

# How to visualise and analyse surfaces using Mercury

CCDC Virtual Workshop

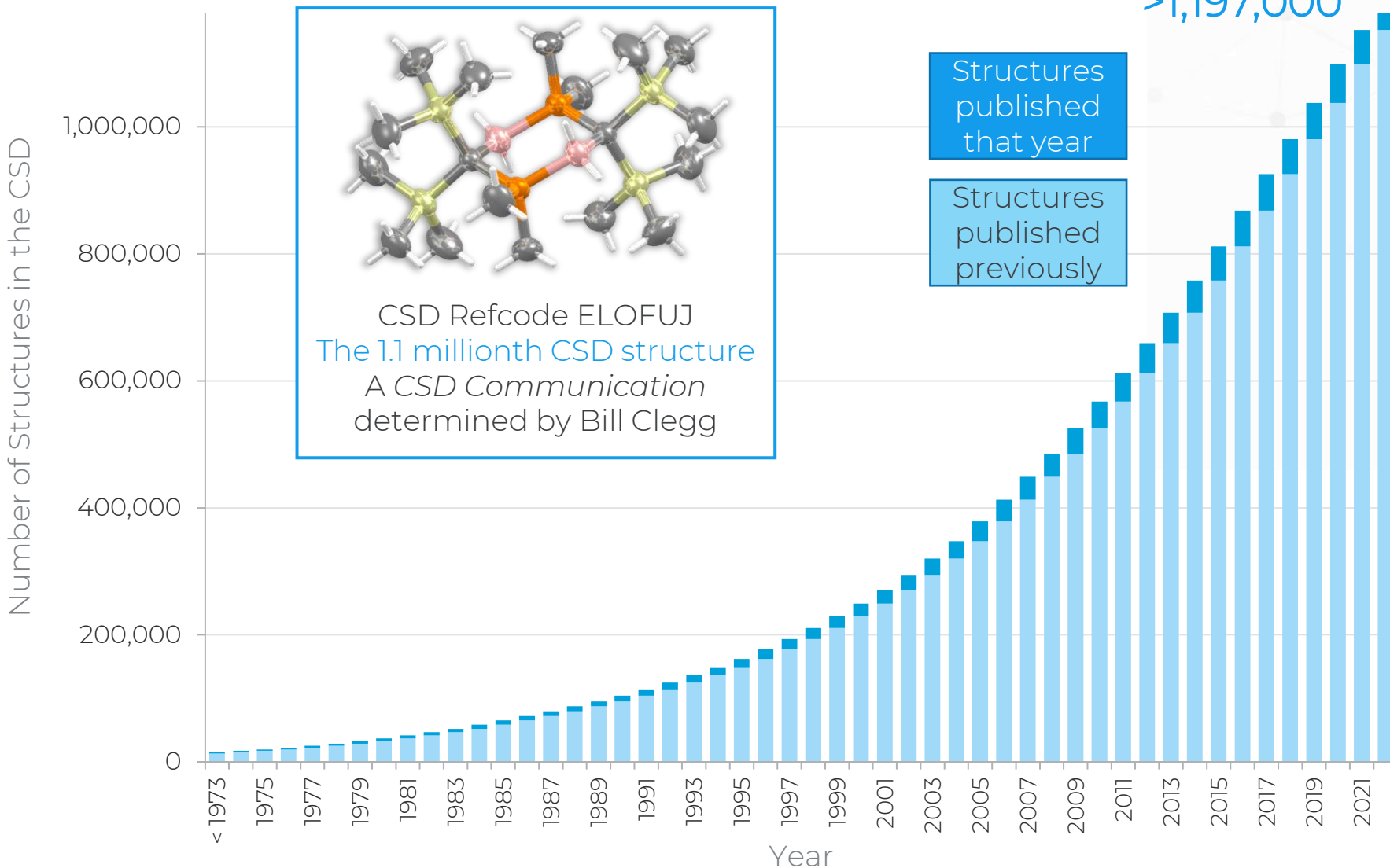
Alex Moldovan, Ilaria Gimondi, Pietro Sacchi, Suzanna Ward, Andy Maloney

October 2022

# 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 and Slip Planes to identify key particle properties.

# The Cambridge Structural Database



- Every published structure
  - Inc. ASAP & early view
  - CSD Communications
  - Patents
  - University repositories
  - Thesis
- Every entry enriched and annotated by experts
- Discoverability of data and knowledge
- Sustainable for over 57 years
- A trusted CoreTrustSeal repository



Certified as Trustworthy  
by CoreTrustSeal

# Inside the Cambridge Structural Database

The CSD is a database of all the published organic and metal-organic experimental crystal structures

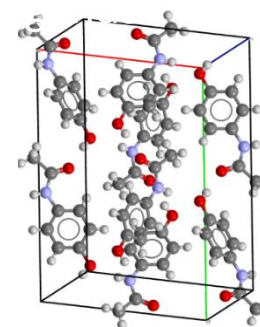
Organic  
43%

Metal-Organic  
57%

At least one transition metal, lanthanide, actinide or any of Al, Ga, In, Tl, Ge, Sn, Pb, Sb, Bi, Po

## Organic

- Drugs
- Agrochemicals
- Pigments
- Explosives
- Protein ligands



## Additional data

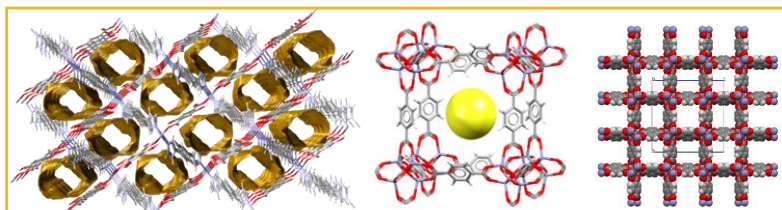
- 11,525 polymorph families
- 171,683 melting points
- 909,992 crystal colours
- 778,663 crystal shapes
- 24,916 bioactivity details
- 11,387 natural source data
- > 250,000 oxidation states

Not Polymeric  
89%

Polymeric: 11%

## Metal-Organic

- Metal Organic Frameworks
- Models for new catalysts
- Porous frameworks for gas storage
- Fundamental chemical bonding

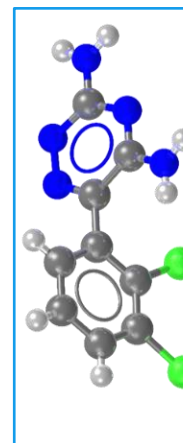


Single  
Component  
56%

Multi  
Component  
44%

## Links and subsets

- DrugBank
- Druglike
- MOFs
- PDB ligands
- PubChem
- ChemSpider
- Pesticide PDB



# The vision

## BERNAL'S VISION: FROM DATA TO INSIGHT

by Dr Olga Kennard OBE FRS

THE J D BERNAL LECTURE 1995  
delivered at  
BIRKBECK COLLEGE, LONDON



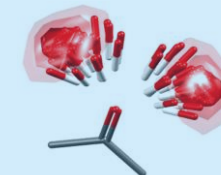
We clearly recognised even in those early days, that data banks have three principal functions. Firstly they must gather together existing knowledge and make it readily available to the scientific community. Secondly they can be used to reduce a large number of observations to a small set of constants and rules, and in this way transform a data base to a knowledge base. Such a knowledge base may obviate the need for further individual experiments in specific areas. Thirdly, they facilitate the comparison and collective analysis of individual results to gain insight into new or as yet unexplained phenomena. These ideas have been at the heart of the work of the Cambridge Crystallographic Data Centre and the driving force for improving methods of data collection, storage and dissemination. Most importantly they influenced development of computer programs and methodologies which are needed for the analysis and transformation of the accumulated information. (5)

# Software to gain new insights



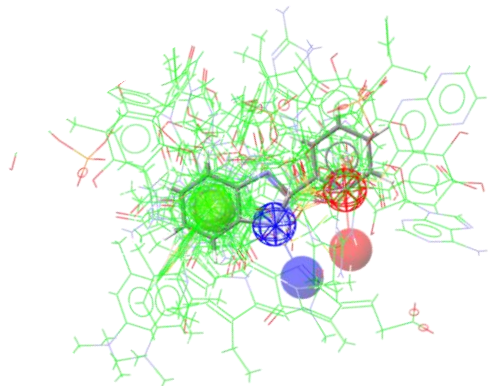
**CSDCore.**

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



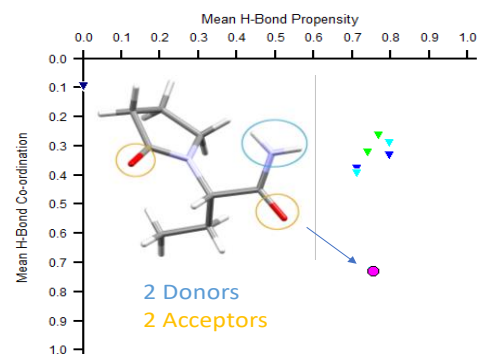
**CSDDiscovery.**

*Design of new molecules*



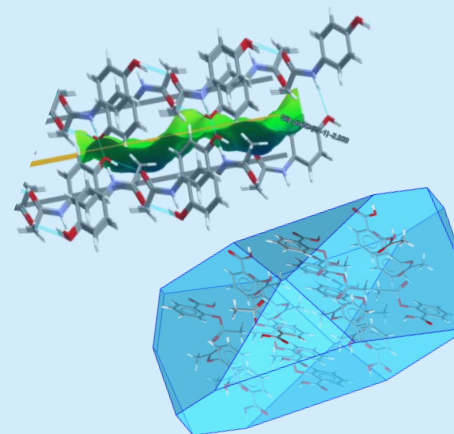
**CSDMaterials.**

*Assessment of solid form stability and properties*



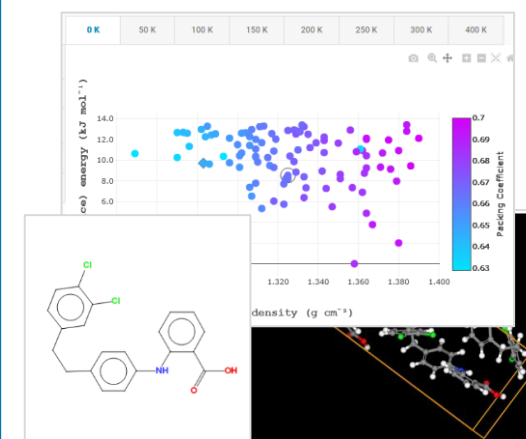
**CSDParticle.**

*Anticipate particle properties and behaviour*



**CSDTheory.**

*Insights from predicted structure landscapes*

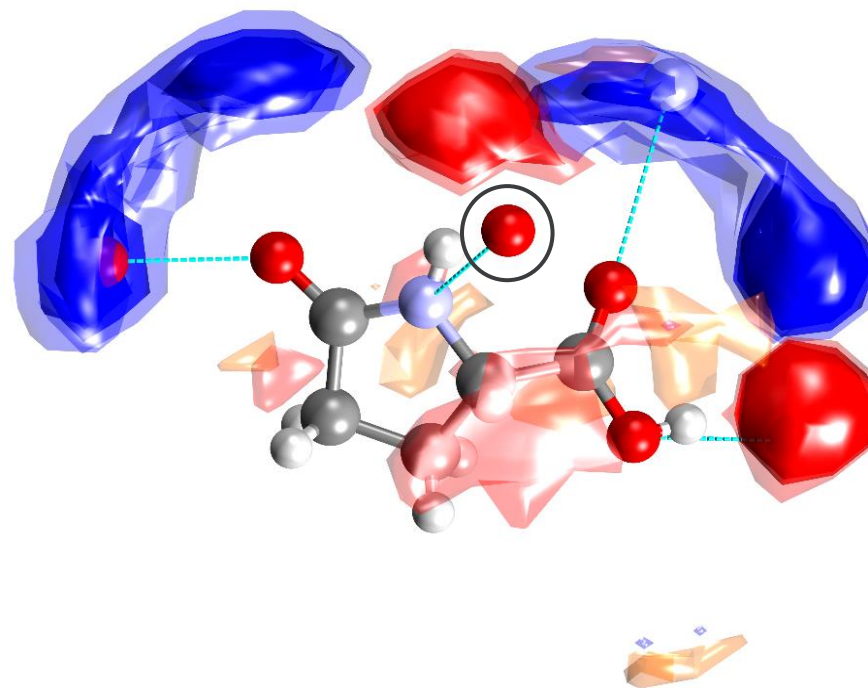


Medicinal & Computational Chemists ♦ Crystallographers & Structural Biologists ♦ Solid Form & Crystallisation Scientists

