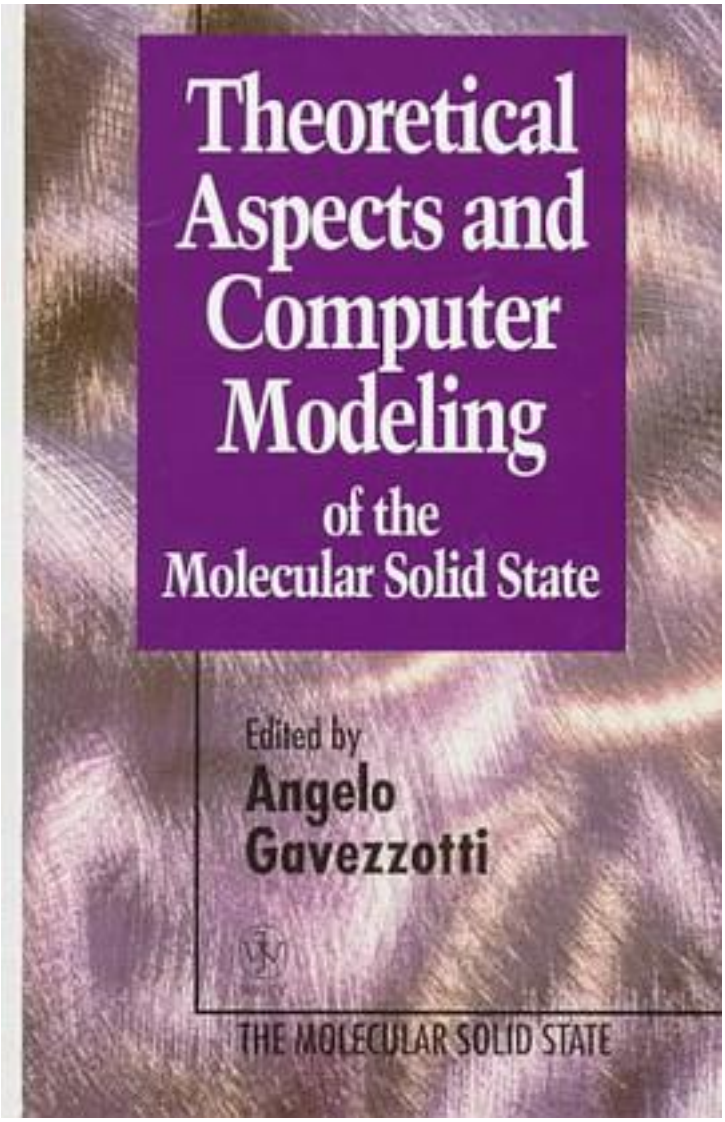
Theoretical Aspects and Computer Modeling of the Molecular Solid State



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The theoretical aspects of crystal packing, the study of the nature and magnitude of the forces that hold molecules together in organic crystals, and of the most favourable arrangements of molecules in crystals are dealt with in this book. After an introductory chapter on the definition and relevance of symmetry in crystal packing, a chapter deals with the physical foundations of weak intermolecular forces and with their simulation by quantum chemical methods. Subsequently, the relationships between crystal structure and crystal thermodynamics are described using empirical intermolecular potentials to bridge the gap by computer modelling.

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