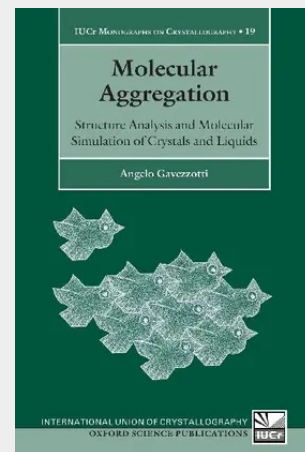


Molecular Aggregation

Structure Analysis and Molecular Simulation of Crystals and Liquids

This book is divided in two parts. Part I provides a brief but accurate summary of all the basic ideas, theories, methods, and conspicuous results of structure analysis and molecular modelling of the condensed phases of organic compounds: quantum chemistry, the intermolecular potential, force field and molecular dynamics methods, structural correlation, and thermodynamics. This Part is written in simple and intuitive form, so that the reader may easily find there the essential background for the discussions in the second part. Part II exposes the present status of studies in the analysis, categorization, prediction and control, at a molecular level, of intermolecular interactions in liquids, solutions, mesophases, and crystals. The main focus is here on the links between energies, structures, and chemical or physical properties.

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