Poster

Correlating particle informatics with surface wetting measurements

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Particle properties are important to a range of formulated product industries such as pharmaceuticals, agrochemicals, and dyes, who expend significant effort in mitigating manufacturing bottlenecks and improving product performance. Particle characteristics impact processes such as flow, compaction, and cohesivity. Shape, size, roughness, and hydrophilicity/hydrophobicity are typical properties of interest in understanding downstream behaviour [1].

Particles are susceptible to solvent deposition that can cause capillary bridges, reducing flowability or impacting the likelihood of agglomerates forming and affecting blend homogeneity. The wettability of surfaces is used to describe the hydrophilicity of a given system. Linking particle surface wettability to molecular and crystal structure using particle informatics can allow for the early detection of challenging systems.

Historically, surface roughness has been studied as a mechanism for adjusting the hydrophobicity of a material. However, surface chemistry can also have an impact on the wettability of a surface [2,3].

In this contribution, we present the findings of correlating surface descriptors and interaction data from the Cambridge Structure Database (CSD) with experimental contact angle measurements.

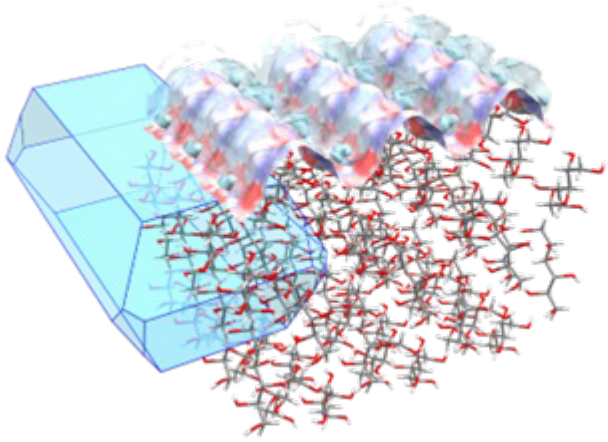

Figure 1. Particle surface properties of D-mannitol (020). Topology colouring shows surface charge. Light blue spheres depict the position of probable water oxygen interactions.

The surface descriptors explain the density of hydrogen forming functional groups, surface roughness, and the probability of interactions with hydrophilic/phobic probes. With the help of these descriptors, the application of predictive tools upstream can quickly determine whether a structure will cause processing problems and reduce the resources required to achieve an optimum formulated product.

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[2] Yang C, Tartaglino U, Persson BNJ. Influence of Surface Roughness on Superhydrophobicity. Phys Rev Lett 2006;97:116103.

[3] Buckton G. Assessment of the wettability of pharmaceutical powders. Journal of Adhesion Science and Technology 1993;7:205–19.