

How to Use Particle Informatics Tools to Connect Crystal Structure to Particle Behaviour

CCDC Virtual Workshop

21st October 2025

Learning outcomes

- ❑ Become familiar with the **CSD**
- ❑ How to use **Mercury** for **Particle Informatics** studies.
- ❑ How to use the **Surface Analysis** tool.
- ❑ How to calculate **Full Interaction Maps** on surfaces.
- ❑ How you can **best use** Mercury and CSD-Particle in your workflows.
- ❑ About **recent advances** and improvements in CSD-Particle tools.

We will make the recording available to you in the next few days.



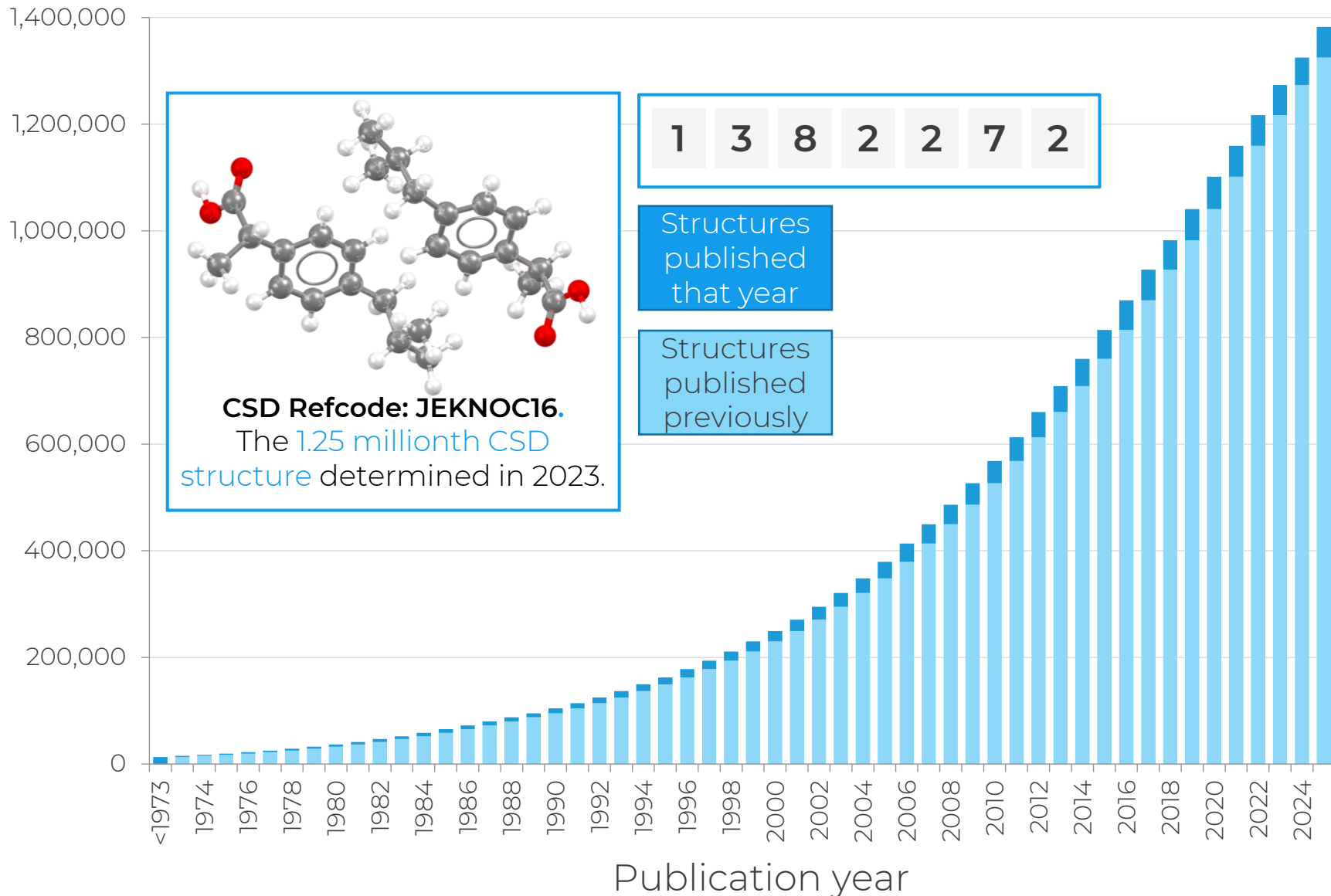
We are recording today's session and will make the recording available to you in the next few days

