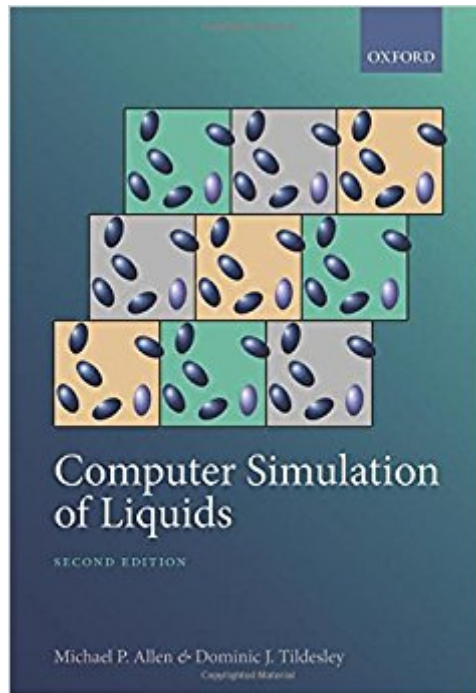




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Computer Simulation Of Liquids



Synopsis

This book provides a practical guide to molecular dynamics and Monte Carlo simulation techniques used in the modelling of simple and complex liquids. Computer simulation is an essential tool in studying the chemistry and physics of condensed matter, complementing and reinforcing both experiment and theory. Simulations provide detailed information about structure and dynamics, essential to understand the many fluid systems that play a key role in our daily lives: polymers, gels, colloidal suspensions, liquid crystals, biological membranes, and glasses. The second edition of this pioneering book aims to explain how simulation programs work, how to use them, and how to interpret the results, with examples of the latest research in this rapidly evolving field.

Accompanying programs in Fortran and Python provide practical, hands-on, illustrations of the ideas in the text.

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Michael P. Allen, Emeritus Professor and Visiting Fellow, University of Warwick and University of Bristol, Dominic J. Tildesley, Director and Titulair Professor of Chemistry, CECAM and Ecole Polytechnique Federale de Lausanne Michael Allen obtained his first degree, and doctorate, in Chemistry at the University of Oxford. After post-doctoral positions at UCLA and Oxford, he was, in 1985, appointed Lecturer, then Reader, and finally Professor in Physics at the University of Bristol. In 2001 he became founding Director of the Centre for Scientific Computing in Warwick, where he stayed in Physics until retirement in 2014. Allen was awarded an Alexander von Humboldt

Foundation Forschungspreis in 1999, visiting Mainz (University and MPI for Polymer Research). He received the 2015 Lennard-Jones award and lectureship from the Royal Society of Chemistry Statistical Mechanics and Thermodynamics Group, and the Thermodynamics Conference series. Dominic Tildesley obtained his first degree at the University of Southampton, and his doctorate in Chemistry at the University of Oxford. After post-doctoral positions at Penn State and Cornell, he was appointed Lecturer, then Reader, and Professor in Chemistry at the University of Southampton. In 1998 he became Head of Physical Sciences at Unilever Research and Development, Port Sunlight and in 2004, Chief Scientist of the Home and Personal Care Division. In 2013, he was appointed as Director of the Centre Europeen de Calcul Atomique et Moleculaire at the EPFL in Switzerland. Tildesley was awarded the Marlow and Tilden medals of the Royal Society of Chemistry and a CBE for services to science, technology and business.

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