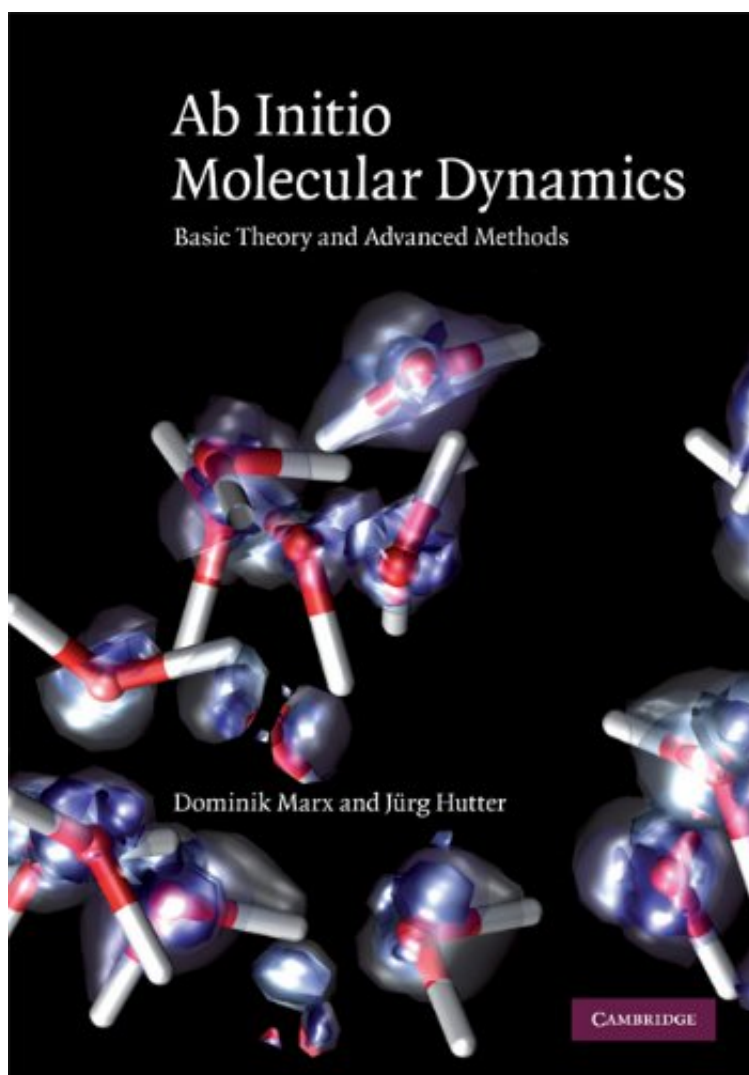


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# Ab Initio Molecular Dynamics: Basic Theory and Advanced Methods



*Par Dominik Marx, Jrg Hutter*  
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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. Revue de presse of the hardback: ' a student or newcomer to the field of molecular dynamics will find the approaches discussed in *Ab Initio Molecular Dynamics* a good place to start [The book is] written clearly and informed by the state-of-the-art research experiences of the authors themselves. Reading it is a valuable experience akin to spending time in their research groups.' *Physics Today* Presentation de l'auteur *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 CarParrinello approach, correcting various misconceptions currently found in 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.