**CSD-Particle - From Crystal Structures to Particle Properties**

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**Purpose:**

Connecting the crystal structure to the surfaces of crystalline organic particles remains of significant interest to this community as it allows for predicting powder behavior and guiding crystal engineering decisions. Particle properties, including shape, hardness, roughness, and chemistry, have been associated with numerous manufacturing and performance challenges. Here, we show how the crystal structure can be used to predict various properties using a simplified set of models to comprehensively describe the particle with the CSD-Particle suite.

**Methods:**

Based on crystallographic data, we predict the properties of particles in molecular systems. Shape predictions are performed using geometric (BFDH) and attachment energy methods (VisualHabit). These guide the determination of relevant particle faces. Mechanical properties are examined by identifying slip planes through inter-slab separations. Lastly, surface chemistry and roughness are quantified through a reticular area representation of each particle facet. All these properties are combined to describe the overall characteristics of the particles.

**Results:**

Using the CSD-Particle suite, we demonstrate a computationally efficient and reproducible method for predicting particle properties directly from crystal structures. The predicted morphologies reveal primary growth directions and exposed facets, while surface chemistry descriptors, based on atomic and functional group distributions, highlight potential interactions with excipients, solvents, and processing equipment. Rugosity is described using a van der Waals contact surface, providing insights into atomistic roughness and potential slip planes that affect mechanical behavior. All descriptors are qualitatively represented by visualizing shapes and surface properties and quantitatively expressed by numerical values. This facilitates better communication across disciplines and offers a comprehensive description of properties.

**Conclusions:**

This approach bridges the gap between crystallographic data and particle-level behavior, offering a computationally efficient framework for particle analysis. By standardizing the description of particle facets and their properties, the method facilitates cross-material comparisons and supports predictive modelling in drug product development. The ability to visualize and quantify surface features provides insight into structure/property relationships and opens new avenues for rational material design.

**Keywords:**

Crystal structure, particle surface, morphology prediction, surface chemistry