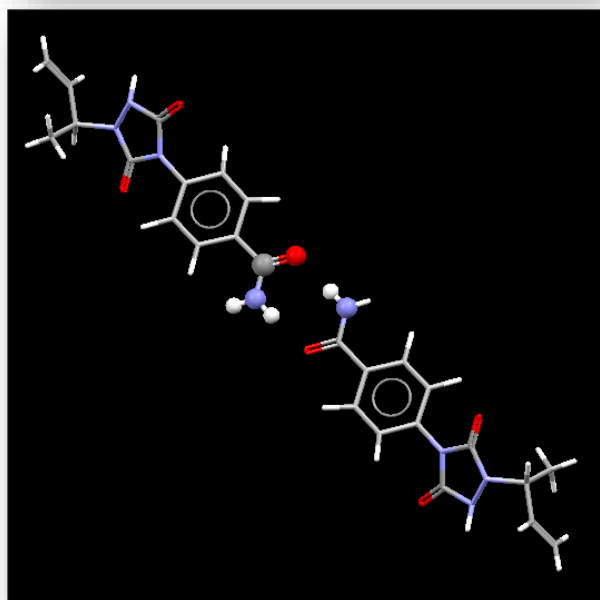
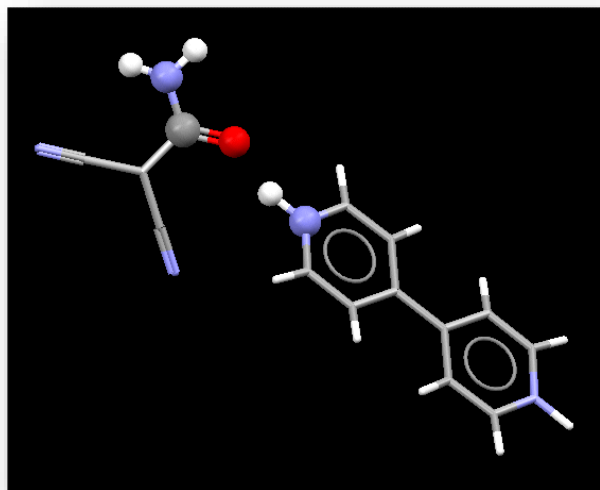
**CCDC**

# Key concepts - Full Interaction Maps

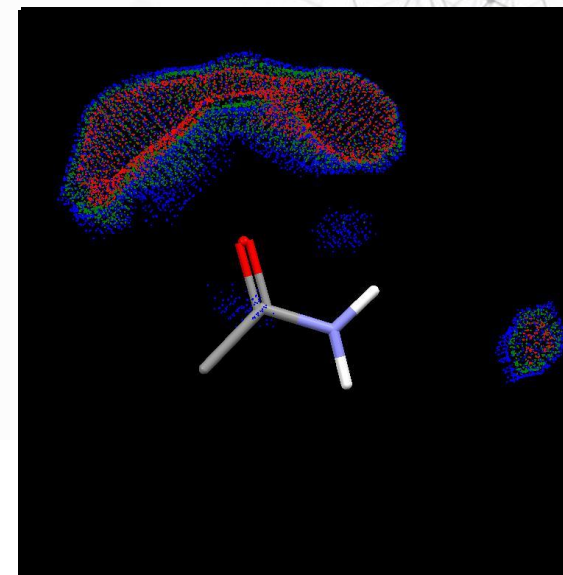
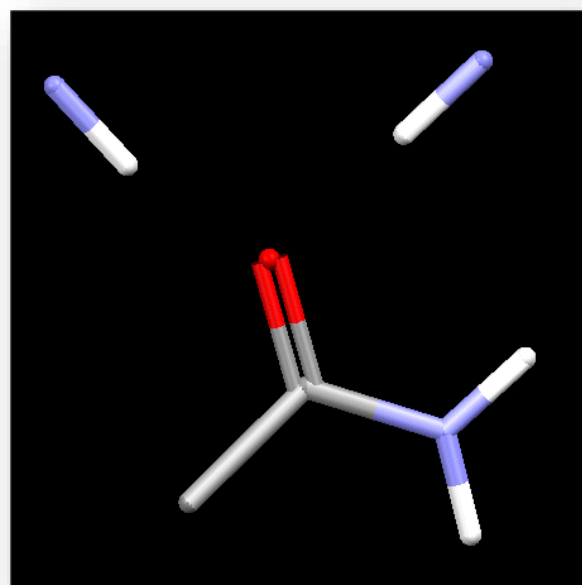
- Map interaction preferences around complete molecules in a crystal structure
- Visualise observed atom-atom contacts with respect to likely geometries in 3D space
- Identify interaction hot-spots around chemical groups



# Key concepts - Full Interaction Maps



central group:  $-\text{CONH}_2$   
contact group: NH



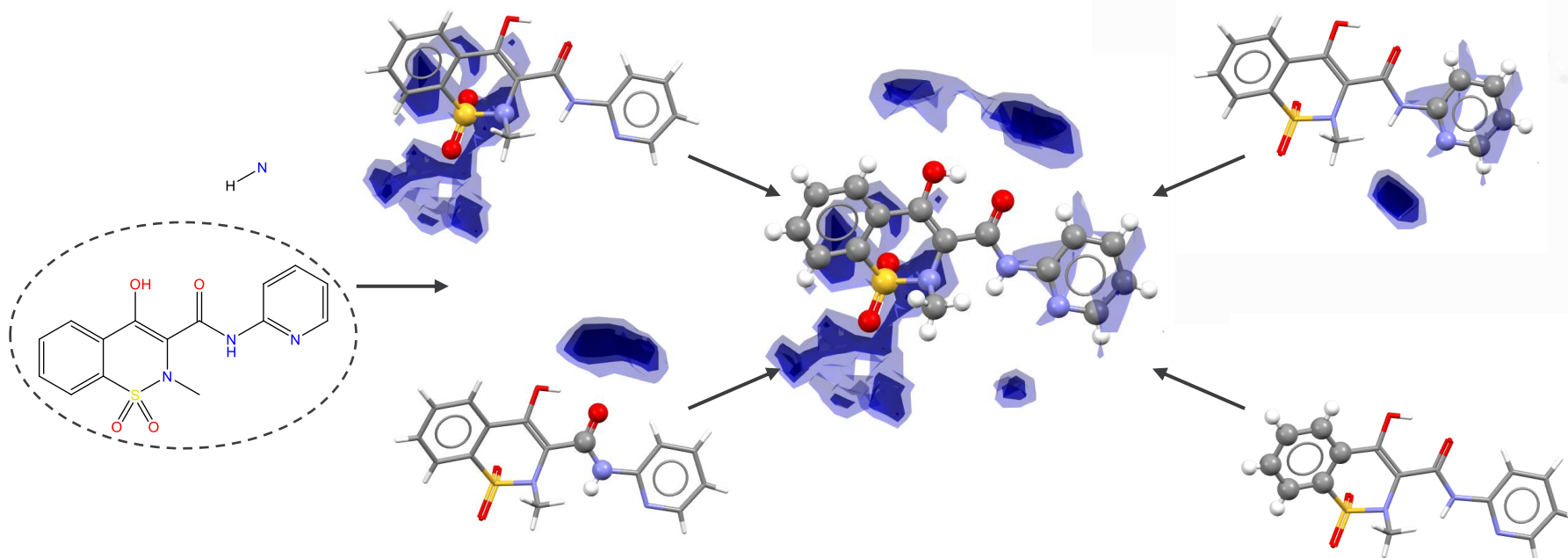
Search for structures containing desired contact

Superimpose hits and display as scatterplots or contour plots



# Key concepts - Full Interaction Maps

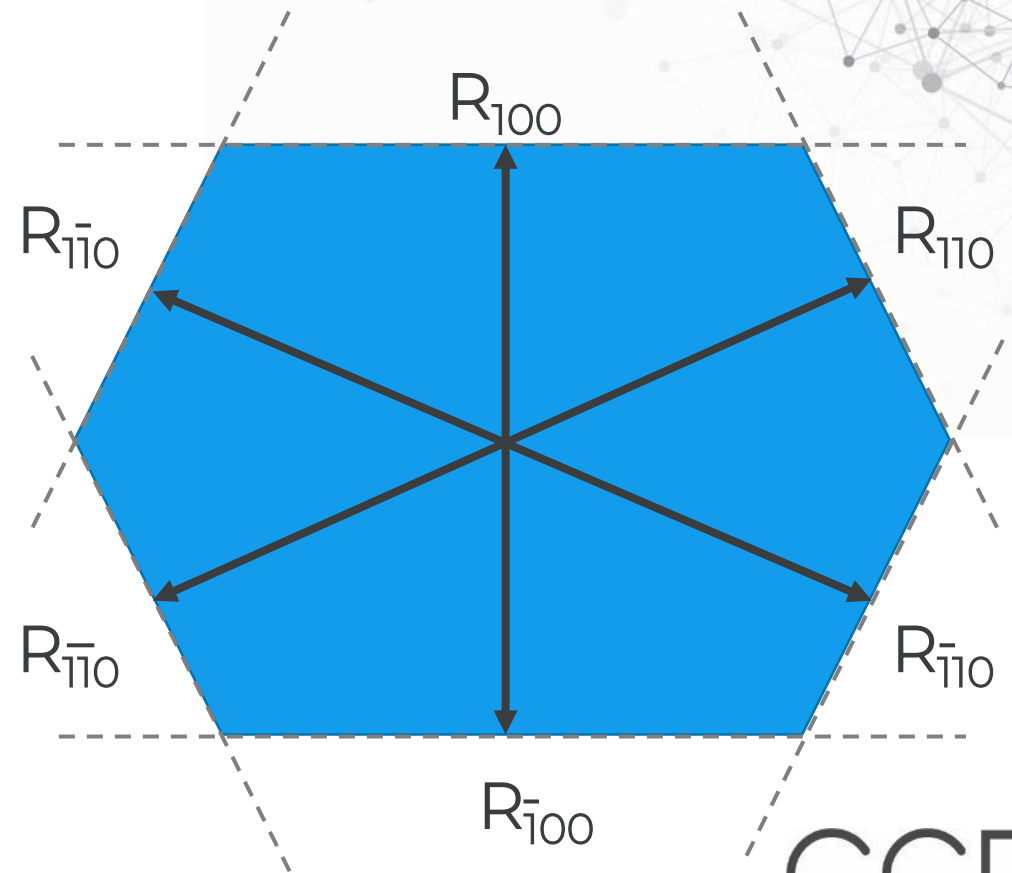
- Molecule is broken down into fragments
- IsoStar maps for each fragment are combined to give the Full Interaction Map



- Multiple maps can be generated for different probes

# Key concepts - How do crystals grow?

- Depends on relative growth rates
  - $R_{hkl}$
  - *Faster growing faces are smaller*
- Growth rates are dependent on many things
  - Supersaturation
  - Solvents
  - Impurities



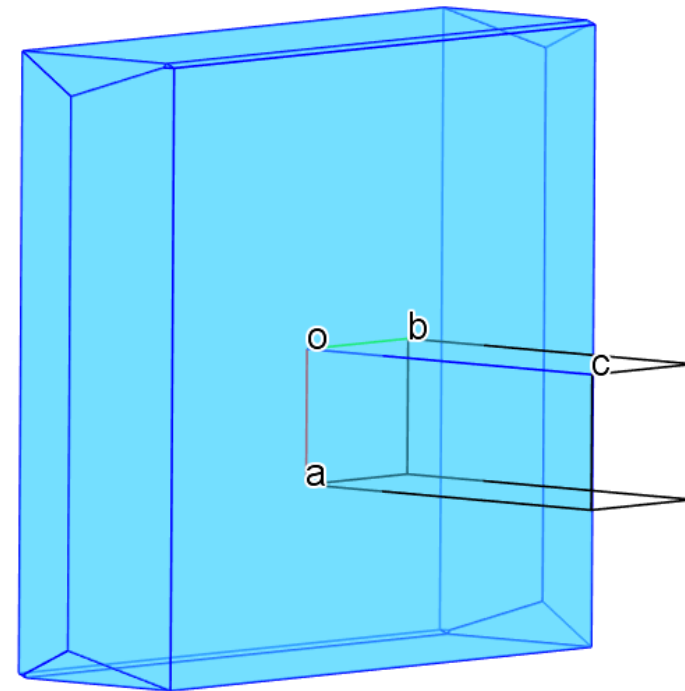
# Key concepts – BFDH morphologies

- 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

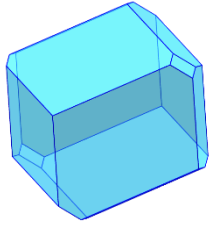
A. Bravais, *Études Crystallographiques*, Gauthier-Villars, Paris, (1866)

M.G. Friedel *Bull. Soc. Franc. Miner.* (1907), 9, 326-455.

