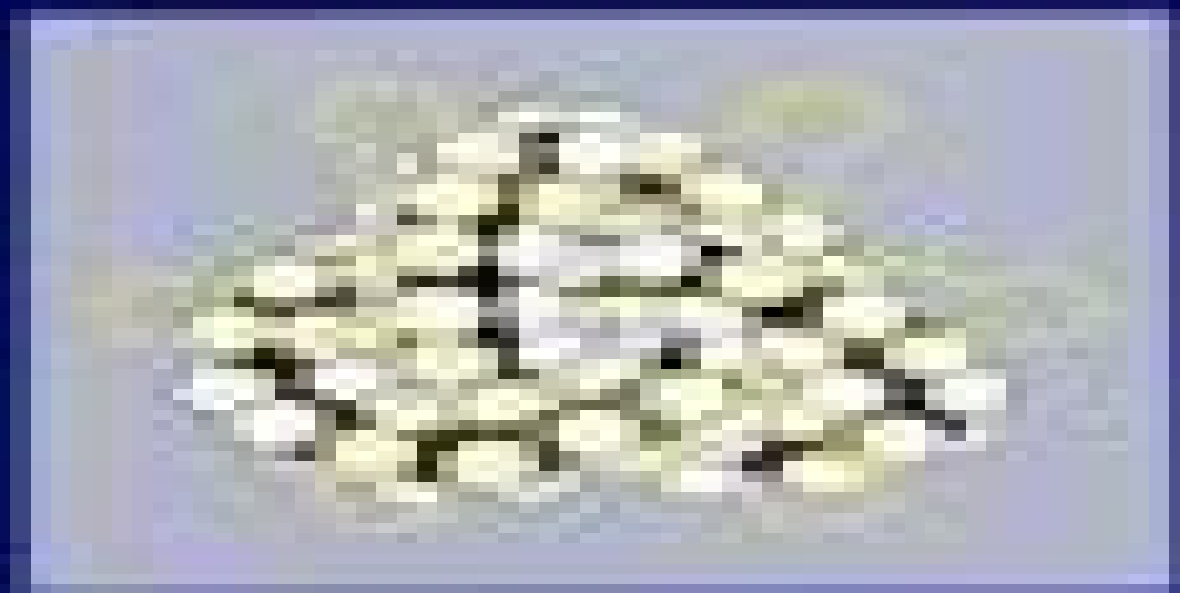


CHEMICAL APPLICATIONS OF MOLECULAR MODELLING



Chemical Applications Of Molecular Modelling

Michael Springborg



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Computational Chemistry and Molecular Modeling K. I. Ramachandran, Gopakumar Deepa, Krishnan Namboori, 2008-05-20 Computational chemistry and molecular modeling is a fast emerging area which is used for the modeling and simulation of small chemical and biological systems in order to understand and predict their behavior at the molecular level It has a wide range of applications in various disciplines of engineering sciences such as materials science chemical engineering biomedical engineering etc Knowledge of computational chemistry is essential to understand the behavior of nanosystems it is probably the easiest route or gateway to the fast growing discipline of nanosciences and nanotechnology which covers many areas of research dealing with objects that are measured in nanometers and which is expected to revolutionize the industrial sector in the coming decades Considering the importance of this discipline computational chemistry is being taught presently as a course at the postgraduate and research level in many universities This book is the result of the need for a comprehensive textbook on the subject which was felt by the authors while teaching the course It covers all the aspects of computational chemistry required for a course with sufficient illustrations numerical examples applications and exercises For a computational chemist scientist or researcher this book will be highly useful in understanding and mastering the art of chemical computation Familiarization with common and commercial software in molecular modeling is also incorporated Moreover the application of the concepts in related fields such as biomedical engineering computational drug designing etc has been added

Molecular Modelling Andrew R. Leach, 2001 Book is in the Baton Rouge Library 08 14 06

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is necessary if one wants to be able to reliably judge the results from molecular modeling calculations Its main objective is the description of the various pitfalls to be avoided Without unnecessary overhead it leads the reader from simple calculations on small molecules to the modeling of proteins and other relevant biomolecules A textbook for beginners as well as an invaluable reference for all those dealing with molecular modeling in their daily work *Molecular Modeling at the Atomic Scale* Ruhong Zhou,2014-08-21 Although molecular modeling has been around for a while the groundbreaking advancement of massively parallel supercomputers and novel algorithms for parallelization is shaping this field into an exciting new area Developments in molecular modeling from experimental and computational techniques have enabled a wide range of biological applications Responding to this renaissance *Molecular Modeling at the Atomic Scale Methods and Applications in Quantitative Biology* includes discussions of advanced techniques of molecular modeling and the latest research advancements in biomolecular applications from leading experts The book begins with a brief introduction of major methods and applications then covers the development of cutting edge methods algorithms new polarizable force fields and massively parallel computing techniques followed by descriptions of how these novel techniques can be applied in various research areas in molecular biology It also examines the self assembly of biomacromolecules including protein folding RNA folding amyloid peptide aggregation and membrane lipid bilayer formation Additional topics highlight biomolecular interactions including protein interactions with DNA RNA membrane ligands and nanoparticles Discussion of emerging topics in biomolecular modeling such as DNA sequencing with solid state nanopores and biological water under nanoconfinement round out the coverage This timely summary contains the perspectives of leading experts on this transformation in molecular biology and includes state of the art examples of how molecular modeling approaches are being applied to critical questions in modern quantitative biology It pulls together the latest research and applications of molecular modeling and real world expertise that can boost your research and development of applications in this rapidly changing field

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Molecular Modeling Hans-Dieter Höltje, 2003

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principle molecular dynamics In the following chapters techniques bridging microscopic and mezosopic modeling scales are presented The authors then illustrate various successful applications of molecular design of new materials drugs biocatalysts etc before presenting challenging topics in molecular materials design

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