



Computer Simulation of Liquids

By M. P. Allen

Oxford University Press Jun 1989, 1989. Taschenbuch. Book Condition: Neu. 238x156x25 mm. Neuware - Computer simulation is an essential tool in studying the chemistry and physics of liquids. Simulations allow us to develop models and to test them against experimental data. They can be used to evaluate approximate theories of liquids, and to provide detailed information on the structure and dynamics of model liquids at the molecular level. This book is an introduction and practical guide to the molecular dynamics and Monte Carlo methods. The first four chapters describe these methods in detail, and provide the essential background in intermolecular forces and statistical mechanics. Chapters 5 and 6 emphasize the practical aspects of writing efficient programs and analysing the simulation results. The remaining chapters cover advanced techniques, non-equilibrium methods, Brownian dynamics, quantum simulations, and some important applications. FORTRAN code is presented in the text. 404 pp. Englisch.



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