Agenda

- *Show One*: Introduction to the CSD, CSD-Particle and Particle Informatics
- *Show One*: Case study by Prof. Elena Simone
- *Show One*: Surface Analysis using CSD-Particle
- *Try One*: Hands-on examples
- *Explore More*: Case studies, tips, quiz and summary
- *Extra time*: More time for hands on and Q&A

The Cambridge Structural Database

Number of structures in the CSD

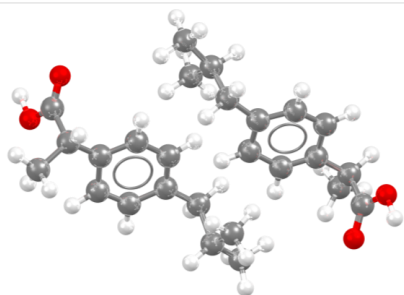


- Small molecule organic and metal-organic structures
- Every published structure
 - Inc. ASAP & early view
 - *CSD Communications*
 - Patents
 - University repositories
 - Thesis
- Every entry enriched and annotated by experts
- Discoverability of data and knowledge
- Sustainable for 60 years
- A trusted CoreTrustSeal repository

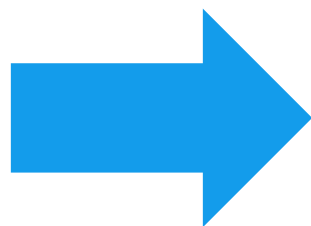


Certified as Trustworthy
by CoreTrustSeal

CSD Refcodes



CSD Refcode -
JEKNOC16



What is JEKNOC16?

- A CSD Refcode
- A database reference code
- Containing 6-8 characters
- Used to identify entries in the CSD

Recode families

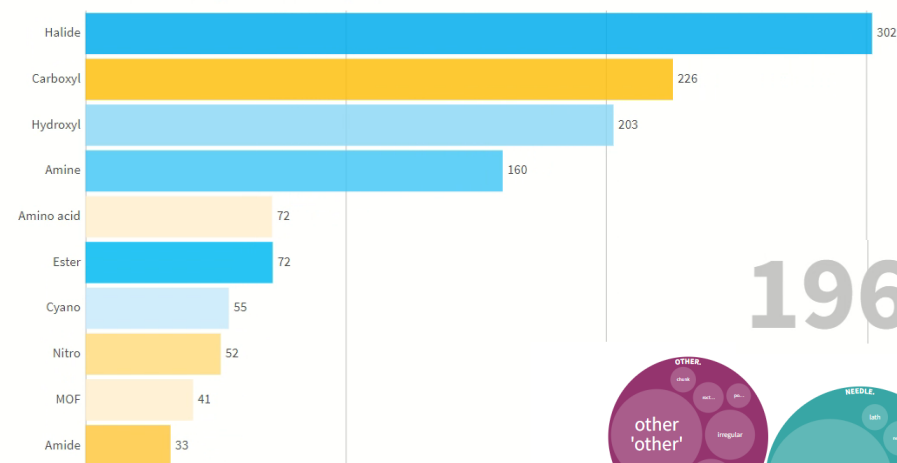
- The same substances are assigned the *same* 6 letter code plus an additional 2 numbers
 - Polymorphs
 - New determinations or re-refinements of the same substance
 - Determinations at different temperatures/pressures
- Stereoisomers or different solvates, co-crystals, etc are assigned *different* recode families