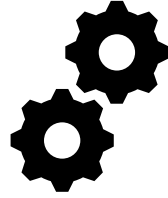
J.D. Donnay, D. Harker, *Amer. Min.* (1937), 22, 446-467.



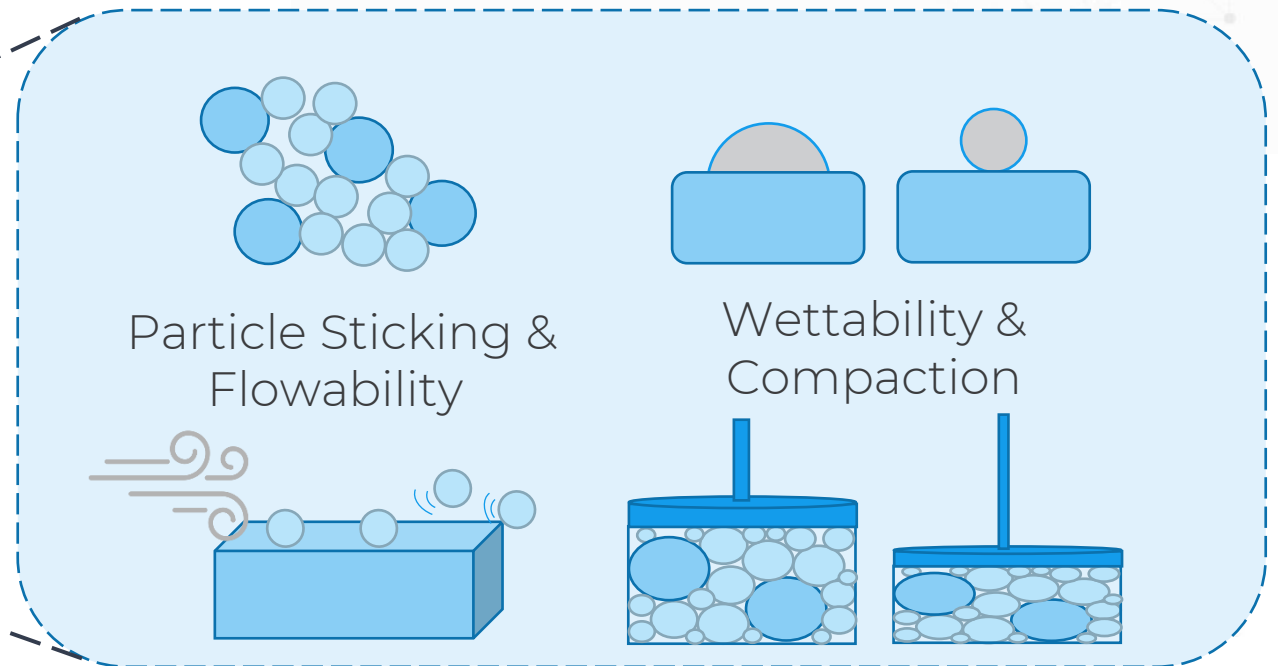
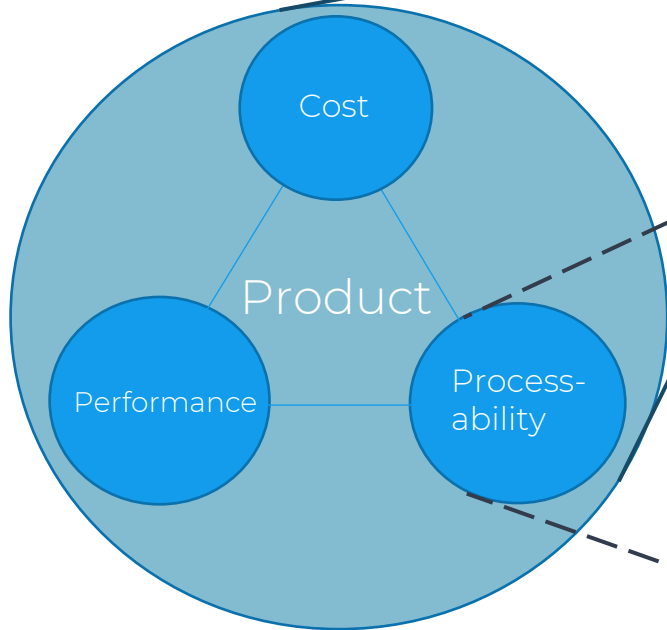
# The field



