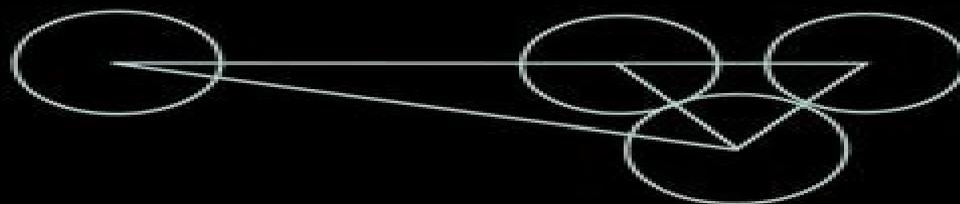


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*Elementary Methods*



J. M. HAILE

# Molecular Dynamics Simulation Elementary Methods

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Computing and Logic Based Methods for Decision Making and Data Mining respectively All chapters in the book discuss theoretical and practical issues connected with computational methods and optimization methods for knowledge engineering

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scientists in fields like biochemistry biophysics physical chemistry or statistical physics and numerical analysts as well as computer scientists working on the advancement of algorithms for a total of over 120 participants from 19 countries In the course of the symposium the speakers agreed to produce a representative volume that combines survey articles and original papers all refereed to give an impression of the present state of the art of Molecular Dynamics The 29 articles of the book reflect the main topics of the Berlin meeting which were i Conformational Dynamics ii Thermodynamic Modelling iii Advanced Time Stepping Algorithms iv Quantum Classical Simulations and Fast Force Field and v Fast Force Field Evaluation

*Molecular Dynamics Simulations of Nucleation and Phase Transitions in Molecular Clusters of Hexafluorides* Shimin Xu,1993

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**Physical Review** ,2000-09

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ITHERM ,2004

Papers Presented at the ... Meeting American Chemical Society. Division of Polymer Chemistry,1996

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