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Crystal Engineering as a tool for rational design of novel sustainable food, agrochemical and pharmaceutical formulations

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Recent progress in pharmacology, plant biology and biotechnology has led to a dramatic increase in potency and specificity of new generation drugs, active agrochemical ingredients and food nutraceuticals. Unfortunately, this has been accompanied by poor bioavailability and water solubility: it is estimated that around 40% of the active pharmaceutical ingredients currently on the market and 60% of the ones still in development are poorly soluble due to their high molecular weight and structural complexity. These issues have pushed scientific research towards the design of complex formulations, with enhanced dissolution rate and bioavailability, which allow more efficient and targeted delivery of active ingredients (AIs). Multiphase systems (e.g., emulsions, foams, creams) are a convenient and effective encapsulation and delivery strategy, particularly for oral and topical formulations. Currently, synthetic excipients, surfactants and specialty polymers are used to create formulations with enhanced properties. However, these compounds are derived from non-renewable resources through some of the most greenhouse gas-intensive manufacturing processes. For this reason it is now necessary to replace the common synthetic stabilizers used for these products with natural, biocompatible and biodegradable materials. These include natural micro and nano-particles (Pickering stabilizers) such as proteins, polysaccharides and various crystalline materials including cellulose, chitin, fat crystals and polyphenol crystals.

Pickering systems are particularly promising since particles adsorb at interfaces more strongly than surfactants, providing significantly more stable formulations. The stability of Pickering systems is strongly affected by particle size and shape, but surface wettability is the most important property of Pickering particles. For faceted, anisotropic crystals surface wettability is not easy to determine. In fact, crystals present multiple crystallographic facets, whose surface properties (e.g., polarity, wettability) depend on the type and directionality of the intermolecular interactions that characterize each facet.

The purpose of the presented work is to understand how crystal properties (size, shape and polymorphism) of Pickering particles affect their surface properties, hence their orientation and adsorption behaviour at interfaces. [1-5] Molecular modelling (synthons analysis from crystallographic data) and experimental work (e.g., characterization using benchtop and synchrotron X-ray techniques, thermal studies, stability studies) were conducted on two model systems: quercetin and cocoa butter.

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[5] Klitou, P., Rosbottom, I., Simone, E. *Crystal Growth and Design*, 2019, 19(8), pp. 4774–4783

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