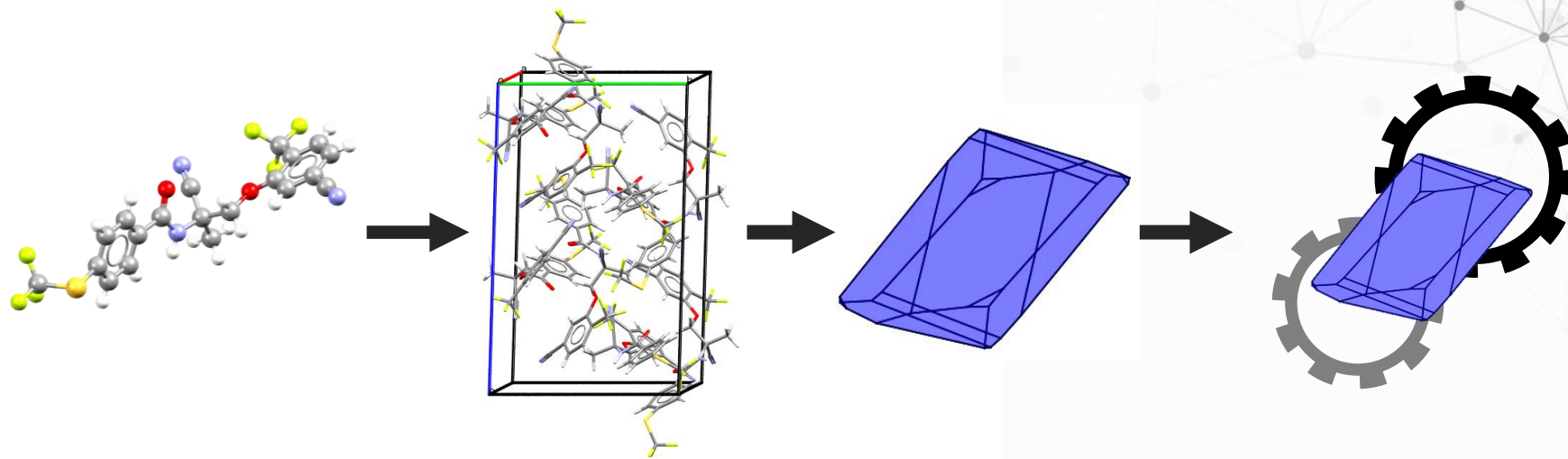
Particle



Product



# From Solid Form to Particle Properties



Molecule

Form

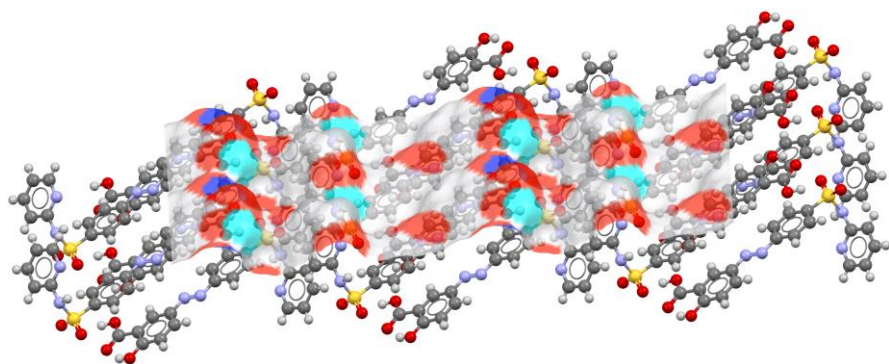
Particle

Properties

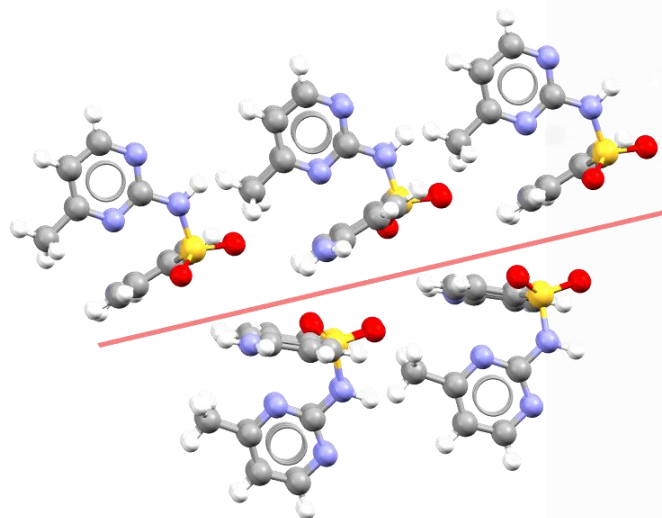
Solid Form Informatics

Particle Informatics

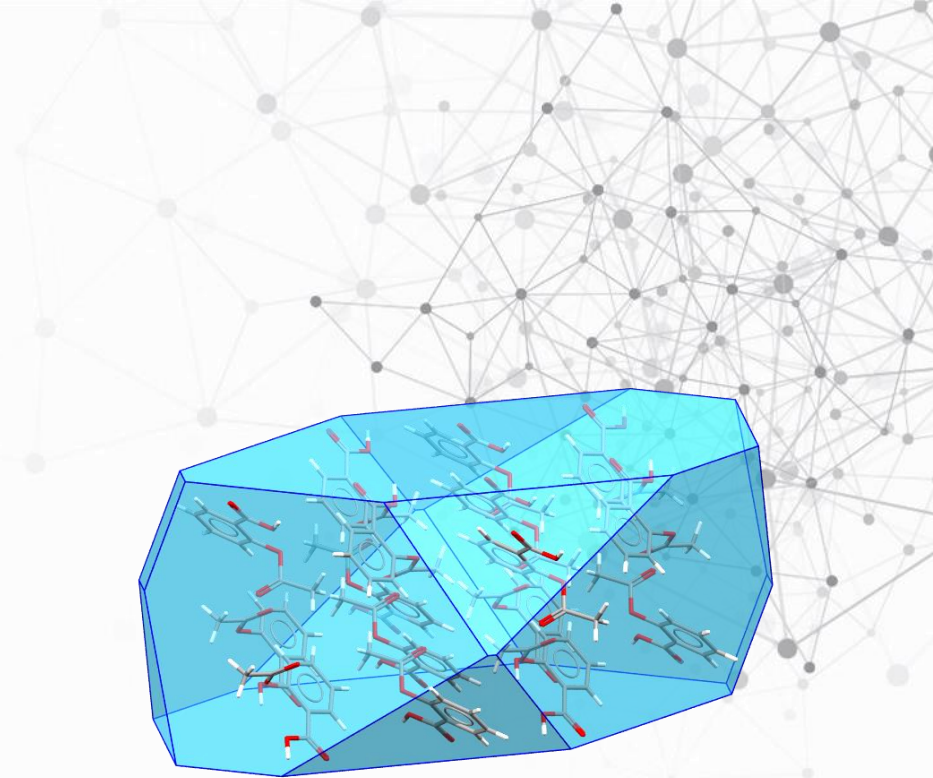
# Particle Informatics



Visualisation and analysis of surface properties

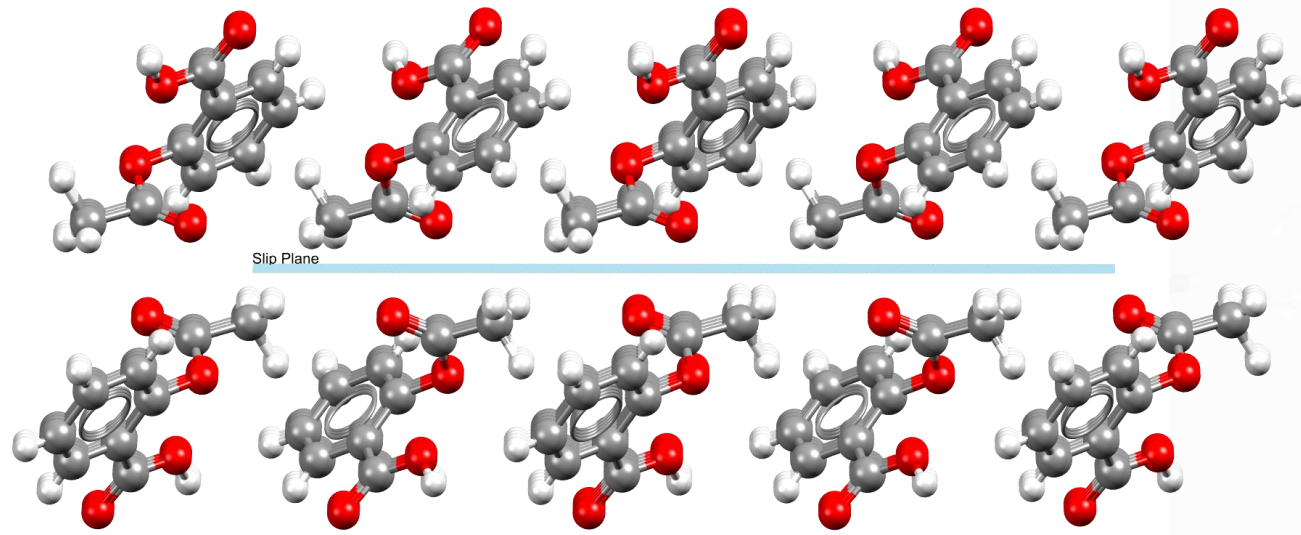


Identification and analysis of potential slip planes



Morphology calculations

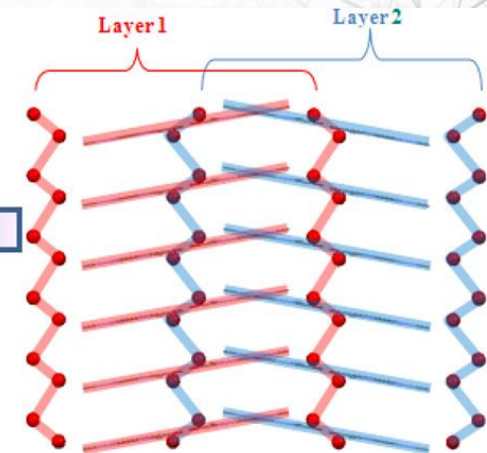
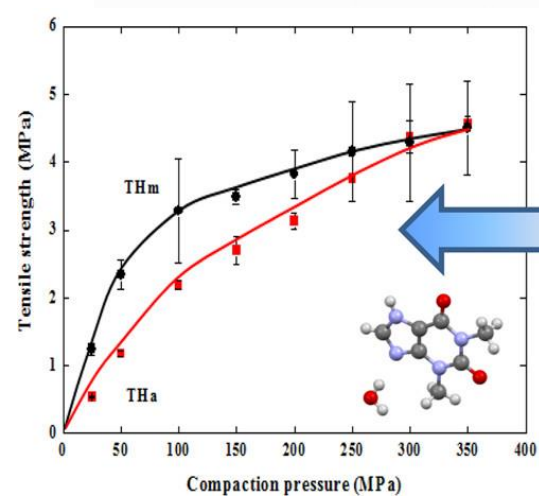
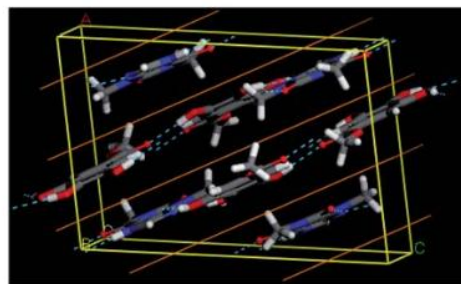
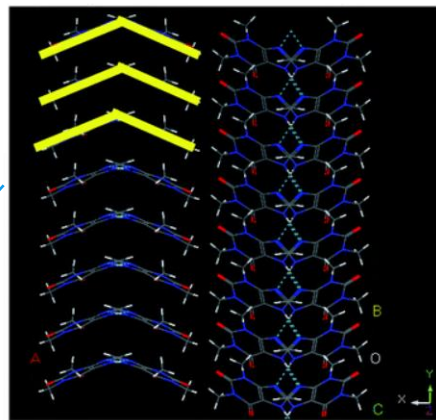
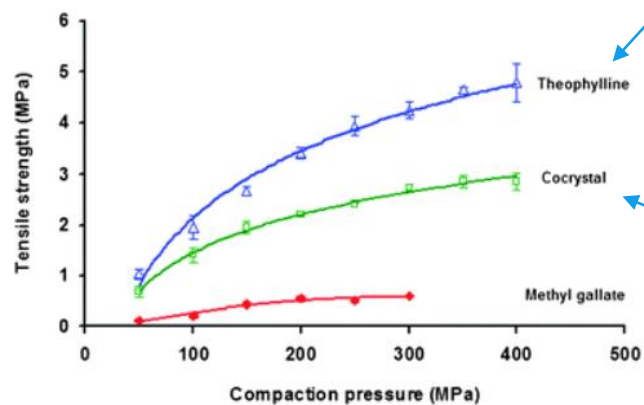
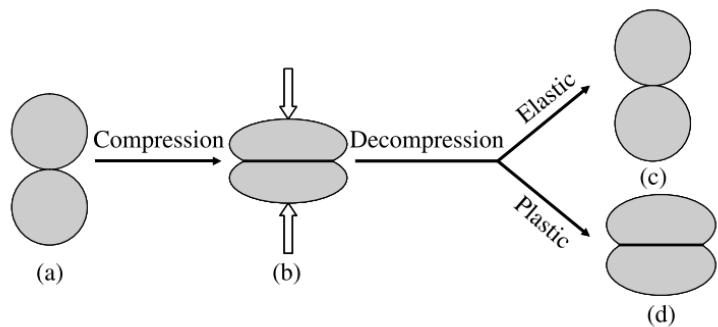
- Ongoing research projects into particle and surface phenomena are developing our understanding of formulation and manufacturing processes
- Application of rapid, informatics-based approaches to understand the link between crystal structure and properties that influence downstream behaviour



# Slip Planes

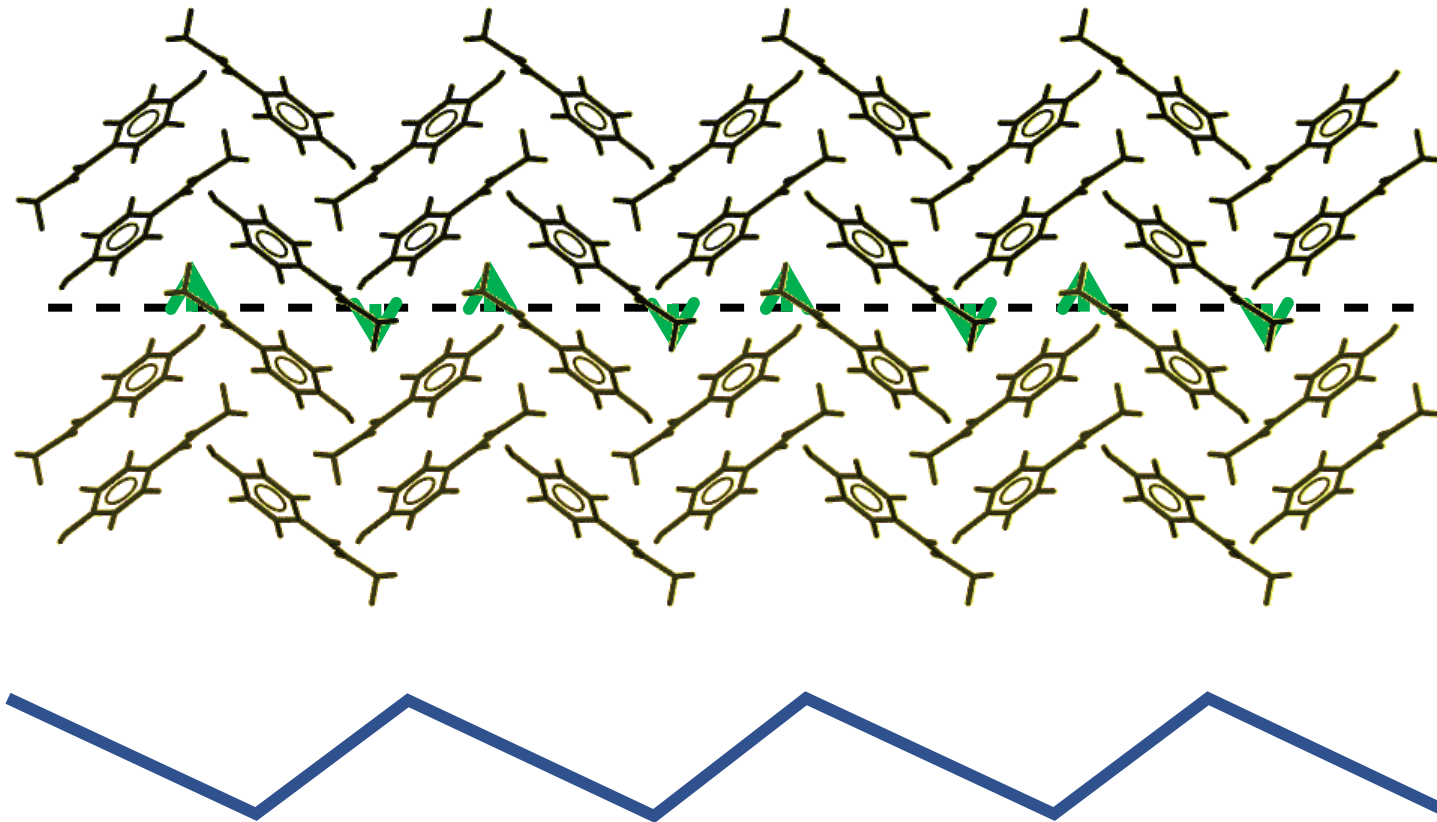
- Identification of Potential Slip Planes
- Analysis of Structure Hydrogen Network

