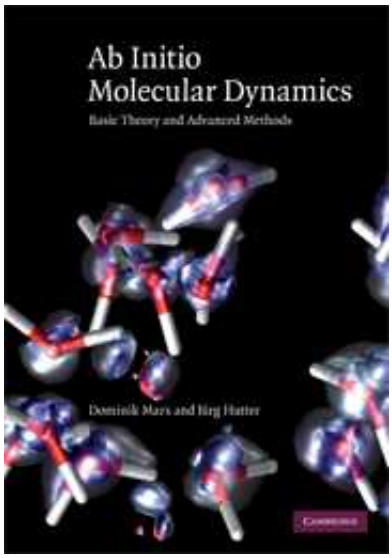
Ab Initio Molecular Dynamics: Basic Theory and Advanced Methods



Blurb cited from the back of the book:
"Ab initio molecular dynamics revolutionized the field of realistic computer simulation of complex molecular systems and processes, including chemical reactions, by unifying molecular dynamics and electronic structure theory. This book provides the first coherent presentation of this rapidly growing field, covering a vast range of methods and their applications, from basic theory to advanced methods. This fascinating text for graduate students and researchers contains systematic derivations of various ab initio molecular dynamics techniques to enable readers to understand and assess the merits and drawbacks of commonly used methods. It also discusses the special features of the widely used Car-Parrinello approach, correcting various misconceptions currently found in the research literature. The book contains pseudo-code and program layout for typical plane wave electronic structure codes, allowing newcomers to the field to understand commonly used program packages, and enabling developers to improve and add new features in their code."

This monograph should be cited as follows:
D. Marx and J. Hutter,
Ab Initio Molecular Dynamics: Basic Theory and Advanced Methods,
(Cambridge University Press, Cambridge 2009)
ISBN: 978--0--521--89863--8, hardback, 578 pages, 1669 references

- CUP Homepage of the book: *http://www.cambridge.org/9780521898638*
- Look inside the book: click here!
- Errata and Addenda of the book: click here!

Ab Initio Molecular Dynamics: Theory and Implementation

This review article describes various types of *ab initio* molecular dynamics techniques (such as e.g. Car-Parrinello molecular dynamics) and the particular implementation of these methods in the `CPMD code`. In addition, lots of references to applications in various fields are compiled. The article can be downloaded as a PDF or as a Postscript file.

This article should be cited as follows:

D. Marx and J. Hutter,
"*Ab Initio* Molecular Dynamics: Theory and Implementation",
in "Modern Methods and Algorithms of Quantum Chemistry" (p. 301-449),
Editor: J. Grotendorst,
(NIC, FZ Jülich 2000).

First Principles Molecular Dynamics Involving Excited States and Nonadiabatic Transitions

Extensions of traditional molecular dynamics to excited electronic states and non-Born-Oppenheimer dynamics are reviewed focussing on applicability to chemical reactions of large molecules, possibly in condensed phases. The review exclusively deals with *ab initio* "on the fly" molecular dynamics methods.
Note: It is illegal to download this PDF file: please contact us at theochem@theochem.rub.de and you will receive a legal reprint of this article as soon as possible.

This article should be cited as follows:

N. L. Doltsinis and D. Marx,
"First Principles Molecular Dynamics Involving Excited States and Nonadiabatic Transitions",
J. Theor. Comput. Chem. **1**, 319-349 (2002).

Computational Nanoscience: Do It Yourself!

NIC Winter School 2006: Computational science plays an ever increasing role in understanding materials and molecular systems. The nanometer scale in particular is governed by the laws of quantum mechanics, which calls for electronic structure theory in order to address questions related to stability of structures, chemical processes or spectral properties. This hands-on NIC Winter School focuses on the application of modern electronic structure calculations and dynamical simulation techniques covering aspects of solid state and surface science, chemical reactions and dynamics, as well as the structure and properties of large molecules and clusters. The School will provide a practical introduction to the theory behind and handling of pertinent software packages through practicals and tutorials in small groups using four codes. The full-potential linearized augmented plane wave code FLEUR and the Korringa-Kohn-Rostocker Green function code KKR-GF, the ab initio (Car-Parrinello) molecular dynamics simulation package CPMD, and the highly efficient quantum chemistry code TURBOMOLE. Although very different in concept and application focus, all these codes are well-known prototypical representatives and are used in various supercomputer centres around the world.

The Lecture Notes can be downloaded for free (as an alternative to ordering a nice hardbound version from the NIC Secretariat).

This book should be cited as follows:

J. Grotendorst, S. Blügel, and D. Marx,
"Computational Nanoscience: Do It Yourself!" (NIC, FZ Jülich 2006)

Quantum Simulations of Complex Many-Body Systems: From Theory to Algorithms

For a broader overview about the state-of-the-art quantum simulation techniques in general see the Lecture Notes of the NIC 2002 Winter School on Quantum Simulations which you can download for free (as an alternative to ordering a nice hardbound version from the NIC Secretariat).

This book should be cited as follows:
J. Grotendorst, D. Marx, and A. Muramatsu, "Quantum Simulations of Complex Many-Body Systems: From Theory to Algorithms" (NIC, FZ Jülich 2002)

In addition, an audio-visual multimedia presentation of the entire NIC 2002 Winter School is available on the web (the corresponding DVD can also be ordered from the NIC Secretariat).

Theoretical Chemistry in the 21st Century: The ’Virtual Lab’

Electronic structure calculation and computer simulation became unified by Car and Parrinello in terms of a dynamical propagation scheme where the orbitals are treated as fictitious scalar fields obeying classical mechanics. This allows the treatment of multicomponent systems with complicated interactions based on first principles. Most importantly within Chemistry, this idea opens an avenue to studying chemical reactions that involve many coupled degrees of freedom, such as those taking place in liquids, in the computer. It is argued that one important branch of Theoretical Chemistry will be devoted to developing and applying such "virtual laboratory methods’’. Two recent examples where chemical reactions are induced by photons (photochemistry) or by an external mechanical force (mechanochemistry) are presented. The article can be downloaded as a PDF file.

This article should be cited as follows:

D. Marx,
Theoretical Chemistry in the 21st Century: The ’Virtual Lab’,
in "Proceedings of the Idea-Finding Symposium: Frankfurt Institute for Advanced Studies" (p. 139-153),
Editors: W. Greiner and J. Reinhardt,
(EP Systema, Debrecen, 2004).

Parrinello Festschrift: From Physics via Chemistry to Biology

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From the Editorial: It is an honor and a pleasure to dedicate this *Festschrift* to Professor Michele Parrinello on the occasion of his 60th birthday. His various original contributions to modern computational methods and algorithms in the realm of molecular sciences are invaluable and we are confident that they will enjoy an ever growing impact on our understanding thereof. Indeed, his work has already opened many new avenues for the study of processes and properties in diverse fields ranging from liquids to chemical reactions and biochemistry, bridging the gap from fundamental methodology to groundbreaking applications. It is instructive to retrace Parrinello’s path in science, from...

The Editorial should be cited as follows:

W. Andreoni, D. Marx, and M. Sprik,
A Tribute to Michele Parrinello: From Physics via Chemistry to Biology (Editorial of the "Parrinello Festschrift’’),
ChemPhysChem **6**, p. 1671-1676 (2005).

The *Festschrift* should be cited as follows:

W. Andreoni, D. Marx, and M. Sprik,
Parrinello Festschrift: From Physics via Chemistry to Biology (Special Issue),
ChemPhysChem Volume **6**, p. 1671-1947 (2005).