Some interesting recodes are: KITTEN, BATMAN, DISNEY, GAUTAM, GLYCIN

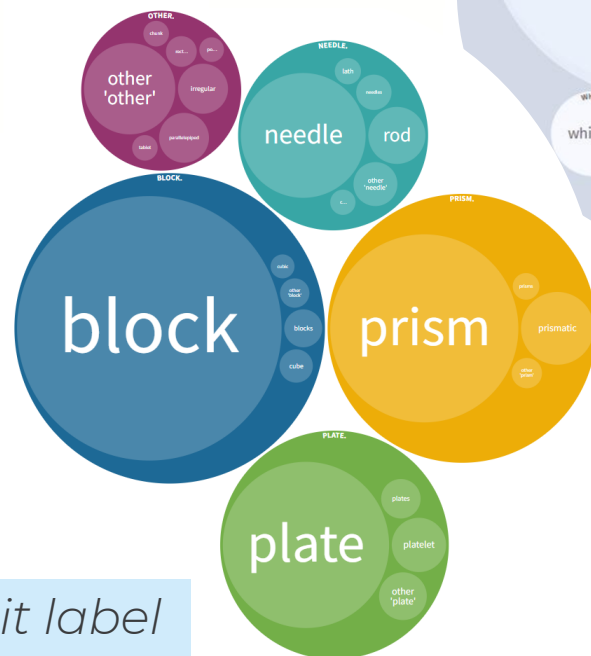
Statistics in the CSD

Chemistry in the CSD

Number of structures containing certain chemical groups



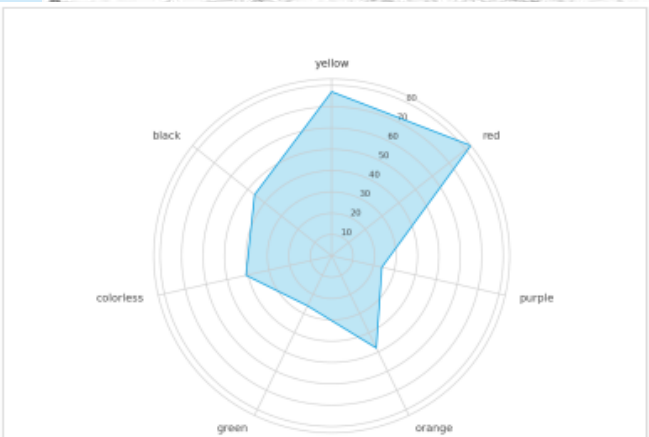
1965



habit label



colour label



ENTRY COMPLETENESS

Of your recent structures, **87.5%** have color labels and **70.2%** have habit labels! This earned you **157,000** points. Check out how many of your submitted structures are your "favorite" colors!

Data collected using the CSD Python API and graphs created with Flourish



From our #CSDLeaderboard at conferences!

The CSD Portfolio

CSDEnterprise.

CSDCore.

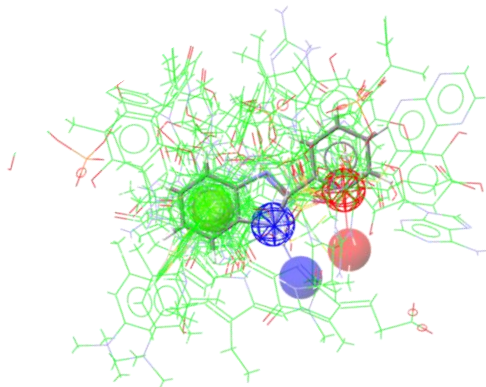


Mercury



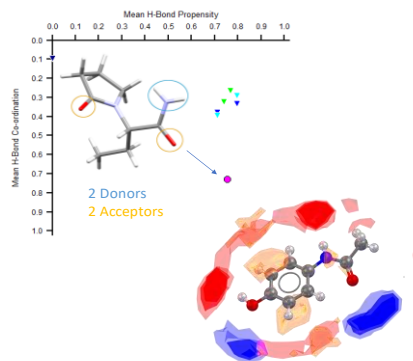
CSDDiscovery.

Design of new molecules



CSDMaterials.

Assessment of solid form stability and properties



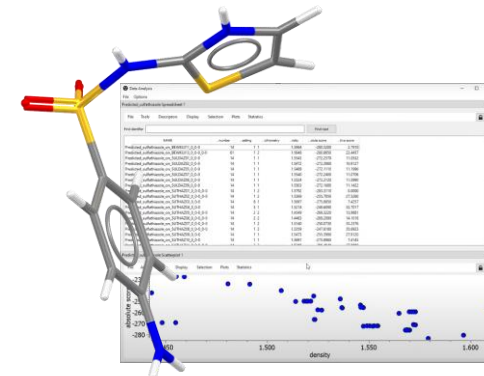
CSDParticle.

