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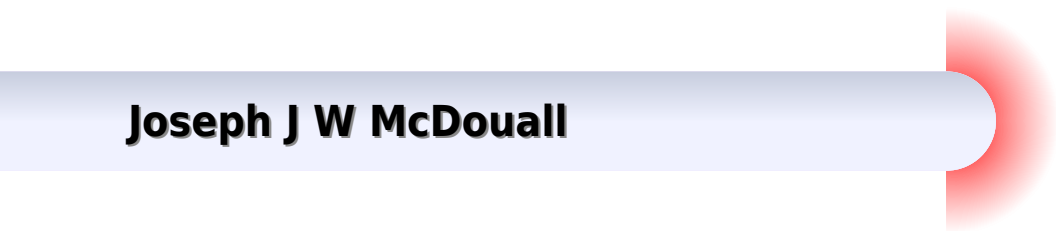
Non-Covalent Interactions

Theory and Experiment



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Joseph J W McDouall



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Non-covalent Interactions Pavel Hobza, Klaus Müller-Dethlefs, 2010 Co authored by an experimentalist Klaus M3ller Dethlefs and theoretician Pavel Hobza the aim of this book is to provide a general introduction into the science behind non covalent interactions and molecular complexes using some important experimental and theoretical methods and approaches

Computational Quantum Chemistry Joseph J W McDouall, 2015-11-09 Computational Quantum Chemistry presents computational electronic structure theory as practised in terms of ab initio waveform methods and density functional approaches Getting a full grasp of the field can often prove difficult since essential topics fall outside of the scope of conventional chemistry education This professional reference book provides a comprehensive introduction to the field Postgraduate students and experienced researchers alike will appreciate Joseph McDouall s engaging writing style The book is divided into five chapters each providing a major aspect of the field Electronic structure methods the computation of molecular properties methods for analysing the output from computations and the importance of relativistic effects on molecular properties are also discussed Links to the websites of widely used software packages are provided so that the reader can gain first hand experience of using the techniques described in the book

Simulating Enzyme Reactivity Inaki Tunon, Vicent Moliner, 2016-11-25 Exploring the theories methodologies and applications in simulations of enzymatic reactions this book is a great resource for postgraduate students and researchers

In Silico Medicinal Chemistry Nathan Brown, 2015-11-02 Exploring the methodologies and applications of computational tools in drug design this book is a practical introduction to chemoinformatics molecular modelling and computational chemistry for researchers

Theory of Molecular Collisions Gabriel G. Balint-Kurti, Alexander P. Palov, 2015-07-03 Almost 100 years have passed since Trautz and Lewis put forward their collision theory of molecular processes Today knowledge of molecular collisions forms a key part of predicting and understanding chemical reactions This book begins by setting out the classical and quantum theories of atom atom collisions Experimentally observable aspects of the scattering processes their relationship to reaction rate constants and the experimental methods used to determine them are described The quantum mechanical theory of reactive scattering is presented and related to experimental observables The role of lasers in the measurement and analysis of reactive molecular collisions is also discussed Written with postgraduates and newcomers to the field in mind mathematics is kept to a minimum and readers are guided to appendices and further reading to gain a deeper understanding of the mathematics involved

Computational Biophysics of Membrane Proteins Carmen Domene, 2016-11-30 Exploring current themes in modern computational and membrane protein biophysics this book presents a comprehensive account of the fundamental principles underlying different methods and techniques used to describe the intriguing mechanisms by which membrane proteins function The book discusses the experimental approaches employed to study these proteins with chapters reviewing recent crucial structural advances that have allowed computational biophysicists to discern how these molecular machines

work The book then explores what computational methods are available to researchers and what these have taught us about three key families of membrane proteins ion channels transporters and receptors The book is ideal for researchers in computational chemistry and computational biophysics

Theoretical Chemistry for Electronic Excited States Michael A. Robb, 2018-03-02 This reference is ideal for both theorists and experimentalists working in theoretical chemistry electronic structure and molecular dynamics

Reaction Rate Constant Computations Keli Han, Tianshu Chi, 2014 The reaction rate constant plays an essential role a wide range of processes in biology chemistry and physics Calculating the reaction rate constant provides considerable understanding to a reaction and this book presents the latest thinking in modern rate computational theory The editors have more than 30 years experience in researching the theoretical computation of chemical reaction rate constants by global dynamics and transition state theories and have brought together a global pool of expertise discussing these in a variety of contexts and across all phases This thorough treatment of the subject provides an essential handbook to students and researchers entering the field and a comprehensive reference to established practitioners across the sciences providing better tools to determining reaction rate constants

Computational Nanoscience Elena Bichoutskaia, 2011-06-09 Nanoscience is one of the most exciting areas of modern physical science as it encompasses a range of techniques rather than a single discipline It stretches across the whole spectrum of science including medicine and health physics engineering and chemistry Providing a deep understanding of the behaviour of matter at the scale of individual atoms and molecules it provides a crucial step towards future applications of nanotechnology The remarkable improvements in both theoretical methods and computational techniques make it possible for modern computational nanoscience to achieve a new level of chemical accuracy It is now a discipline capable of leading and guiding experimental efforts rather than just following others Computational Nanoscience addresses modern challenges in computational science within the context of the rapidly evolving field of nanotechnology It satisfies the need for a comprehensive yet concise and up to date survey of new developments and applications presented by the world's leading academics It documents major recent advances in scientific computation mathematical models and theory development that specifically target the applications in nanotechnology Suitable for theoreticians researchers and students the book shows readers what computational nanoscience can achieve and how it may be applied in their own work The twelve chapters cover topics including the concepts behind recent breakthroughs the development of cutting edge simulation tools and the variety of new applications

σ - and π -Hole Interactions Antonio Frontera, 2021-03-30 This book describes unconventional noncovalent interactions and analyzes their importance for crystal growth in organic and hybrid organic inorganic systems Several examples illustrate how the combination of theory and experiment allows rationalizing the strength and directionality of noncovalent interactions This book elegantly describes the results of a survey of X ray structures of main group element compounds M Sn Pb As Sb Bi and Te exhibiting intermolecular M Se noncovalent interactions in one of its chapters Moreover it provides a consistent

description of noncovalent interactions covering most groups of the periodic table The interactions are described and discussed using their trivial names That is a comprehensive and accurate description is provided for alkali alkaline earth regium spodium triel tetrel pnictogen chalcogen halogen and aerogen bonding interactions No other book is available covering such an extensive number of interactions and examples where these interactions are relevant relevant

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