CHEMICAL ENGINEERING

Relating crystal structure to surface properties

Funded By	Dipartimento DISAT
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Context of the research activity	Crystallization of organic compounds is a separation and purification technique widely used across industrial sectors: pharmaceuticals, agrochemicals, foods, healthcare, and many formulated household products contain crystalline particulate components. Their relevant physical properties, such as stability, texture, solubility, and dissolution rates, are related to interlinked multi-scale properties. Many of these are readily determined, such as chemical composition, size distribution, morphology, and internal crystal structure (including polymorphism) of particles. However, surface and interfacial properties, which are widely recognised to have critical influence on downstream processing, are not. Molecular level variations in surface properties determine critical macroscopic observables (e.g., wettability, polarity) and impact virtually every step of manufacturing (blending, milling, granulation, tableting) and ultimately product performance (e.g. stability, powder caking, dissolution profiles). Poor control of surface properties is believed to be one of the most common modes of manufacturing and product failure across all the relevant industrial sectors. This project seeks to investigate, using both computational and experimental techniques, the relationship between crystallographic structure and interfacial properties of small organic molecular crystals.
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Objectives	product failure across all the relevant industrial sectors. Progress with the underpinning molecular science has been slow due to the complex nature of surfaces in organic crystalline particles. Additionally, every crystalline particle is inherently anisotropic, potentially exposing a molecularly different surface structure for each of its crystal facets. With the advent of the latest generation of surface analysis techniques [1-3] and the recent development of molecular modelling techniques that attempts to describe the surface structure of crystalline particles [4,5], we can now realistically hope to make progress. This project seeks to investigate, using both computational and experimental techniques, the relationship between crystallographic structure and interfacial properties of small organic molecular crystals. The effects of crystal morphology, polymorphism, co-crystallization, surface features (roughness, defects), adsorbed impurities and additives will be considered. The prospective student will have the chance to work alongside an international multi-disciplinary team of chemists, engineers, and materials scientists, and to take advantage of the cutting-edge crystallization and characterization facilities available in Dr Elena Simone's brand new laboratory at Politecnico di Torino. For this project we are currently seeking for financial support from the Cambridge Crystallographic Data Centre (https://www.ccdc.cam.ac.uk/). Aims and Objectives The main aim of the project is to investigate how crystal structure affects the surface structure and properties of particulate materials. The objectives identified to achieve this aim are: O1. To develop computational modelling methodologies to realistically describe the chemical nature of crystalline facets, starting from crystallographic information. O2. To experimentally validate the methodologies developed in O1 experimentally, considering the effect of possible interfering parameters such as microscopic surface roughness/defects and adsorbed impurities of crystal facets. O3. To determine how and to what extent facet-specific surface structure dictates macroscopic particle properties, in particular as polarity and wettability. O4. To determine the effect of polymorphism, co-crystallization, and solvation on the facet-specific surface molecular structure of organic crystals. Programme of Work This PhD scholarship will involve both experimental and modelling work. A preliminary literature and crystal structure search will be performed to select a suitable model molecule based on its ability to form polymorphs, solvates and co-crystals, its solubility in different solvents and the rate of crystal growth of its different solid forms. This preliminary search will focus on polyphenol molecules [6,7], saccharide derivatives [8] or similar extracts, which are of interest for the nutraceutical and food industry. Existing computational methods alongside molecular modelling approaches [9], will be used as a starting point to pursue objective O1, providing computational surface characterisation through chemical and topological descriptors alongside energetic analysis. Crystal engineering (e.g., optimal cooling, solvent choice, growth modifiers) and the use of dedicated equipment available at the Politecnico (Technobis CrystalBreeder platform) will generate the required mm-sized faceted reference crystals to validate the modelling results (objective O2). The topography and chemical nature of crystal facets will be characterized via atomic force microscopy. The effect of sample preparation and storage conditions will be studied through this set of experiments to understand their relevance on crystal surface properties. Further facet-specific chemical information will be gained by X-ray photoelectron spectroscopy, tip-enhanced Raman spectr

Skills and competencies for the	Master degree (or equivalent) in Chemistry, Chemical Engineering, Pharmacy of Physics (Physical Chemistry). Some basic knowledge of computational

development of the activity	chemistry and crystallography might be desirable.