Anticipate particle properties and behaviour



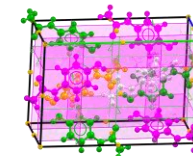
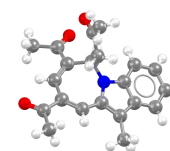
CSDTheory.

Generate solid form landscapes



CSDCommunity.

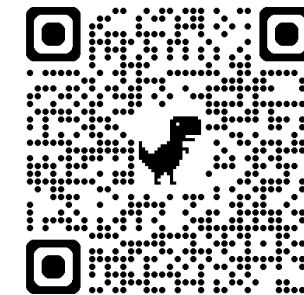
*Deposit, publish, access and visualise structural data
Free functionality to share and learn from structures*



Medicinal & Computational Chemists ♦ Crystallographers & Structural Biologists ♦ Solid Form & Crystallisation Scientists ♦ Functional Materials Scientists ♦ Educators ♦ Industry and Academia

CCDC

What can you do with a licence?



CCDC

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How CSD Licences Work

About CSD Licences

A licence allows you to use the Cambridge Structural Database (CSD) data and software in your research.

We offer a range of data and software to support molecular discovery, materials design, and crystallography research. This includes open source, free, and paid software.

CSD licences are available for academic universities and research institutions, government organizations, and commercial companies. The exact licence terms and what tools are included depend on the licence type. We can help advise you what licence is best for your needs.

Academic CSD Licence Types	Commercial CSD Licence Types	View Standard CSD Licence Agreement
For academic users we offer a range of free tools, including free Mercury, or a full licence enables even more search and analysis tools. The full licence is provided at a heavy discount to all academic users. This table compares the free CSD-Community and full CSD-Enterprise licences.	Commercial users can select from a range of licence levels depending on your field. Specialist packages for data and search, drug discovery, materials design, crystal structure prediction, and particle / manufacturing analysis are available. This table compares the commercial CSD licences available.	View the standard CSD licence agreement. Note that this may not match your own agreement. If you want a copy of your personal agreement, please contact us.

- **Supporting research:** The CSD Portfolio enables bulk access to the CSD and large-scale structural surveys to advance your research.
- **Responsible data use:** We encourage and support use for research and analysis, but redistribution and large-scale publication are restricted to protect the CSD's sustainability.
- **Publication guidelines:** Small extracts and visualizations can be shared, as can refcode lists but full datasets require permission.
- **Supporting you:** More information is available on our website, but if in doubt, contact us—we're happy to help!

<https://www.ccdc.cam.ac.uk/solutions/csd-licence/>

support@ccdc.cam.ac.uk

CCDC



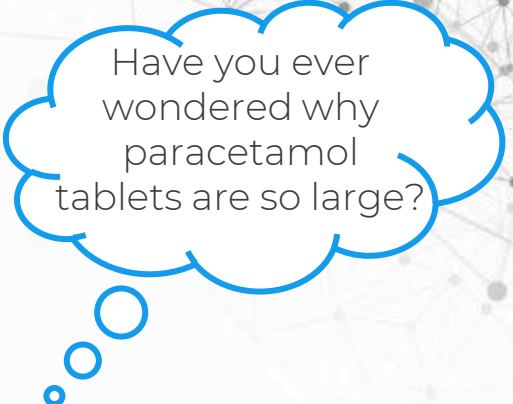
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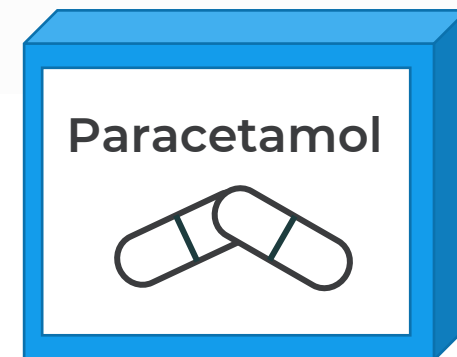
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Why does particle shape matter?

