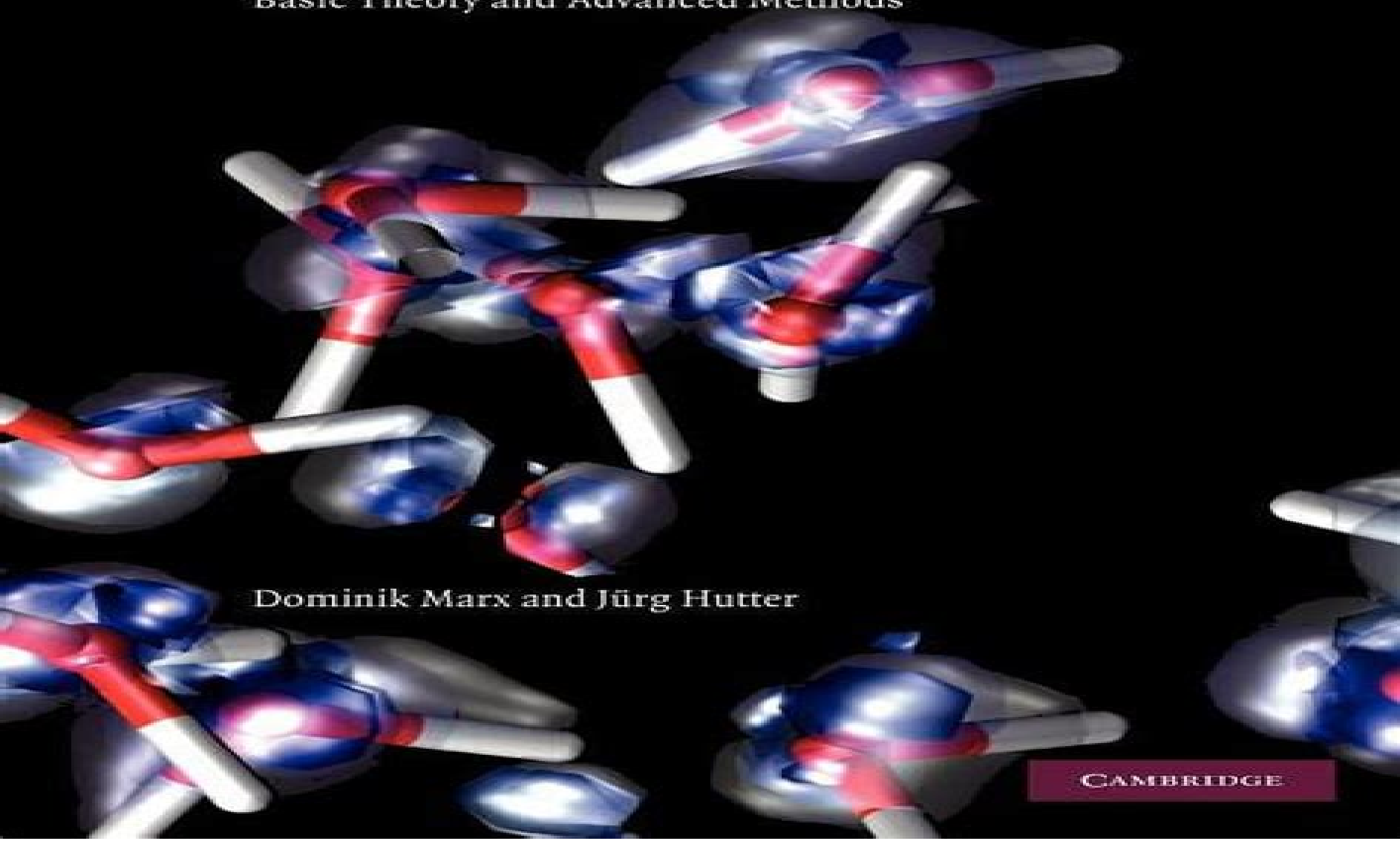


Ab Initio Molecular Dynamics

Basic Theory and Advanced Methods

Dominik Marx and Jürg Hutter

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several characterization techniques with an understanding at the molecular level of chemical and physical phenomena are the main focal point of the subject matter

Dynamics of Gas-Surface Interactions Ricardo Diez Muino, Heriberto Fabio Busnengo, 2013-02-26 This book gives a representative survey of the state of the art of research on gas surface interactions. It provides an overview of the current understanding of gas surface dynamics and in particular of the reactive and non reactive processes of atoms and small molecules at surfaces. Leading scientists in the field both from the theoretical and the experimental sides write in this book about their most recent advances. Surface science grew as an interdisciplinary research area over the last decades mostly because of new experimental technologies: ultra high vacuum for instance as well as because of a novel paradigm: the surface science approach. The book describes the second transformation which is now taking place pushed by the availability of powerful quantum mechanical theoretical methods implemented numerically. In the book experiment and theory progress hand in hand with an unprecedented degree of accuracy and control. The book presents how modern surface science targets the atomic level understanding of physical and chemical processes at surfaces with particular emphasis on dynamical aspects. This book is a reference in the field.

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