MS35-05 | Surface Properties of Organic Crystals Based on a Guantum Chemical Treatment of Crystal Facets

Van de Velde, Jasper (University of Antwerp, Antwerp, BEL); Blockhuys, Frank (University of Antwerp, Antwerp, BEL)

The differences in reactivity of the different facets of a crystal to solute and/or solvent molecules is a rich source of information in the development of new materials based on small organic molecules for technological or pharmaceutical applications. Indeed, many macroscopic crystal properties such as morphology, interfacial stability, growth direction and speed, polarity, sticking propensity, wetting etc. are directly related to the susceptibility of the crystal facets to other molecular moieties during the crystallization process. In turn, controlling these properties is important for downstream unit processes associated with *e.g.* pharmaceutical product manufacture, such as filtration, granulation and compression.

A computational treatment of different crystal facets of materials ranging from small pharmaceuticals to large organic oligomers for optical applications, was performed at the level of DFT under Periodic Boundary Conditions. In the case of solute probe molecules, in which the attachment of solvated molecules to the crystal structure is simulated, an approach based on strong intermolecular synthons was used. In the case of solvent probes, in which the wetting and solubility of the crystal is central, a free relaxation mechanism was applied. The interactions between different probe molecules and the crystal surfaces results in energy profiles that can be directly linked to the growth direction of the crystal and hence the morphological importance of the different crystal facets. Although it is not a dynamic simulation of the crystallization process, this thermodynamic description allows a relatively fast screening of a large number of interactions on the surface.