Preface

This book is written for both theoretical and experimental scientist (chemists and physicists) to help understand chemical bonding and electronic structure, from the viewpoint of molecular orbital theory. A long time ago, quantum theory was applied to very simple atoms. To connect quantum theory with complex systems, there were many research activities in the fields of quantum chemistry and physics: the Bohr model, wave-function, Schrödinger's equation, the Hartree-Fock method, Mulliken charge density analysis, density functional theory, etc. Due to this research, we are now able to perform molecular orbital calculations from small molecules through to advanced materials including transition metals. In this book, chemical bonding and electronic structure are explained with the use of concrete calculation results, density functional theory, and coupled cluster methods.

In Part I the theoretical background of quantum chemistry is clearly explained. In Part II we introduce molecular orbital analysis of atoms and diatomic molecules via concrete calculation results. After introducing the theoretical background of inorganic chemistry in Part III, the concrete calculation results for advanced materials such as photocatalysts, secondary batteries, and fuel cells are introduced in Part IV. Finally, helium chemistry and the future of the subject are considered in Part V.

Acknowledgements

My research work has been supported by the Research Council of Norway (RCN) through CoE Grant No. 179568/V30 (CTCC) and through NOTUR Grant No. NN4654K for HPC resources. I thank Professor Trygve Helgaker for his kind research support and encouragement since my first stay in Norway.

I wrote most of the book during my research stay at the Centre for Theoretical and Computational Chemistry (CTCC), University of Oslo, Norway, and Department of Applied Physics, Graduate School of Engineering, Osaka University, Japan.

Finally, I am especially grateful for the constructive discussions I had with TO.

Quantum chemistry is not virtual but real

Research is first discovery

Kobe, Japan Taku Onishi
May 2017

http://www.springer.com/978-981-10-5932-2

Quantum Computational Chemistry
Modelling and Calculation for Functional Materials
Onishi, T.
2018, XIII, 290 p. 171 illus., 147 illus. in color.,
Hardcover
ISBN: 978-981-10-5932-2