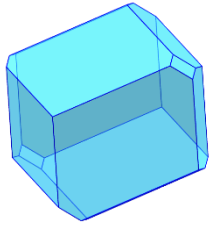
- The shape of a particle can impact:
 - Pharmaceutical solubility and stability.
 - Packing behaviour.
 - Flowability.
 - Processing and manufacturing efficiency/ability.
- CSD-Particle and data-driven design can help to:
 - Anticipate manufacturing bottlenecks.
 - Guide formulation decisions.
 - Predict particle shape and properties.

A blue-outlined thought bubble containing text, with three smaller circles leading to it from the bottom left.

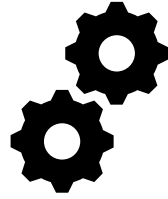
Have you ever wondered why paracetamol tablets are so large?



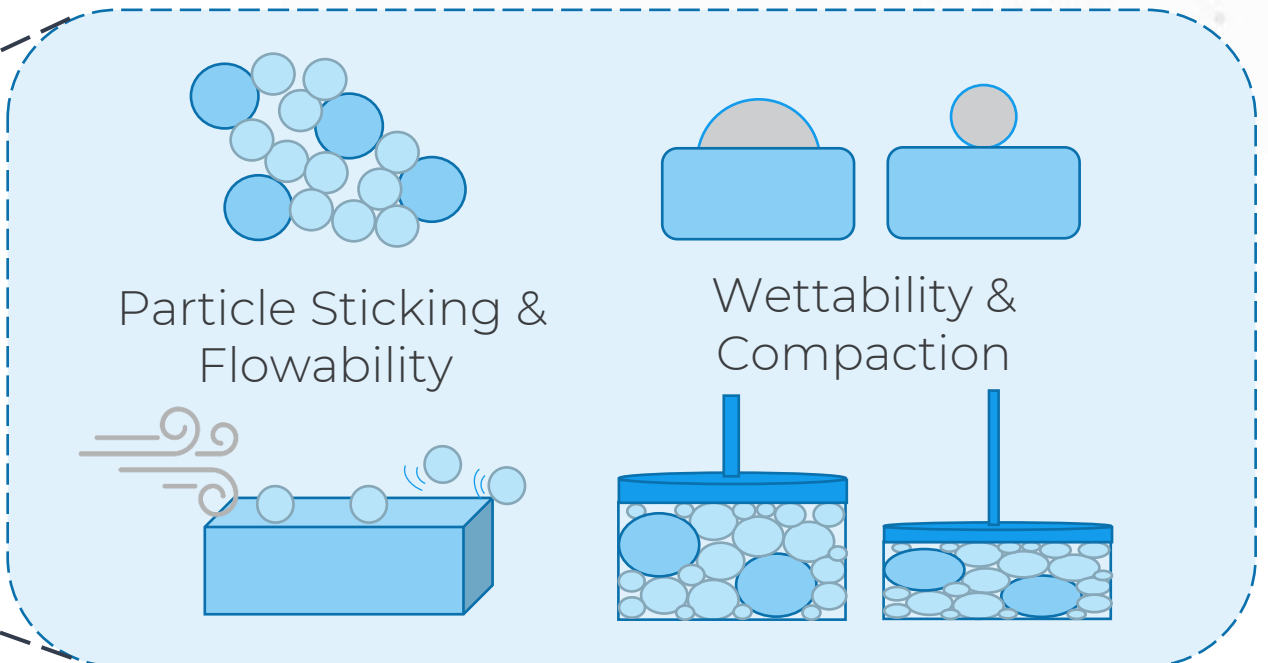
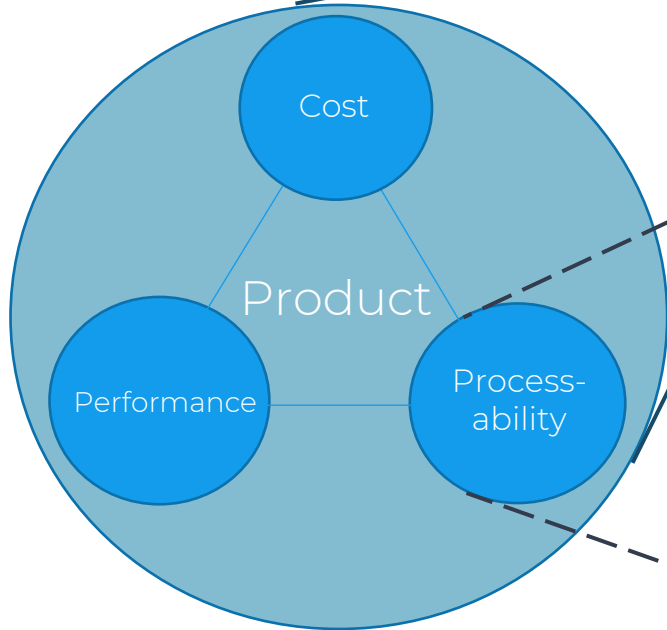
The field