# Compaction and Bending

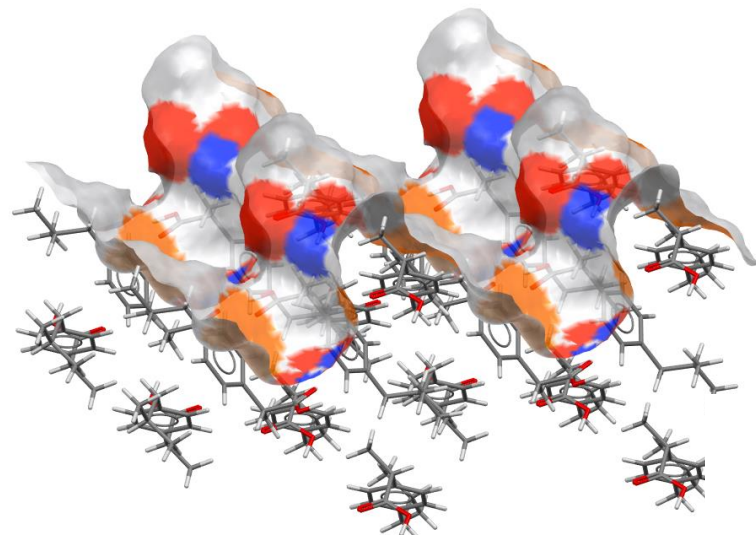




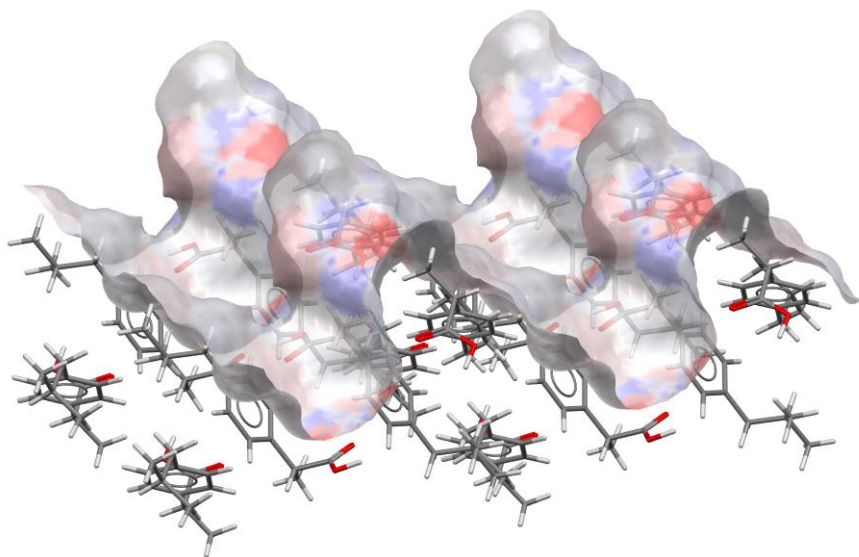
# Predicting slip planes



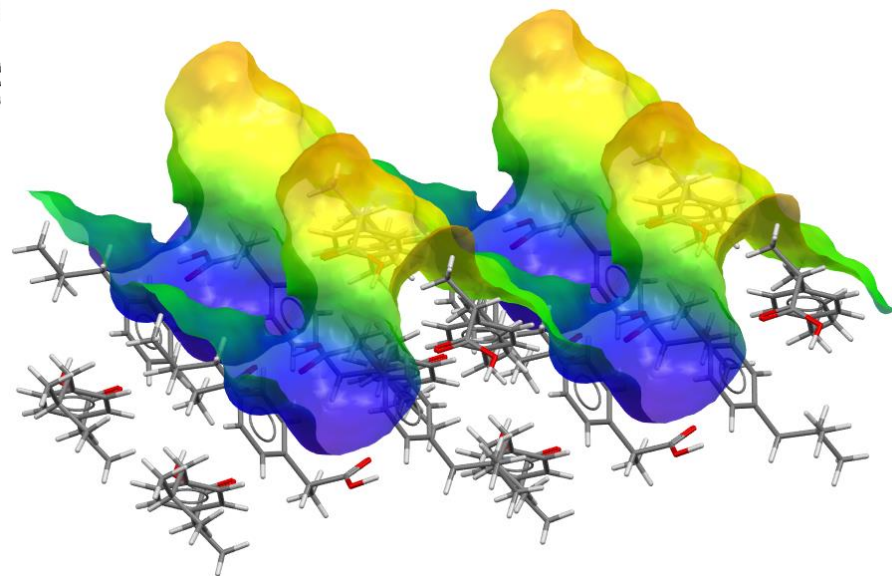
# Surface Analysis



Surface Chemistry

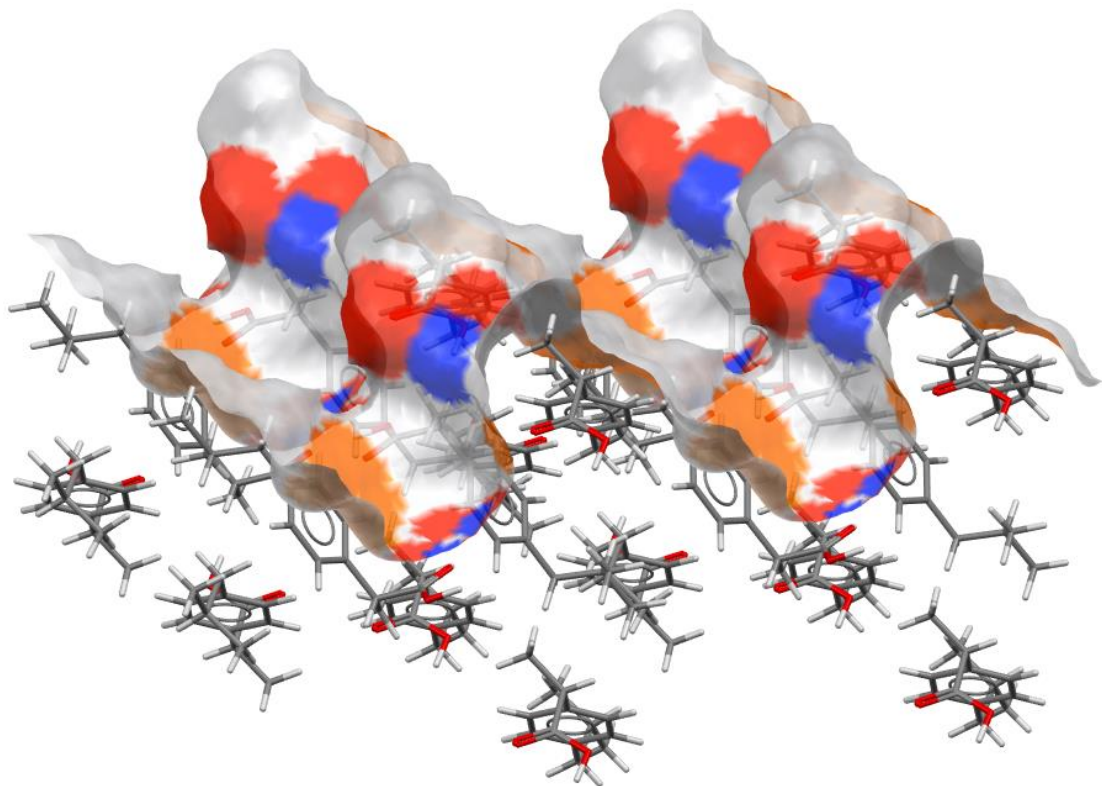


Surface Charge



Surface Roughness

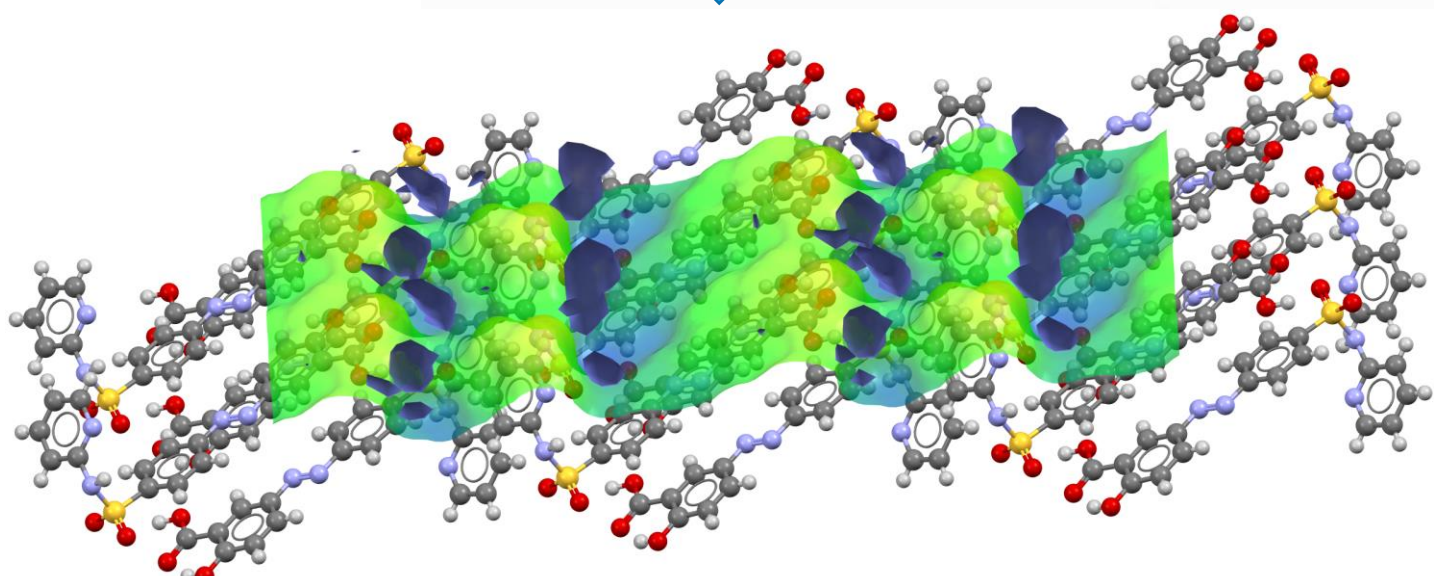
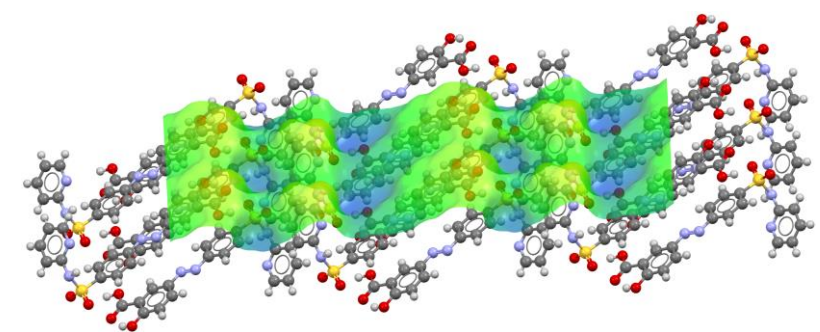
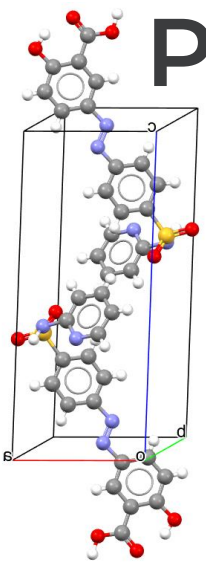
# Surface Analysis



## Descriptors

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

# Particle Informatics



## Descriptors

Physical

Chemical

Reticular Surface Area

Hydrogen Bond Donor/Acceptor Density

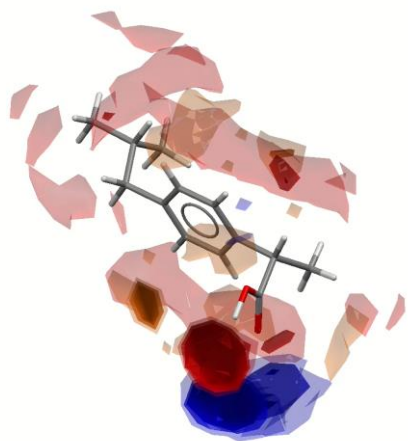
Rugosity

Aromatic Bond Density

RMSD, Skewness, and Kurtosis

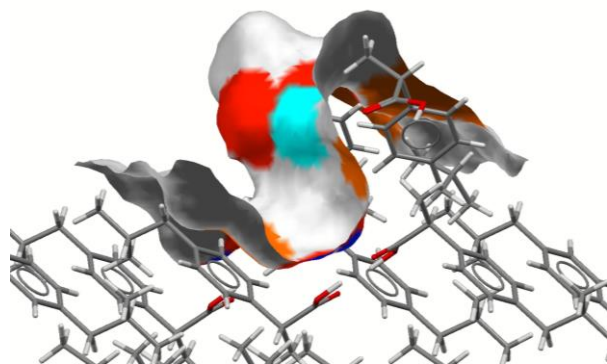
FIMs on Surface

# FIMs on Surface



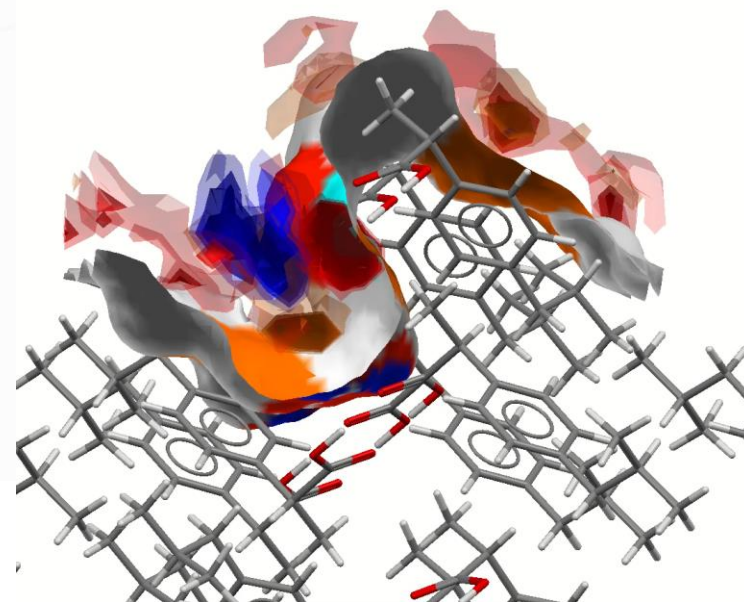
FIM

+



Surface

=



FIM on Surface

# 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

Picking Mode: Pick Atoms Clear Measurements  Show Labels for All atoms with Atom Label

Style: Ball and Stick Colour: by Element or Suppression Manage Styles... Work Atom selections:

Animate... Default view: b a b c a\* b\* c\* x- x+ y- y+ z- z+ x-90 x+90 y-90 y+90 z-90 z+90 ← → ↓ ↑ zoom- zoom+ Select by SMARTS: [c]

Structure Navigator

AABHTZ Find

Crystal Structures	Spacegroup
AABHTZ	P-1
AACANI10	P21/c
AACANI11	P21/c
AACFAZ	Pbcn
AACFAZ10	Pbcn
AACMAL	P21/c
AACMHX10	Pbca
AACRHA	Pncm
AACRHC	P-1
AACRUB	Cc
AACRUB01	C2/c
AADAMC	P21/c
AADMPY	P-1
AADMPY10	P-1
AADRIB	P21
AAGAGG10	P212121
AAGGAG10	P21

Display Options

Display

Packing  Short Contact < (sum of vdW radii) Contacts...  
 Asymmetric Unit  H-Bond Default definition More Info  
 Auto centre Reset Powder...

Options

Show hydrogens  Depth cue  
 Show cell axes  Z-Clipping  
 Label atoms  Stereo

Tree View  Multiple Structures Structures...

