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Novel Methods in Soft Matter Simulations



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Novel Methods In Soft Matter Simulations Lecture Notes In Physics

**Purushottam D. Gujrati, Arkady I.
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New Algorithms for Macromolecular Simulation Benedict Leimkuhler, Christophe Chipot, Ron Elber, Aatto Laaksonen, Alan Mark, Tamar Schlick, Christoph Schütte, Robert Skeel, 2006-03-22 Molecular simulation is a widely used tool in biology chemistry physics and engineering This book contains a collection of articles by leading researchers who are developing new methods for molecular modelling and simulation Topics addressed here include multiscale formulations for biomolecular modelling such as quantum classical methods and advanced solvation techniques protein folding methods and schemes for sampling complex landscapes membrane simulations free energy calculation and techniques for improving ergodicity The book is meant to be useful for practitioners in the simulation community and for those new to molecular simulation who require a broad introduction to the state of the art

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

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