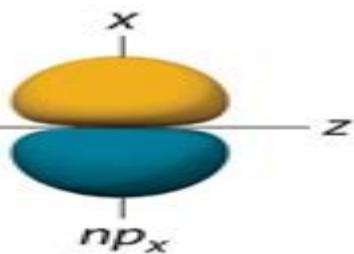
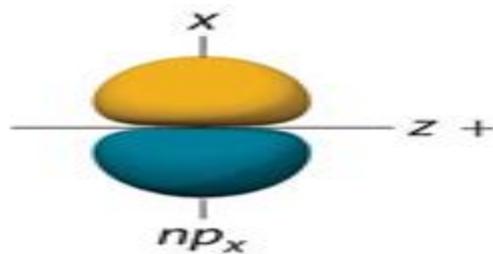
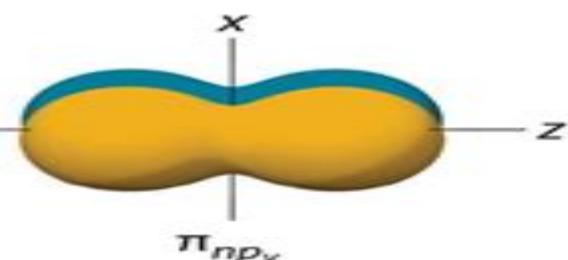
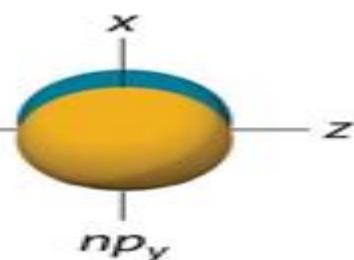
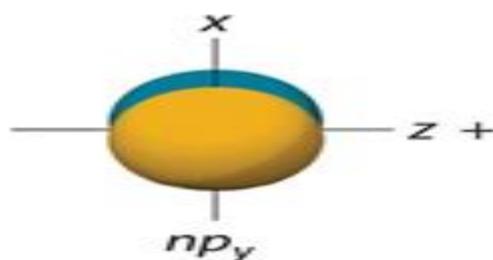
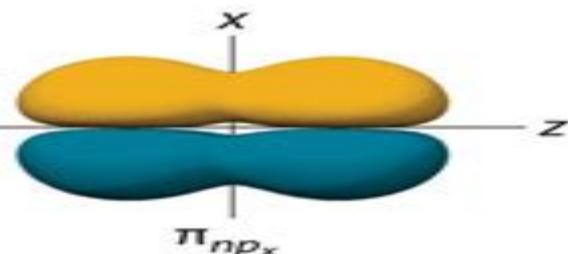


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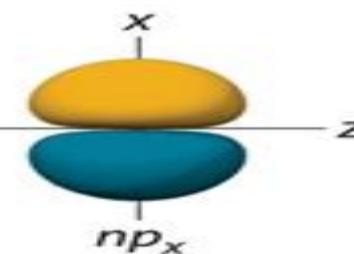
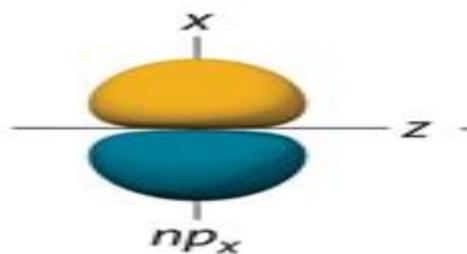


