NEW! Includes free modeling software on CD-ROM

The Fragment Molecular Orbital Method
Practical Applications to Large Molecular Systems

Dmitri G. Fedorov • RICS, AIST Tsukuba, Japan
Kazuo Kitaura • Graduate School of Pharmaceutical Sciences, Kyoto University, Japan

FEATURES

• Focuses on practical guidelines for those who wish to apply the FMO method
• Includes a CD-ROM with data samples and application software
• Collects information found scattered in the literature and in software manuals
• Offers the expertise of the authors who are co-inventors of the FMO method

CONTENTS

Chapter 1: Introduction; Kazuo Kitaura and Dmitri G. Fedorov
Chapter 2: Theoretical Background of the Fragment Molecular Orbital (FMO) Method and Its Implementation in GAMESS; Dmitri G. Fedorov and Kazuo Kitaura
Chapter 3: Developments of FMO Methodology and Graphical User Interface in ABINIT-MP; Tatsuya Nakano, Yuji Mochizuki, Akifumi Kato, Kaori Fukuzawa, Takeshi Ishikawa, Shinji Amari, Ikuo Kurisaki, and Shigenori Tanaka
Chapter 4: Excited States of Photoactive Proteins by Configuration Interaction Studies; Yuji Mochizuki, Tatsuya Nakano, Naoki Taguchi, and Shigenori Tanaka
Chapter 5: The Fragment Molecular Orbital–Based Time-Dependent Density Functional Theory for Excited States in Large Systems; Mahito Chiba, Dmitri G. Fedorov, and Kazuo Kitaura
Chapter 6: FMO-MD: An Ab Initio-Based Molecular Dynamics of Large Systems; Yuto Komeiji
Chapter 7: Application of the FMO Method to Specific Molecular Recognition of Biomacromolecules; Kaori Fukuzawa, Yuji Mochizuki, Tatsuya Nakano, and Shigenori Tanaka

See reverse side for continuation of Contents, About The Authors and ordering information

The Fragment Molecular Orbital Method: Practical Applications to Large Molecular Systems is for those researchers eager to obtain useful information from electronic structure calculations of large systems, and for those who wish to know what can be elucidated with the calculations at present and in the near future. The text emphasizes the practical aspects, with as little mathematical detail as possible and in language that is easy to understand.

CD-ROM Included!

The free modeling software Facio, in which FMO-related functions are implemented, is provided on the accompanying CD-ROM, which also provides input file samples, usage hints, annotated output from typical calculations, easy-to-follow tutorial material, and AppliGuide movies that show the sequence of mouse operations for data processing.

The book encourages readers to perform their own calculations — describing the features of the freely available FMO programs (GAMESS and ABINIT-MP) and reviewing many successful applications of the FMO method to practical problems. Filled with practical advice from the inventors of the method and from world-renowned contributors, this reference provides general scientists with the foundation required to use FMO computational methods in a wide range of biomolecular applications, including drug design, protein–ligand binding, enzyme reactivity, and light-driven processes.

Developers interested in extending FMO capabilities or in advancing their own methods will find sufficient information and mathematical detail to encourage method development.
Chapter 8: Detailed Electronic Structure Studies Revealing the Nature of Protein–Ligand Binding; Isao Nakamishi, Dmitri G. Fedorov, and Kazuo Kitaura

Chapter 9: How Does the FMO Method Help in Studying Viruses and Their Binding to Receptors?; Toshihiko Sawada, Tomohiro Hashimoto, Hiroaki Tokiya, Tohru Suzuki, Hirofumi Nakano, Hideharu Ishida, Makoto Kiso, and Yasuo Suzuki

Chapter 10: FMO as a Tool for Structure-Based Drug Design; Tomonaga Ozawa, Koike Okazaki, and Motohiro Nishio

Chapter 11: Modeling a Protein Environment in an Enzymatic Catalysis: A Case Study of the Chorismate Mutase Reaction; Toyokazu Ishida

Index

About The Authors

Dmitri G. Fedorov received his M.S. in quantum chemistry from St. Petersburg State University in Russia in 1993. He was awarded a Ph.D. in physical chemistry at Iowa State University in 1999, working under the guidance of Mark Gordon. He spent 2 years at the University of Tokyo as a Japan Society for the Promotion of Science (JSPS) Postdoctoral Research Fellow, where he worked with Kimihiko Hiroa. He then moved to the Research Institute for Computational Sciences (RICS) at the National Institute of Advanced Industrial Science and Technology (AIST) in Japan in 2002, where he is currently employed as senior research scientist. Dr. Fedorov’s research interests include the relativistic effects in chemistry as well as the quantum-mechanical method development for describing large systems, such as proteins.

Kazuo Kitaura received his Ph.D. in quantum chemistry in 1976 from Osaka City University. After working in Japan as a research associate at the Institute for Molecular Science and Osaka City University, he became associate professor in 1989 at the Institute for Molecular Science. In 1993, Dr. Kitaura was appointed professor at Osaka Prefecture University. In 2001, he moved to the Research Institute for Computational Sciences at AIST, where he serves as group leader and director, and is presently the principal research scientist. Since 2006, he has also been a professor at the School of Pharmaceutical Sciences, Kyoto University. Dr. Kitaura’s research interests include intermolecular interactions, structure and reactivity of transition metal complexes, and electronic structure theory for large molecules and molecular clusters.