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

# Reminder: Basic navigation in Mercury



- **Left mouse** button and move – rotate molecules



- **Middle Mouse** wheel – move molecules up and down



- **Right mouse** button and move up and down – zoom in and out of molecules

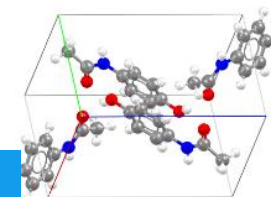


- **Shift + Left mouse** button and move – rotate in the plane molecules



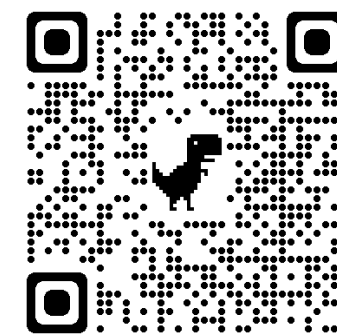
- **Ctrl + Left mouse** button and move – translate molecules

Visualisation 101 - Visualising structural chemistry data with Mercury



Learn more in this CSDU on-demand course

[Begin module](#)

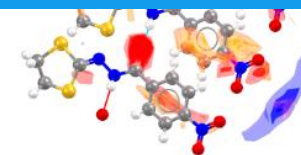


# Creating a Full Interaction Map

The screenshot displays the Mercury software interface. The main window shows a ball-and-stick model of a molecule with a Full Interaction Map overlaid, featuring red and blue electron density surfaces. The 'Full Interaction Maps...' menu option is highlighted in blue. The 'Full Interaction Maps' dialog box is open, showing the 'Maps' tab. The 'Map Contour Levels' section has three checked options: 'Display first contour with initial level of 2.0', 'Display second contour with initial level of 4.0', and 'Display third contour with initial level of 6.0'. The 'Hotspots' section has 'Generate hotspots in the map' unchecked. The 'Probe' section has several checked options: 'Uncharged NH Nitrogen', 'Carbonyl Oxygen', 'Water Oxygen', 'Aromatic CH Carbon', and 'C-F Fluorine'. A color scale legend is visible next to the probe list. The 'Calculate Maps' button is highlighted in blue. The 'Options' section at the bottom right has 'Show hydrogens', 'Show cell axes', and 'Label atoms' checked, while 'Depth cue', 'Z-Clipping', and 'Stereo' are unchecked.

Analysing intermolecular interactions 101 - Full Interaction Maps

Learn more in this CSDU on-demand course



Begin module

<https://www.ccdc.cam.ac.uk/Community/blog/getting-started-with-FIMS/>

CCDC



# CSD-Particle Menu

The screenshot displays the Mercury software interface. The main window shows a ball-and-stick model of a crystal structure. A blue box highlights the 'CSD-Particle' menu, which is open, showing options: 'Morphology', 'Slip Planes...', and 'Surface Analysis...'. The 'Morphology' option has a right-pointing arrow. The 'Structure Navigator' panel on the right lists various crystal structures and their space groups. The 'Display Options' panel at the bottom provides settings for the visualization, including 'Display' and 'Options' sections.

**Structure Navigator**

Crystal Structures	Spacegroup
AABHTZ	P-1
AACANI10	P21/c
AACANI11	P21/c
AACFAZ	Pbcn
AACFAZ10	Pbcn
AACMAL	P21/c
AACMHX10	Pbca
AACRHA	Pnmc
AACRHC	P-1
AACRUB	Cc
AACRUB01	C2/c
AADAMC	P21/c
AADMPY	P-1
AADMPY10	P-1
AADRIB	P21
AAGAGG10	P212121
AAGGAG10	P21
AALCFE	P21/c
AALPRO	P21/c
AAMAND	P212121
AAMTCO	P-1
AAMTCO10	P-1
AAMTXP	P21/n
AANHGX	Pna21
AANHGX01	Pna21
AANOPM	P21
AAPUNI	P21/a
AAPYPE	P21/c
AARBOX	P21
AAXTHP	P212121

**Display Options**

Display

- Packing
- Asymmetric Unit
- Auto centre
- Short Contact < (sum of vdW radii)
- H-Bond User defined

Options

- Show hydrogens
- Show cell axes
- Label atoms
- Depth cue
- Z-Clipping
- Stereo

# CSD-Particle – Morphology - BFDH

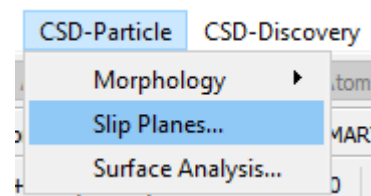
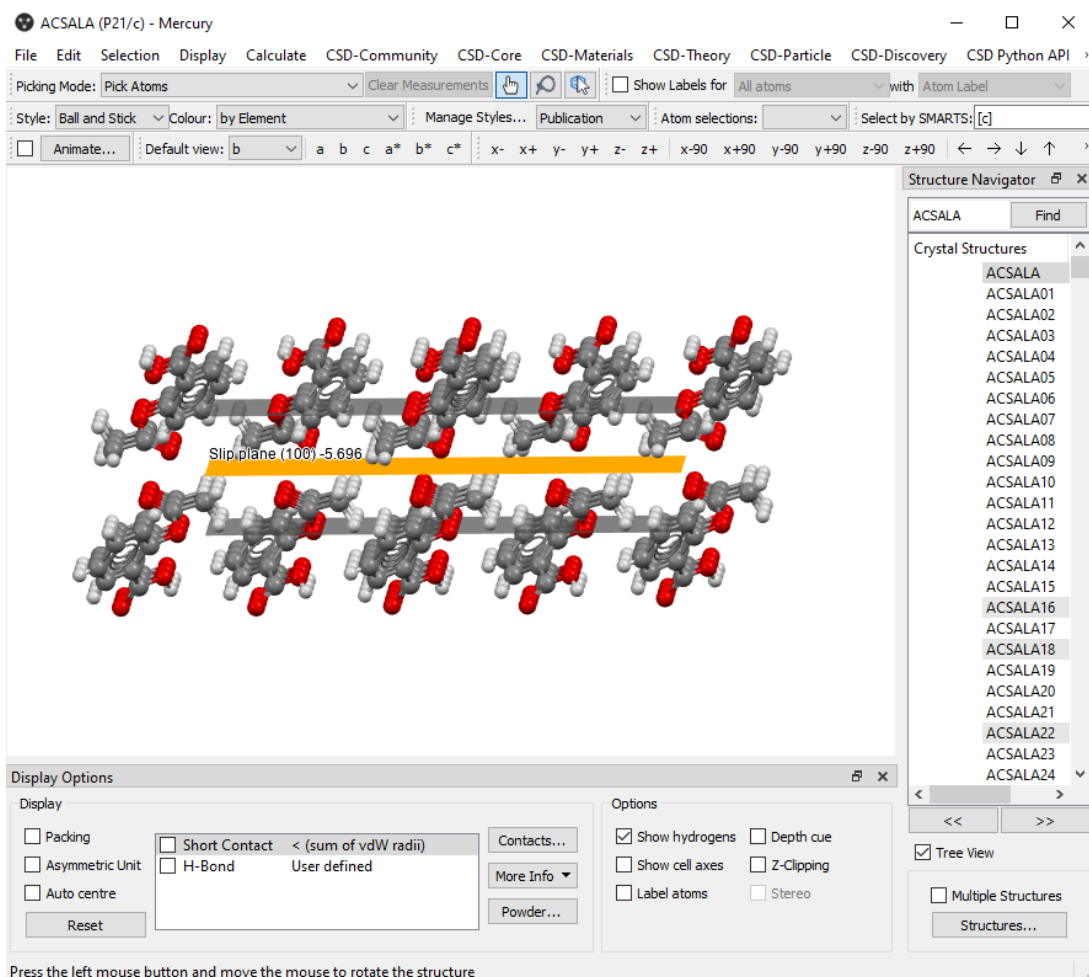
The screenshot displays the CSD-Particle software interface. The main window shows a 3D model of a crystal morphology with a central molecular structure and a surrounding blue polyhedral shape representing the morphology. The morphology is labeled with crystallographic planes: (-110), (-11-1), (-100), (010), (001), (0-11), (0-10), (01-1), (00-1), (101), (1-11), (1-10), and (100). The interface includes a menu bar with options like File, Edit, Selection, Display, Calculate, CSD-Community, CSD-Core, CSD-Materials, CSD-Theory, CSD-Particle, CSD-Discovery, and CSD Python API. A dropdown menu is open under 'Morphology', showing options: Morphology, Slip Planes..., Surface Analysis..., and BFDH... (selected). Below the menu is a 'Structure Navigator' panel listing crystal structures, with 'AABHTZ' selected. A 'Morphology' control panel is open, showing options:  Show Morphology, Scale factor: 100 (with 'Auto scale' checked),  Show (hkl) labels,  Draw faces (Colour: light blue, 0.5),  Shadows,  Draw edges (Colour: blue), and  Fill morphology with molecules. Buttons for 'Open...', 'Save...', 'Defaults', and 'OK' are visible. At the bottom left, a 'Display Options' panel is partially visible, showing options for Packing, Asymmetric Unit, Auto centre, Short Contact, H-Bond, and User defined. A footer note reads: 'Press the left mouse button and move the mouse to rotate the structure'.

Display Options

Save and Load

Learn more on [BFDH Morphology](#) in the *Glossary* in the handout.

# CSD-Particle – Slip Planes



Slip Planes... ACSALA

Minimum slab separation 0.0 Reset

Status Calculation completed

	Orientation	Slab separation	Repeat distance	Offset	H-bonded	Perpendicular planes
1	(100)	1.574	11.392	-5.696	no	
2	(100)	0.242	11.392	0.000	yes	

H-bond dimensionality: 0D discrete

Analyse Surface Export... Calculate Close

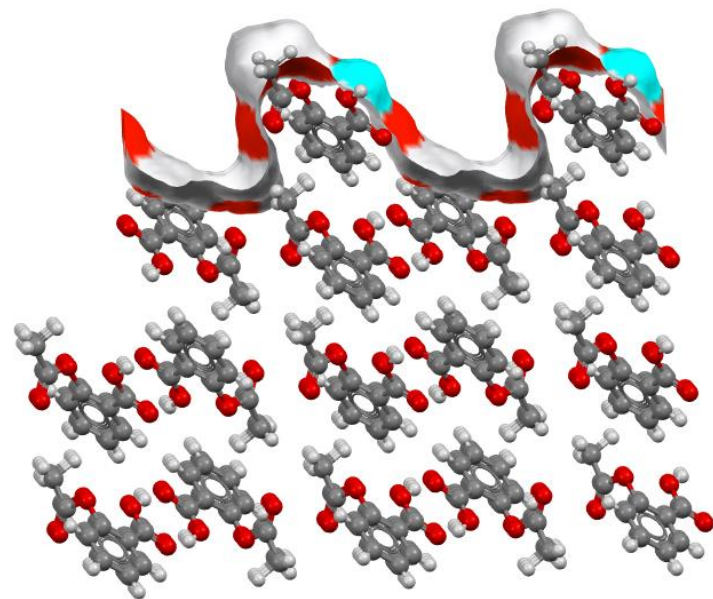
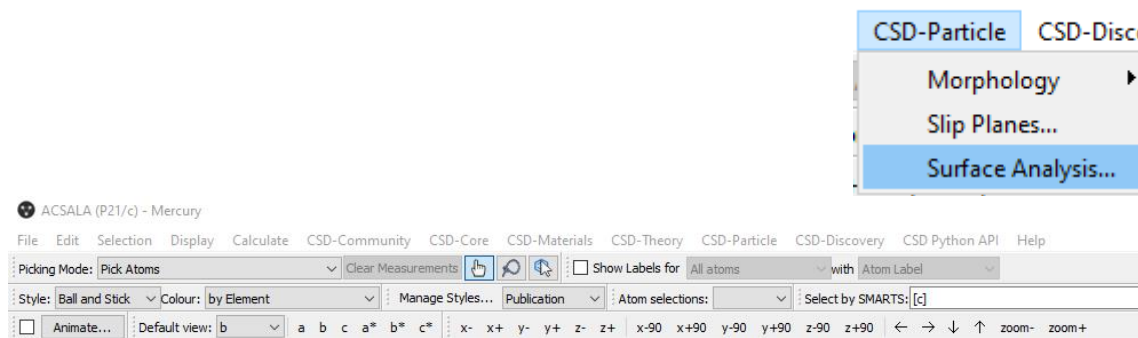
Possible Slip Planes

H-Bond System

Export Table

Learn more on [Slip Planes](#) in the *Glossary* in the handout.

