This article was downloaded by:

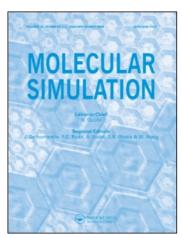
On: 14 January 2011

Access details: Access Details: Free Access

Publisher Taylor & Francis

Informa Ltd Registered in England and Wales Registered Number: 1072954 Registered office: Mortimer House, 37-

41 Mortimer Street, London W1T 3JH, UK



Molecular Simulation

Publication details, including instructions for authors and subscription information: http://www.informaworld.com/smpp/title~content=t713644482

Guest Editorial

Sanat Kumar

To cite this Article Kumar, Sanat(1994) 'Guest Editorial', Molecular Simulation, 13: 4, 243

To link to this Article: DOI: 10.1080/08927029408021990 URL: http://dx.doi.org/10.1080/08927029408021990

PLEASE SCROLL DOWN FOR ARTICLE

Full terms and conditions of use: http://www.informaworld.com/terms-and-conditions-of-access.pdf

This article may be used for research, teaching and private study purposes. Any substantial or systematic reproduction, re-distribution, re-selling, loan or sub-licensing, systematic supply or distribution in any form to anyone is expressly forbidden.

The publisher does not give any warranty express or implied or make any representation that the contents will be complete or accurate or up to date. The accuracy of any instructions, formulae and drug doses should be independently verified with primary sources. The publisher shall not be liable for any loss, actions, claims, proceedings, demand or costs or damages whatsoever or howsoever caused arising directly or indirectly in connection with or arising out of the use of this material.

Molecular Simulation, 1994, Vol. 13, pp. 243 Reprints available directly from the publisher Photocopying permitted by license only

Downloaded At: 19:28 14 January 2011

GUEST EDITORIAL

The computer simulation of macromolecular systems has experienced very rapid progress in the last decade; with the advent of large computers as well as the development of new algorithms which make the simulation of real systems an attainable goal. The practical value of such work cannot be stressed enough, and the existence of at least three different software packages marketed primarily to industrial professionals is suitable testament to this fact. Recent pioneering work has allowed the simulation of polymeric glasses, the Monte Carlo simulations of chains with realistic architectures, as well as the calculation of the free energies and the phase diagrams of these soft condensed phases with fully delineated molecular structures. In view of this progress it might appear that the field of polymer modeling is mature: rather, it is a field still under development with many problems, such as polyelectreolytes, which have not even been explored perfunctorily. It is with this background that the current issue of Molecular Simulation was assembled: a diverse field of experts have contributed papers ranging from diblock copolymers, to electrophoresis and to biopolymers. It is hoped that these articles will provide a vision of a future in which molecular modeling can supply researchers with effective tools for solving important practical problems.

Sanat Kumar Pennsylvania