DESCRIPTION

Molecular modeling encompasses applied theoretical approaches and computational techniques to model structures and properties of molecular compounds and materials in order to predict and / or interpret their properties. The modeling covered in this book ranges from methods for small chemical to large biological molecules and materials. With its comprehensive coverage of important research fields in molecular and materials science, this is a must-have for all organic, inorganic and biochemists as well as materials scientists interested in applied theoretical and computational chemistry. The 28 chapters, written by an international group of experienced theoretically oriented chemists, are grouped into four parts: Theory and Concepts; Applications in Homogeneous Catalysis; Applications in Pharmaceutical and Biological Chemistry; and Applications in Main Group, Organic and Organometallic Chemistry. The various chapters include concept papers, tutorials, and research reports.

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chemistry - molecular modeling, spectroscopy, thermodynamics, magnetochemistry, kinetics and mechanisms, synthesis and catalysis.

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