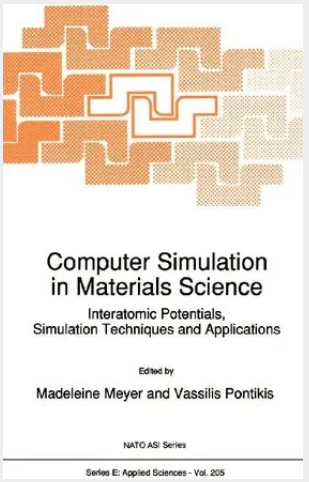
Meyer / Pontikis

Computer Simulation in Materials Science

Interatomic Potentials, Simulation Techniques and Applications

This volume collects the contributions! to the NATO Advanced Study Institute (ASI) held in Aussois (France) by March 25 - April 5, 1991. This NATO ASI was intended to present and illustrate recent advances in computer simulation techniques applied to the study of materials science problems. Introductory lectures have been devoted to classical simulations with special reference to recent technical improvements, in view of their application to complex systems (glasses, molecular systems.). Several other lectures and seminars focused on the methods of elaboration of interatomic potentials and to a critical presentation of quantum simulation techniques. On the other hand, seminars and poster sessions offered the opportunity to discuss the results of a great variety of simulation studies dealing with materials and complex systems. We hope that these proceedings will be of some help for those interested in simulations of material properties. The scientific committee advises have been of crucial importance in determining the conference program. The directors of the ASI express their gratitude to the colleagues who have participated to the committee: Y. Adda, A. Bellemans, G. Bleris, J. Castaing, C. R. A. Catlow, G. Ciccotti, J. Friedel, M. Gillan, J. P. Hansen, M. L. Klein, G. Martin, S. Nose, L. Rull-Fernandez, J. Valleau, J. Villain. The main financial support has been provided by the NATO Scientific Affairs Division and the Commission of European Communities (plan Science).

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