Engineering Crystallography: From Molecule to Crystal to Functional Form [

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Chemical engineering | Pharmaceutical technology | Industrial Chemistry /Chemical Engineering | Pharmaceutical Sciences/Technology

Monografía

This book highlights the current state-of-the-art regarding the application of applied crystallographic methodologies for understanding, predicting and controlling the transformation from the molecular to crystalline state with the latter exhibiting pre-defined properties. This philosophy is built around the fundamental principles underpinning the three inter-connected themes of Form (what), Formation (how) and Function (why). Topics covered include: molecular and crystal structure, chirality and ferromagnetism, supramolecular assembly, defects and reactivity, morphology and surface energetics. Approaches for preparing crystals and nano-crystals with novel physical, chemical and mechanical properties include: crystallisation, seeding, phase diagrams, polymorphic control, chiral separation, ultrasonic techniques and mechano-chemistry. The vision is realised through examination of a range of advanced analytical characterisation techniques including in-situ studies. The work is underpinned through an unprecedented structural perspective of molecular features, solid-state packing arrangements and surface energetics as well as in-situ studies. This work will be of interest to researchers, industrialists, intellectual property specialists and policy makers interested in the latest developments in the design and supply of advanced high added-value organic solid-form materials and product composites

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Contenido: Form -- 1. Crystal Science Fundamentals -- Molecular Structure, Chirality and Chiral Crystals -- Supramolecular Assembly and Solid State Chemistry -- Solid Form Landscape and Design of Physical Properties -- Design of Physical Properties and Solid Form Design -- Modelling Route Map: from Molecule through the Solution State to Crystals -- Crystal Growth and Morphology of Molecular Crystals -- Determining Surface Energetics of Solid Surfaces -- Crystal Effects Influencing the Course of Organic Solid State Reactions: Perfect, Imperfect and Surface Effects -- Synthonic Engineering Modelling Tools for Product and Process Design -- Formation -- Crystallisation Route Map -- Phase Diagrams for Process Design -- Seeding in Crystallisation -- Preparation, Stabilisation and Advantages of Metastable Polymorphs -- Crystallisation Control by Process Analytical Technology -- Methods for Nano-Crystals Preparation -- Crystallisation Control Approaches and Models -- Application of Ultrasound in Crystallization (Sonocrystallization) -- Continuous Pharmaceutical Crystallization from Solution -- Viedma Ripening and its Role in the Chiral Separation of Optical Isomers -- Mechanochemistry and its Role in Novel Crystal Form Discovery -- Innovative Spontaneous Chiral Resolution Phenomenon: Preferential Enrichment -- Function -- Pharmaceutical Solid State Characterisation Techniques -- Techniques for Crystal Optical Characterisation: Chiroptical Spectroscopy -- Unique Ferromagnetic Properties Observed in All-Organic Radical Liquid Crystals -- Mechanical Deformation Chemistry of Crystals: Designing Mechanical Performance -- DEM Analysis of the Effects of Die Shape and Orientation on Die Filling Processes -- Finite Element Modeling of Powder Compaction -- From Molecules to Crystals to Functional Form: Science of Scale

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