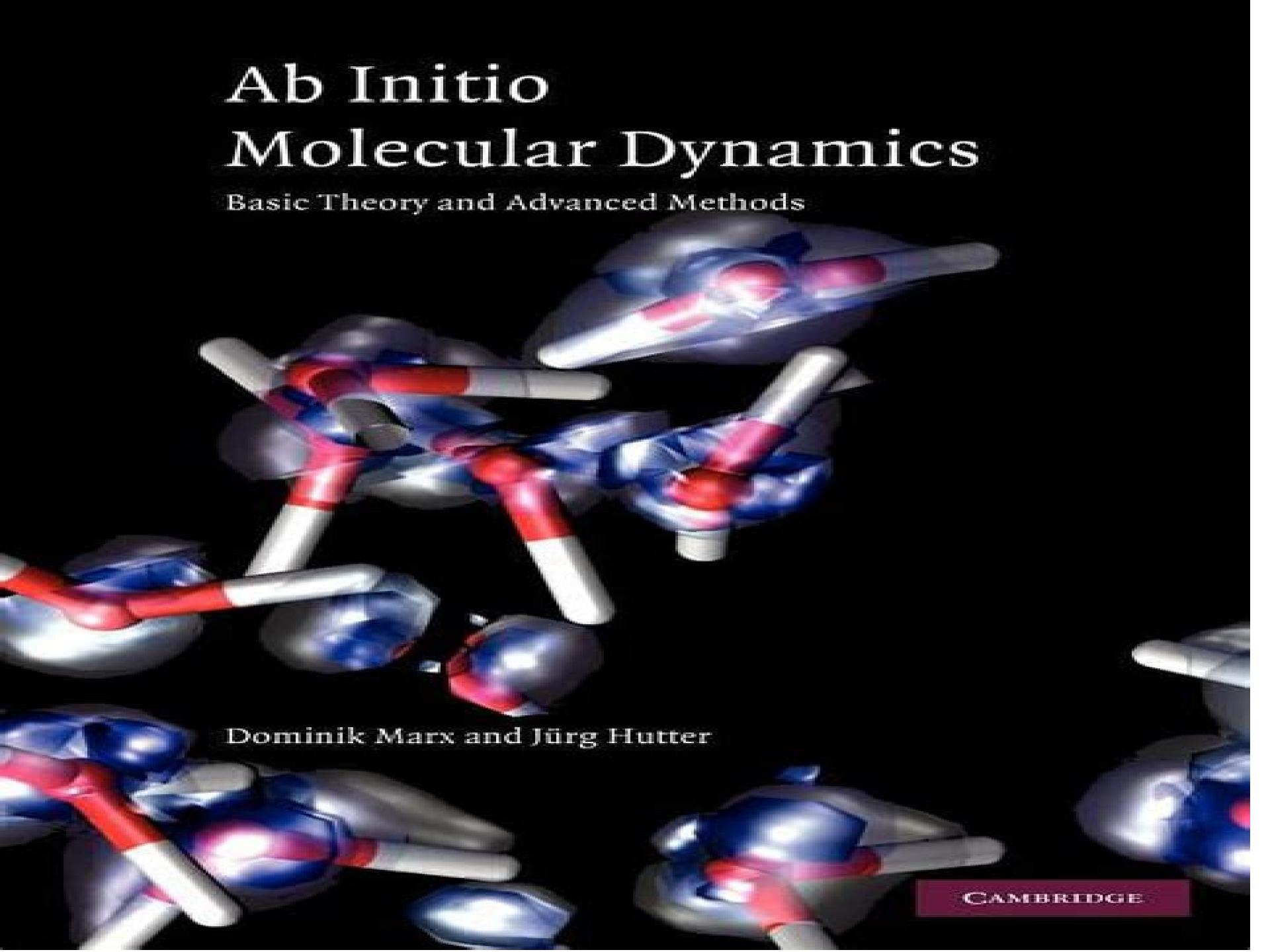


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Basic Theory and Advanced Methods



Dominik Marx and Jürg Hutter

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Ab Initio Molecular Dynamics Dominik Marx,Jürg Hutter,2010-01-29 Focusing on a breakthrough combination methodology this handbook and ready reference is the first book to collect and present all facets of the important Car Parrinello approach Clearly divided into three sections the text covers basic and advanced techniques before finishing with applications A must have for all computational researchers and producers of pharmaceuticals and other complex molecules

Advances in Density Functional Theory and Beyond for Computational Chemistry Wei Hu,Mohan Chen,2021-09-13 [Advanced Methods in Ab-initio Molecular Dynamics](#) Fawzi Roberto Mohamed,2006 [Exploration on Quantum Chemical Potential Energy Surfaces](#) Koichi Ohno,Hiroko Satoh,2022-12-12 Written chemical formulas such as C2H6O can tell us the constituent atoms a molecule contains but they cannot differentiate between the possible geometrical arrangements isomers of these models Yet the chemical properties of different isomers can vary hugely Therefore to understand the world of chemistry we need to ask what kind of isomers can be produced from a given atomic composition how are isomers converted into each other how do they decompose into smaller pieces and how can they be made from smaller pieces The answers to these questions will help us to discover new chemistry and new molecules A potential energy surface PES describes a system such as a molecule based on geometrical parameters The mathematical properties of the PES can be used to calculate probable isomer structures as well as how they are formed and how they might behave Exploration on Quantum Chemical Potential Energy Surfaces focuses on the PES search based on quantum chemical calculations It describes how to explore the chemical world on PES discusses fundamental methods and specific techniques developed for efficient exploration on PES and demonstrates several examples of the PES search for chemical structures and reaction routes [Annual Reports on Computational Chemistry](#) David A. Dixon,2023-11-29 Annual Report in Computational Chemistry Volume 19 the latest release in this highly regarded series highlights new advances in the field with this new volume presenting interesting chapters written by an international board of authors Provides the authority and expertise of

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