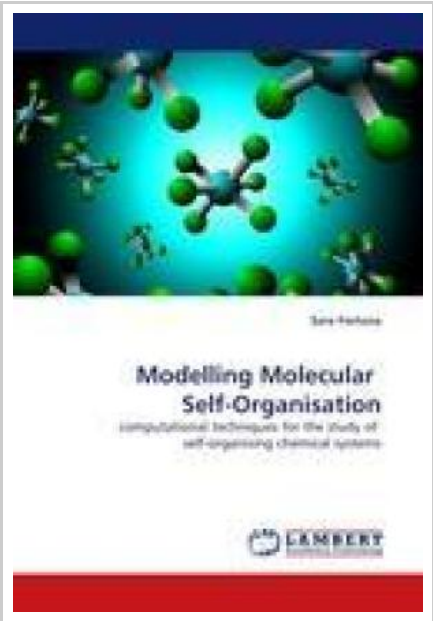

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Modelling Molecular Self-Organisation

By Sara Fortuna

LAP Lambert Acad. Publ. Dez 2010, 2010. Taschenbuch. Book Condition: Neu. 220x150x10 mm. This item is printed on demand - Print on Demand Neuware - The study of self-organising chemical systems merges together concepts and techniques from different fields. This book focuses on those in use in soft matter and complexity science, which are introduced after a short review of the current nanotechnological applications of molecular self-assembly and the main problems encountered in modelling the self-organised behaviour of chemical systems. The attention is on Monte Carlo (MC) based methods. The MC method is first applied to two systems of experimental interest, showing that simplified models are able to reproduce the experimental observations, and predict phase diagrams and bonding motif. Follows the description of our new Agent Based (AB) algorithm for the study of molecular self-organisation. The AB algorithm, which can include elements of artificial intelligence and is traditionally used for the study of complex systems, is capable of driving the system towards a lowest energy con guration with respect to traditional MC methods. Finally, it is shown how the AB algorithm can be used as a part of the protocol to calculate the phase diagram of a rigid organic molecule...

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