# CSD-Particle – Surface Analysis



Surface Analysis... ACSALA

**Analyse**

Select surface orientation (hkl) and offset (o)

h: 0 k: 0 l: 2 o: 0.00  Preview Slab

Show Advanced Options

Full Interaction Map Calculate Surface

**Input**

## Results - ACSALA (002)[0.00]

### Density Info (count/Å<sup>2</sup>)

H-Bond Acceptors: 0.079	Aromatic Bonds: 0.159
H-Bond Donors: 0.013	Unsatisfied H-Bond Donors: 0.013

### Topology Info

Surface Area (Å <sup>2</sup> ): 637.558	Projected Area (Å <sup>2</sup> ): 301.991
Rugosity: 2.111	RMSD: 2.273
Skewness: 0.052	Kurtosis: 1.729

### Display Options

Surface colouring: Atom Properties

Opacity: (%) 100

Periodic View  Hide Molecules

Atom Properties

Charge  H-Bond Acceptors

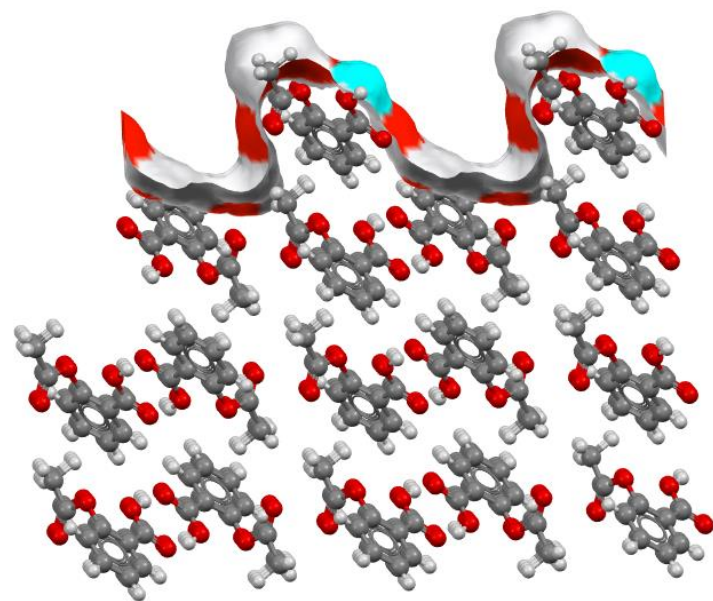
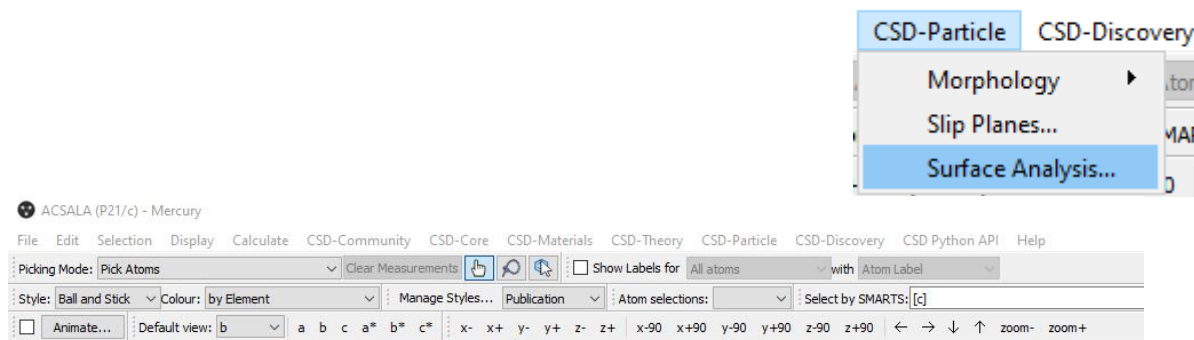
Aromatic  H-Bond Donors

Unsatisfied H-Bond Donors

Reset

Close

# CSD-Particle – Surface Analysis



Surface Analysis... ACSALA

**Analyse**

Select surface orientation (hkl) and offset (o)

h: 0 k: 0 l: 2 o: 0.00  Preview Slab

Show Advanced Options

Full Interaction Map Calculate Surface

**Results - ACSALA (002)[0.00]**

Density Info (count/Å<sup>2</sup>)

H-Bond Acceptors: 0.079	Aromatic Bonds: 0.159
H-Bond Donors: 0.013	Unsatisfied H-Bond Donors: 0.013

Topology Info

Surface Area (Å <sup>2</sup> ): 637.558	Projected Area (Å <sup>2</sup> ): 301.991
Rugosity: 2.111	RMSD: 2.273
Skewness: 0.052	Kurtosis: 1.729

**Display Options**

Surface colouring: Atom Properties

Opacity: (%) 100

Periodic View  Hide Molecules

Atom Properties

Charge  H-Bond Acceptors

Aromatic  H-Bond Donors

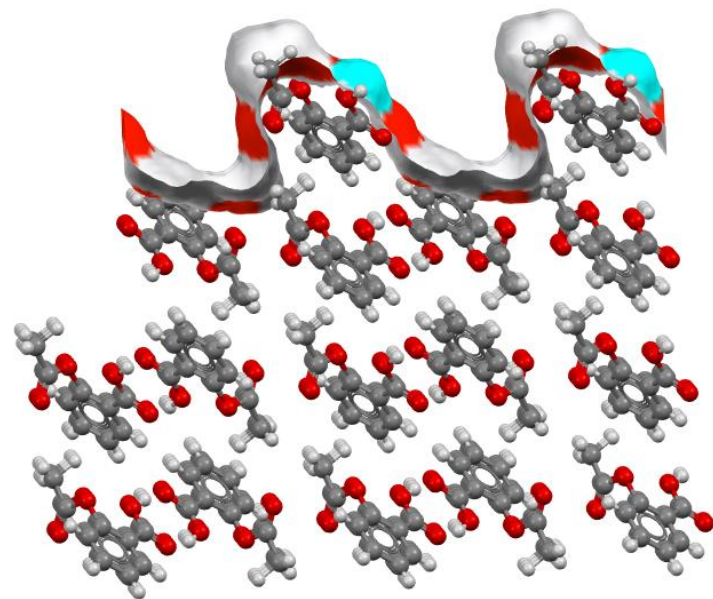
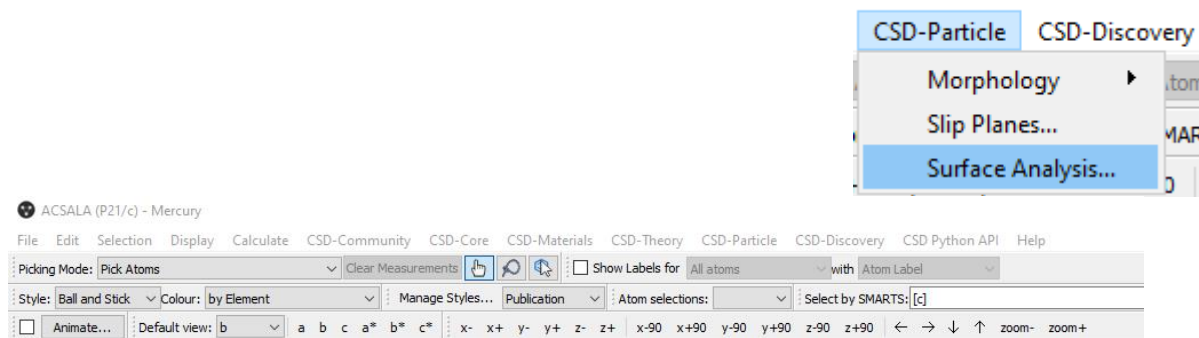
Unsatisfied H-Bond Donors

Reset Close

Results

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

# CSD-Particle – Surface Analysis



Surface Analysis... ACSALA

**Analyse**

Select surface orientation (hkl) and offset (o)

h: 0 k: 0 l: 2 o: 0.00  Preview Slab

Show Advanced Options

Full Interaction Map Calculate Surface

**Results - ACSALA (002)[0.00]**

Density Info (count/Å<sup>2</sup>)

H-Bond Acceptors: 0.079	Aromatic Bonds: 0.159
H-Bond Donors: 0.013	Unsatisfied H-Bond Donors: 0.013

Topology Info

Surface Area (Å <sup>2</sup> ): 637.558	Projected Area (Å <sup>2</sup> ): 301.991
Rugosity: 2.111	RMSD: 2.273
Skewness: 0.052	Kurtosis: 1.729

**Display Options**

Surface colouring: Atom Properties

Opacity: (%) 100

Periodic View  Hide Molecules

Atom Properties

Charge  H-Bond Acceptors

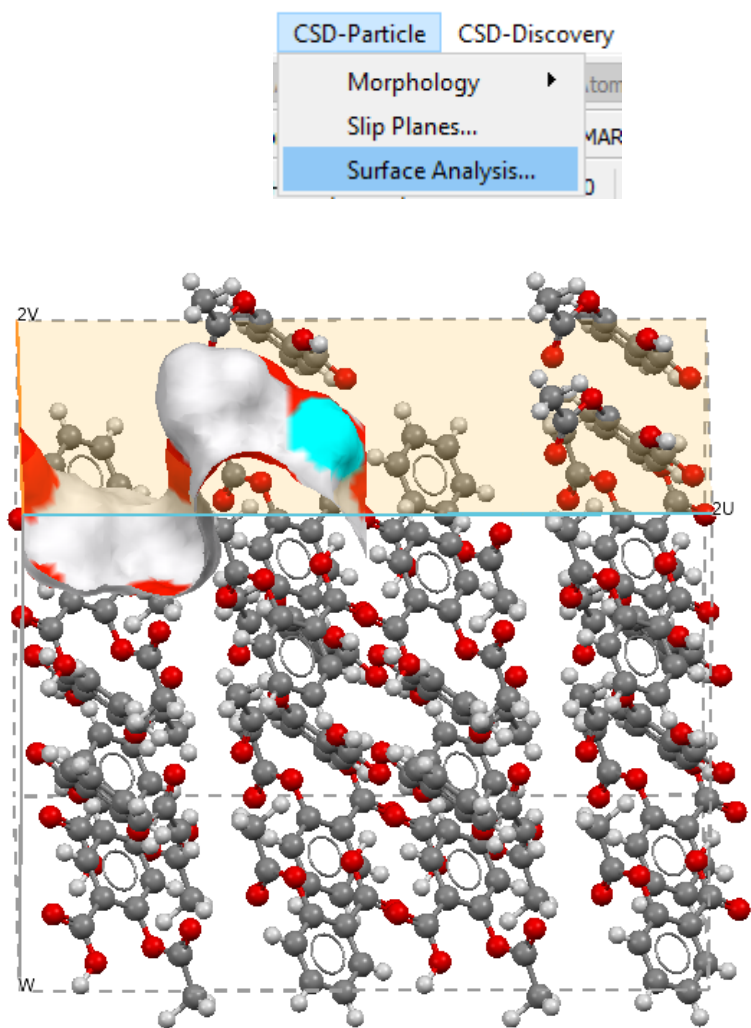
Aromatic  H-Bond Donors

Unsatisfied H-Bond Donors

Reset Close

Display Options

# CSD-Particle – Surface Analysis



The 'Surface Analysis... ACSALA' dialog box is shown. The 'Analyse' section is active, with 'Show Advanced Options' checked. The 'Size of Surface' is set to U: 2 and V: 2. The 'Probe Radius' is 1.2 and 'Grid Spacing' is 0.3. The 'Thickness (W) Factor' is 1.60. The 'Results - ACSALA (002)[0.00]' section displays the following data:

Density Info (count/Å <sup>3</sup> )	
H-Bond Acceptors: 0.079	Aromatic Bonds: 0.159
H-Bond Donors: 0.013	Unsatisfied H-Bond Donors: 0.013

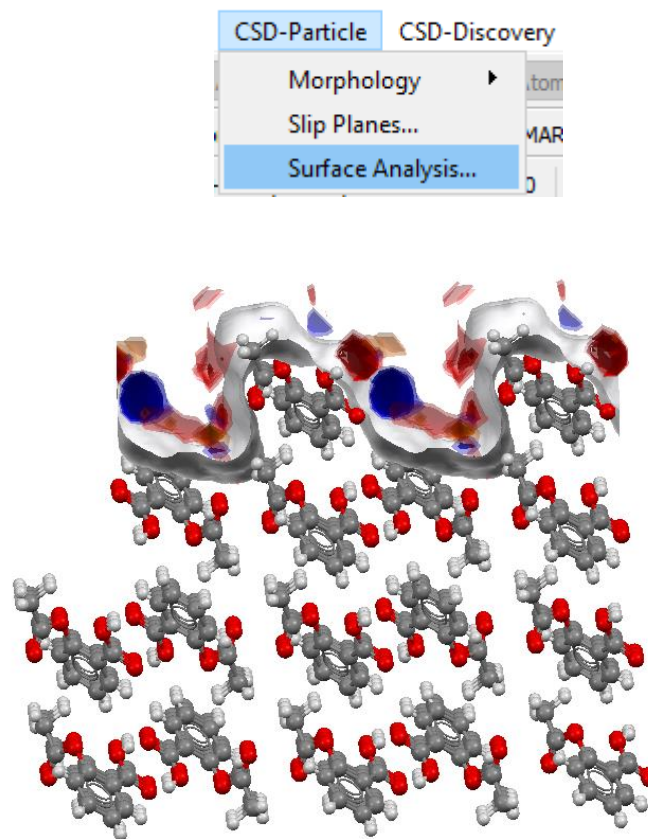
  

Topology Info	
Surface Area (Å <sup>2</sup> ): 159.389	Projected Area (Å <sup>2</sup> ): 75.498
Rugosity: 2.111	RMSD: 2.273
Skewness: 0.052	Kurtosis: 1.729

The 'Display Options' section shows 'Surface colouring' set to 'Atom Properties' and 'Opacity (%)' set to 100. The 'Atom Properties' section has 'Charge' and 'Aromatic' unchecked, and 'H-Bond Acceptors', 'H-Bond Donors', and 'Unsatisfied H-Bond Donors' checked. 'Reset' and 'Close' buttons are at the bottom.

