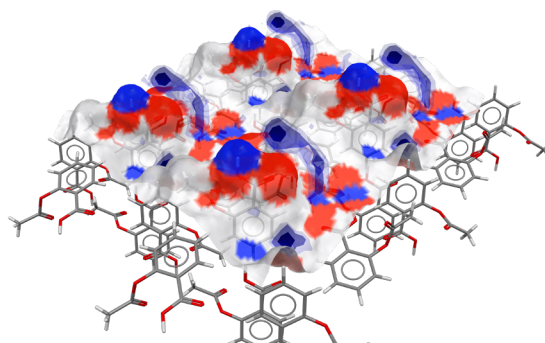
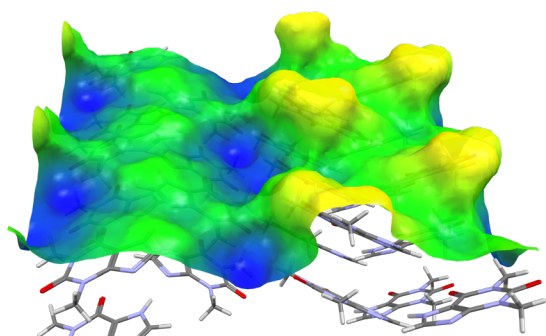


# CSD-Particle

Anticipate manufacturing bottlenecks and guide formulation decisions with a deep understanding of particle behaviour.



Rapidly analyse the mechanical and chemical properties of crystalline particles with a suite of visual and statistical tools. Perform particle shape and surface analyses to anticipate manufacturing issues such as sticking, wettability, and tabletability. Communicate findings across your team with visual displays of surface chemistry, charge and topology.

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## • Predict Particle Facets

- Predict the particle shape by predicting which facets are available.

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## • Visualize Surface Chemistry and Charge

- Communicate the distribution of H-bond donors and acceptors on the surface with clear, colour-coded graphics.
- See the potential causes of wettability, stickiness, flow, and electrostatic issues easily.

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## • Identify Potential Slip Planes, Fast

- Determine mechanical properties and guide formulation choices to support better tableting, flow, and milling.

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## • Evaluate Particle Surface Interactions

- Gain insights into wettability, tabletability, flow, and sticking by understanding the interactions at the particle surface.

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## • Visually Map Surface Interactions

- Calculate and visualize full interaction maps (FIMs) on the surface, showing the positions a given probe is most likely to interact. Change probes to explore interaction types, e.g. assess hydrophilicity with the water oxygen probe, or hydrophobicity with methyl carbon.

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## • Understand Interactions Within the Crystal Lattice

- Explore system shape and stability, and see how internal bonding impacts surface termination and exposed groups on a given facet.



- **Determine H-bond Dimensionality**

- Assess hydrogen bonding dimensionality, and how discreet, 3D, or sheet hydrogen bonding impacts the mechanical properties of your product.
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- **Visualize Surface Topology**

- See surface roughness in clear, 3D graphics.
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- **Quantify Surface Chemistry and Topology**

- Compare facets, particles, or structures easily by quantifying the density of H-bond donors, acceptors, aromatic bonds, unsatisfied H-bond donors, RMSD, surface area, rugosity, kurtosis, and skewness.
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- **Access via Python API**

- Access all these features in the CSD Python API for fully customizable analyses.

## FAQs

### How can CSD-Particle predict manufacturing bottlenecks for pharmaceuticals and fine chemicals?

By understanding the mechanical and chemical properties of your product, potential issues in wettability, flow or sticking, tabletability, and electrostatic interactions can be identified at an early stage. Explore how the formulation and solid form impacts these properties computationally, to reduce costs and understand your product earlier.

### What form are CSD-Particle results given in?

Visual and numerical results are possible. Examine surface chemistry, topology, and interactions through interactive 3D visualizations. Quickly compare facets, particles, or structures by quantifying the density of H-bond donors, acceptors, aromatic bonds, unsatisfied H-bond donors, RMSD, surface area, rugosity, kurtosis, and skewness.

### How is CSD-Particle accessed?

The analytical tools in CSD-Particle can be accessed through our desktop program Mercury, or via the CSD Python API. The functions are available to all academic researchers, non-academic users require a CSD-Particle licence—contact us here to request a quote, demo, or trial.

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## Learn More

- Email [hello@ccdc.cam.ac.uk](mailto:hello@ccdc.cam.ac.uk) to ask a question or request an online demo.
  - Visit [www.ccdc.cam.ac.uk](http://www.ccdc.cam.ac.uk) for more information.
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