





## Analyse Surfaces using CSD-Particle





## Learning outcomes for today

- Learn how informatics and data-driven approaches can be used to understand particle properties.
- Familiarise yourself with what tools are available in the CSD-Particle suite and what they can be used to do.
- Learn how to use Surface Analysis to identify key particle properties.





## **From Solid Form to Particle Properties**



MoleculeFormParticlePropertiesSolid Form Informatics

Particle Informatics

## **Particle Informatics**





Visualisation and analysis of surface properties

Identification and analysis of potential slip planes

Morphology calculations

CCDC

- Ongoing research projects into particle and surface phenomena are developing our understanding of formulation and manufacturing processes
- Application of rapid, informatics-based approaches to understand the link between crystal structure and properties that influence downstream behaviour

M. J. Bryant et al., Cryst. Growth Des. (2019), 19, 9, 5258-5266

## Software to gain new insights

**CSD**Core.

Search, visualise, analyse and communicate structural data Insights into molecular and crystal shape and interactions



Medicinal & Computational Chemists ♦ Crystallographers & Structural Biologists ♦ Solid Form & Crystallisation Scientists

## Key concepts for this module



## **Key concepts - Full Interaction Maps**

- Map interaction preferences around complete molecules in a crystal structure
- Visualise observed atom-atom contacts with respect to likely geometries in 3D space
- Identify interaction hot-spots around chemical groups





## Key concepts - How do crystals grow?

- Depends on relative growth rates
  - R<sub>hkl</sub>
  - Faster growing faces are smaller
- Growth rates are dependent on many things
  - Supersaturation
  - Solvents
  - Impurities



## Key concepts – BFDH morphologies

- Simplest morphology model
  - Essentially based on unit cell
- Point molecules
- Growth rates inversely proportional to distance between Miller planes
- Layer-on-layer growth
- Independent of growth environment

A. Bravais, *Études Crystallographiques*, Gauthier-Villars, Paris, (1866)
M.G. Friedel *Bull. Soc. Franc. Miner.* (1907), 9, 326-455.
J.D. Donnay, D. Harker, *Amer. Min.* (1937), 22, 446-467.









Surface Charge



Surface Roughness



## **Surface Analysis**



Descri	ptors
Physical	Chemical
Reticular Surface Area	Hydrogen Bond Donor/Acceptor Density
Rugosity	Aromatic Rond
RMSD, Skewness, and Kurtosis	Density
Statistically Derived	d Interaction Data





## Accessing CSD-Particle through Mercury

### AABHTZ (P-1) - Mercury

File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Theory CSD-Particle CSD-Discovery CSD Python API Help

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Press the left mouse button and move the mouse to rotate the structure

## **CSD-Particle Menu**

### AABHTZ (P-1) - Mercury

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# Learn more about these parameters in the Glossary in the handout.

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Preview Slab

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CSD-Particle CSD-Discovery

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H-Bond Donors

## Advanced Options

## **CSD-Particle – FIMs on Surface**

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