Advance Options

# CSD-Particle – FIMs on Surface



Surface Analysis... ACSALA

**Analyse**

Select surface orientation (hkl) and offset (o)  
h: 0 k: 0 l: 2 o: 0.00  Preview Slab  
 Show Advanced Options

Size of Surface: U: 2 V: 2  
Default values for the following settings have been optimised for small molecule organic systems.

Probe Radius: 1.2 Grid Spacing: 0.3  
Thickness (W) Factor  1.60

**Results - ACSALA (002)[0.00]**

Density Info (count/Å<sup>2</sup>)

H-Bond Acceptors: 0.079	Aromatic Bonds: 0.159
H-Bond Donors: 0.013	Unsatisfied H-Bond Donors: 0.013

Topology Info

Surface Area (Å <sup>2</sup> ): 159.389	Projected Area (Å <sup>2</sup> ): 75.498
Rugosity: 2.111	RMSD: 2.273
Skewness: 0.052	Kurtosis: 1.729

**Display Options**

Surface colouring: Atom Properties  
Opacity: (%)  100

Periodic View  Hide Molecules

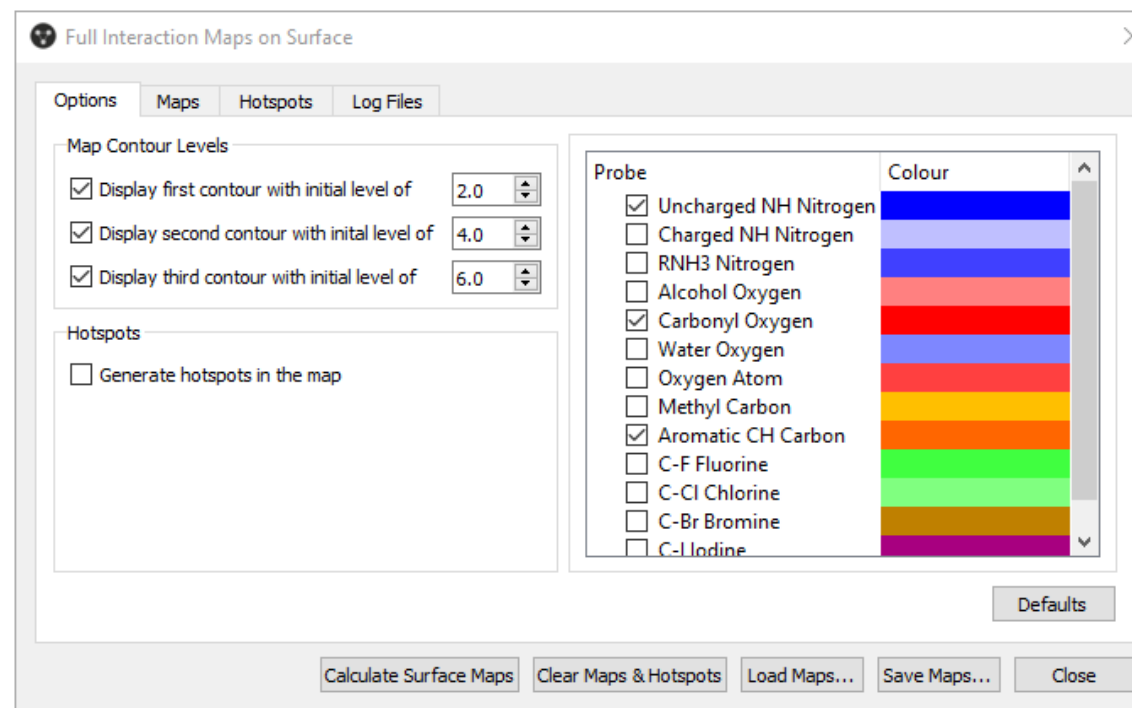
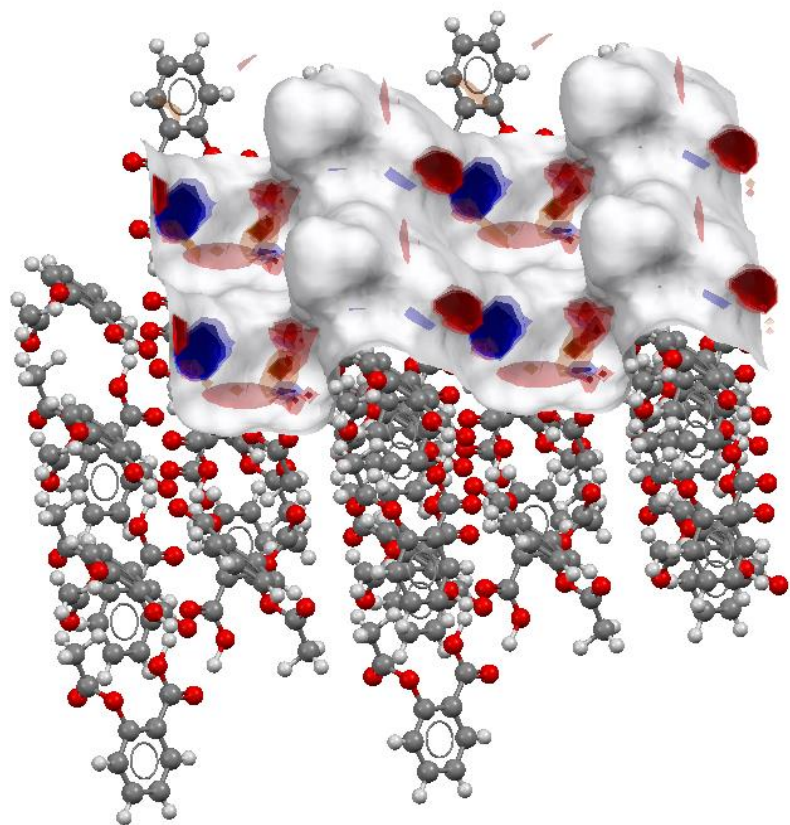
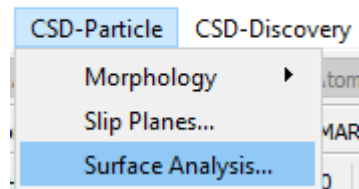
Atom Properties

<input type="checkbox"/> Charge	<input checked="" type="checkbox"/> H-Bond Acceptors
<input type="checkbox"/> Aromatic	<input checked="" type="checkbox"/> H-Bond Donors
	<input checked="" type="checkbox"/> Unsatisfied H-Bond Donors

Full Interaction Map on Surface



# CSD-Particle – FIMs on Surface



# Want to explore more?

## Training and Educational Resources

The wealth of information contained within the Cambridge Structural Database (CSD) extends far beyond a collection of crystal structures. Knowledge derived from these materials informs much of chemistry, biochemistry, and biology. Chemical and structural concepts are often difficult to grasp without real world, interactive examples for students to explore.

The CCDC and our colleagues continually produce educational materials for use in classroom and computer lab settings, or as independent study modules. Many of these materials make use of the Teaching Subset - a freely available set of over 750 structures that can be investigated with the free version of our Mercury visualisation and analysis program. Of course, our database of over one million entries are available for free through our Access Structures portal.

If you are an educator looking for supplementary teaching materials, find out more about the Teaching Database [here](#). If you have developed your own modules using the CSD and would like to share them with the broader community, please contact us at [education@ccdc.cam.ac.uk](mailto:education@ccdc.cam.ac.uk).

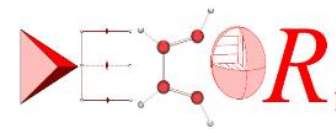
To keep up to date with the latest news from education and outreach at the CCDC, sign up for the Education and Outreach Newsletter [here](#).



Information on the Teaching Subset



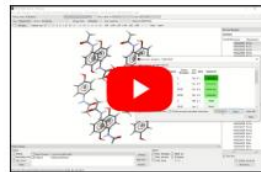
Access a series of teaching modules for use in the classroom



DECOR: Educational Resources for Teaching Crystallography



Download a series of self-guided workshop materials for CCDC tools and features



Watch software training and support videos



CSDU modules - Explore our on-demand training courses



Access fun science activities for kids through the CCDC Home learning page



Explore the Periodic Table through Crystal Structures



Bound! a Protein-Drug matching card game

Register for E&O newsletter

On-demand modules with completion certificate

A new docking card game

Self-guided workshops

YouTube and LabTube channels

# CSDU



- **On-demand** modules to learn how to use the CSD Software at your own pace.
- **Completion certificate** after a final quiz!



UWatch

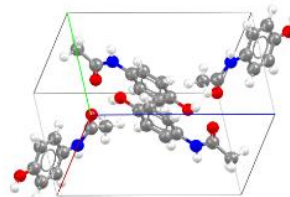


UTry



UTest

### Visualisation 101 - Visualising structural chemistry data with Mercury



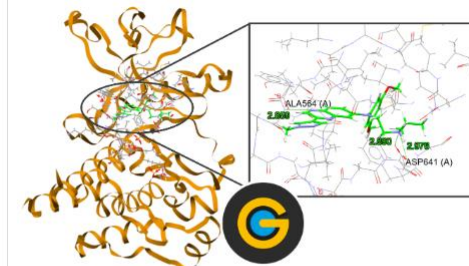
Begin module

### Programmatic access to the CSD 101 – CSD Python API



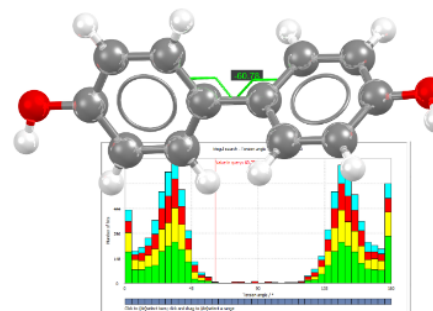
Begin module

### Protein-ligand docking 101 - Running a simulation in GOLD



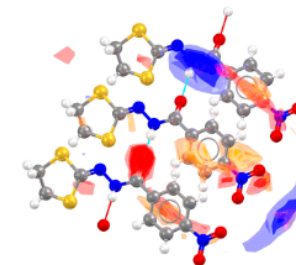
Begin module

### Analysing molecular geometries 101 - basics of Mogul



Begin module

### Analysing intermolecular interactions 101 - Full Interaction Maps

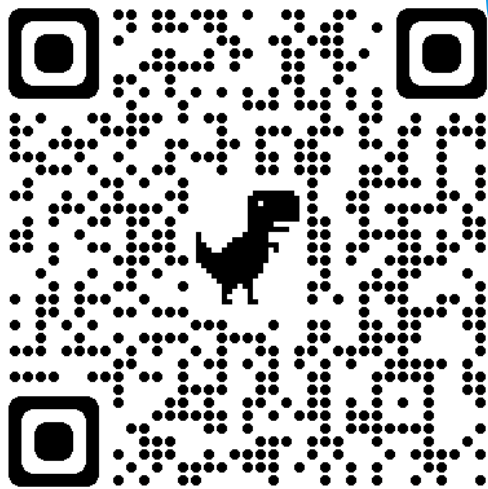


Begin module



# CCDC Engagement Grants

**Engage, inspire, share!**



Applications  
and all  
information  
on the  
website!

Ask us at  
the booth!

- Do you wish to inspire others with your love of crystallography or structural science?
- CCDC Engagement Grants cover costs for you to produce resources or activities to increase schools and public engagement in crystallography and structural science.