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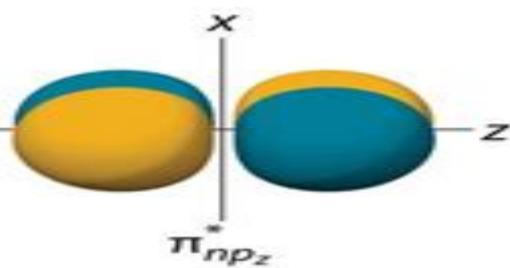
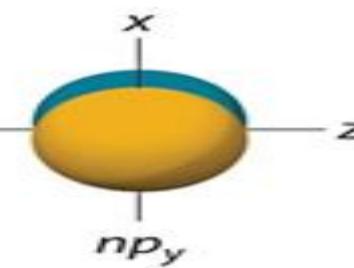
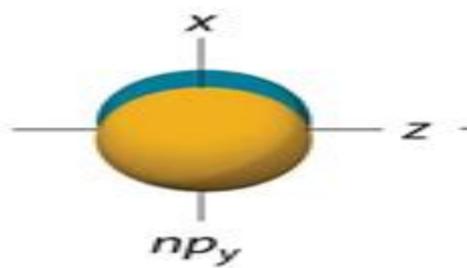
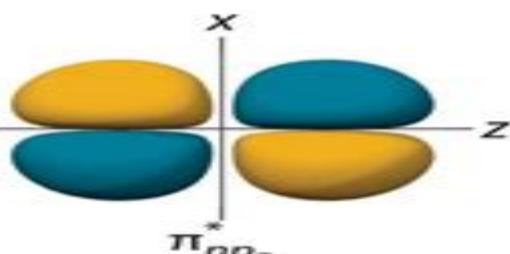


(a) Bonding

Atomic orbitals



Molecular orbitals



(b) Antibonding

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Molecular Orbitals in Chemistry, Physics, and Biology Robert Sanderson Mulliken, 1964

Frontier Orbitals And Reaction Paths: Selected Papers Of Kenichi Fukui Hiroshi Fujimoto, Kenichi Fukui, 1997-11-26 This book is a collection of selected papers on the Frontier Orbital Theory by Nobel prizewinner Kenichi Fukui Chemistry 1981 with introductory notes It provides the basic concept and formulation of the theory and the physical and chemical significance of the frontier orbital interactions in chemistry together with many practical applications The formulation of the Intrinsic Reaction Coordinate and applications to some simple systems are also presented The aim of this volume is to show by what forces chemical reactions are driven and to demonstrate how the regio and stereo selectivities are determined in chemical reactions Students and senior investigators will gain insight into the nature of chemical reactions and find out how quantum chemical calculations are connected with chemical intuition

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Molecular Orbitals and their Energies, Studied by the Semiempirical HAM Method Einar Lindholm, Leif Asbrink, 2012-12-06 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 f_{5y} were parametrized using Slater's shielding concept The self repulsion was compensated by a term $1/2 \sum_{i,j} f_{ij}^2 E_{HAM}$ 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 F_{pv} were then obtained from E in a conventional way

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Introduction to Elementary Molecular Orbital Theory and to Semiempirical Methods G.H. Wagniere, 2012-12-06 These notes summarize in part lectures held regularly at the University of Zurich and in the Summer of 1974 at the Seminario Latinoamericano de Quimica Cuantica in Mexico I am grateful to those who have encouraged me to publish these lectures or have contributed to them by their suggestions In particular I wish to thank Professor J Keller of the Universidad 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 provide 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 properties and in the search for regularities within given classes of larger molecules The reader is supposed to have had some previous basic instruction in quantum mechanics such as is now offered in many universities 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

The Quantum Theory of Atoms, Molecules and Photons John Avery, 1972

International Physics & Astronomy Directory, 1969 Intended as a comprehensive current source of professional information for the use of physicists and astronomers Faculty and brief biographical data listed under institutions which are arranged alphabetically Data about laboratories international organizations societies meetings financial support awards research and books and journals Faculty index Geographical index of universities and colleges

Physical Organic Chemistry Neil S. Isaacs, 1987 Physical Organic Chemistry deals with reaction mechanisms and with the experimental techniques and logical connections used in the establishment of a consistent theory of organic chemistry

Molecular Orbitals in Chemistry, Physics, and Biology Per-Olov Löwdin, Robert Sanderson Mulliken,

U.S. Government Research & Development Reports, 1970

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