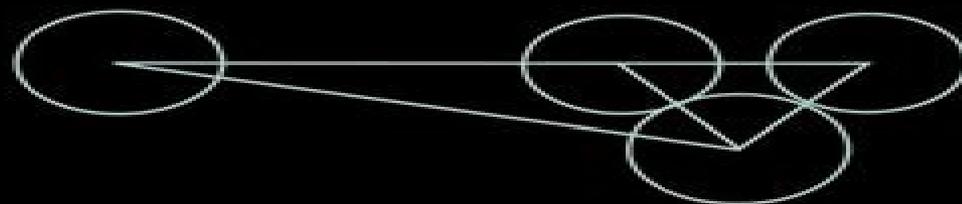


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Computer Simulation of Biomolecular Systems W.F. van Gunsteren,P.K. Weiner,A.J. Wilkinson,1994-01-31 The long range goal of molecular approaches to biology is to describe living systems in terms of chemistry and physics Over the last fifty years great progress has been made in applying the equations representing the underlying physical laws to chemical problems involving the structures and reactions of small molecules Corresponding studies of mesoscopic systems have been undertaken much more recently Molecular dynamics simulations which are the primary focus of this volume represent the most important theoretical approach to macromolecules of biological interest Now that molecular dynamics of macromolecules is a flourishing field serious questions have to be asked concerning what more can be done with the methodology What is the present and the future role of molecular dynamics in the development of our knowledge of macromolecules of biological interest How does the methodology need to be improved to make it applicable to important problems The present volume is concerned with providing some answers with its primary focus on the methodology and its recent developments

Physical Review,2000-09

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