



Computer Simulation in Chemical Physics (NATO Science Series C: (closed))

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Computer Simulation in Chemical Physics contains the proceedings of a NATO Advanced Study Institute held at CORISA, Alghero, Sardinia, in September 1992. In the five years that have elapsed since the field was last summarized there have been a number of remarkable advances which have significantly expanded the scope of the methods. Good examples are the Car--Parrinello method, which allows the study of materials with itinerant electrons; the Gibbs technique for the direct simulation of liquid--vapor phase equilibria; the transfer of scaling concepts from simulations of spin models to more complex systems; and the development of the configurational--biased Monte-Carlo methods for studying dense polymers. The field has also been stimulated by an enormous increase in available computing power and the provision of new software.

All these exciting developments, an more, are discussed in an accessible way here, making the book indispensable reading for graduate students and research scientists in both academic and industrial settings.



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