to many frustrations.The main focus of the book is to build a solid bridge connecting FMO users to GAMESS, by giving a helpful introduction of various FMO methods as needed for particular problems found in computational chemistry, and describing in detail how to do these simulations and understand the results from the output of the program. The book also covers parallelization strategies for attaining high parallel efficiency in massively parallel computations, and provides means to analyze performance and design a solution for overcoming performance bottlenecks. A special section is devoted to dealing with problems in executing GAMESS, arising from computational environment and user errors. Finally, 14 carefully selected types of applications are discussed in detail, describing the input keywords and explaining where to find the main results in the text-based output. This multi-author contributed volume contains chapters featuring the development of the DV-Xα method and its application to a variety of problems in Materials Science and Spectroscopy written by leaders of the respective fields. The volume contains a Foreword written by the Chairs of Japanese and Korea DV-X alpha Societies. This book is aimed at

individuals working in Quantum Chemistry. This book is aiming at filling the gap between the different languages of the physics and chemistry communities to understand the electronic structure of solids. How structure and properties of solids are related is illustrated by considering in detail a large number of real examples. These notes summarize in part lectures held regularly at the University of Zurich and, in the Summer of 1974, at the Semi nario Latinoamericano de QUimica Cuantica in Mexico. I am grateful to those who have encouraged me to publish these lec tures or have contributed to them by their suggestions. In particular, I wish to thank Professor J. Keller of the Univer sidad Nacional Autonoma in Mexico, Professor H. Labhart and Professor H. Fischer of the University of Zurich, as well as my former students Dr. J. Kuhn, Dr. W. Hug and Dr. R. Geiger. The aim of these notes is to provtde a summary and concise introduction to elementary molecular orbital theory, with an emphasis on semiempirical methods. Within the last decade the development and refinement of ab initio computations has tended to overshadow the usefulness of semiempirical methods. However, both approaches have their justification. Ab initio methods are designed for accurate predictions, at the expense of greater computational labor. The aim of semiempirical methods mainly lies in a semiquantitative classification of electronic pro perties and in the search for regularities within given classes of larger molecules. The reader is supposed to have had some previous basic instruc tion in quantum mechanics, such as is now offered in many uni versities to chemists in their third or fourth year of study. The bibliography should encourage the reader to consult other texts, in particular also selected publications in scientific journals. Answering the need to facilitate quantum-chemical calculations of systems with thousands of atoms, Kazuo Kitaura and his coworkers developed the Fragment Molecular Orbital (FMO) method in 1999. Today, the FMO method can be applied to the study of whole proteins and protein-ligand interactions, and is extremely effective in calculating the propertie During the past few years, there has been dramatic progress in theoretical and computational studies of large molecules and local ized states in solids. Various semi-empirical and first-principles methods well known in quantum chemistry have been applied with considerable success to ever larger and more complex molecules, including some of biological importance, as well as to selected solid state problems involving localized electronic states. In creasingly, solid state physicists are adopting a molecular point of view in attempting to understand the nature of electronic states associated with (a) isolated structural and chemical defects in solids; (b) surfaces and interfaces; and (c) bulk disordered solids, most notably amorphous semiconductors. Moreover, many concepts and methods already widely used in solid state physics are being adapted to molecular problems. These adaptations include pseudopotentials, statistical exchange approxi mations, muffin-tin model potentials, and multiple scattering and cellular methods. In addition, many new approaches are being de vised to deal with progressively more complex molecular and local ized electronic state problems. Describes the essence of the orbit method for non-experts and gives a detailed exposition of the method. This work can be used as a text for a graduate course, as well as a handbook for non-experts and a reference book for research mathematicians and mathematical physicists. Ever since its introduction around 1960 by Kirillov, the orbit method has played a major role in representation theory of Lie groups and Lie algebras. This book contains the proceedings of a conference held from August 29 to September 2, 1988, at the University of Copenhagen, about "the orbit method in representation theory." It contains ten articles, most of which are original research papers, by well-known mathematicians in the field, and it reflects the fact that the orbit method plays an important role in the representation theory of semisimple Lie groups, solvable Lie groups, and even more general Lie groups, and also in the theory of enveloping algebras. Fragmentation: Toward Accurate Calculations on Complex Molecular Systems introduces the reader to the broad array of fragmentation and embedding methods that are currently available or under development to facilitate accurate calculations on large, complex systems such as proteins, polymers, liquids and nanoparticles. These methods work by subdividing a system into subunits, called fragments or subsystems or domains. Calculations

are performed on each fragment and then the results are combined to predict properties for the whole system. Topics covered include: Fragmentation methods Embedding methods Explicitly correlated local electron correlation methods Fragment molecular orbital method Methods for treating large molecules This book is aimed at academic researchers who are interested in computational chemistry, computational biology, computational materials science and related fields, as well as graduate students in these fields.

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