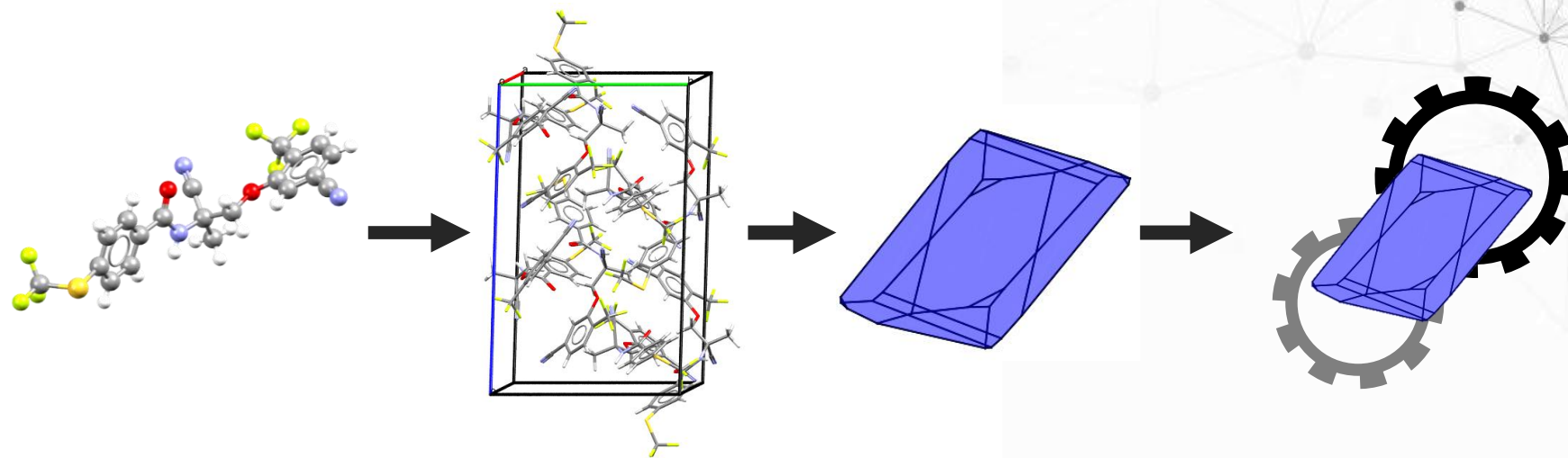
Particle



Product



From solid form to particle properties



Molecule

Form

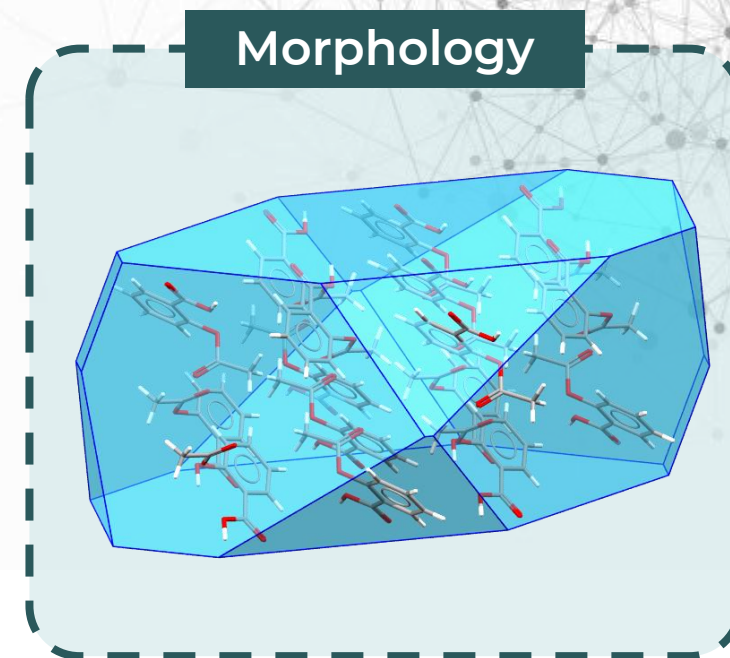
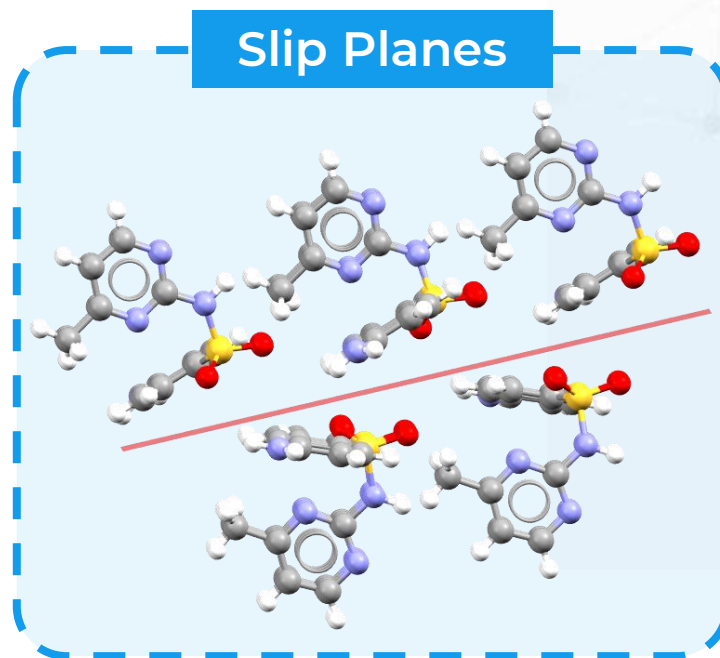
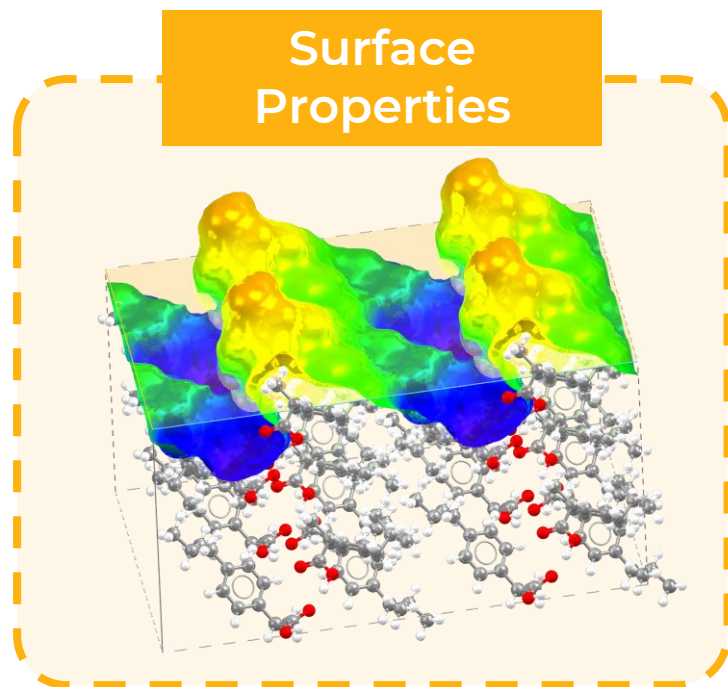
Particle

Properties

Solid Form Informatics

Particle Informatics

Analysing particle properties



- 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.

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Please add your questions for Prof. Simone in the chat and she will answer either in writing or verbally during the hands-on part.



Prof. Elena Simone
Politecnico di Torino

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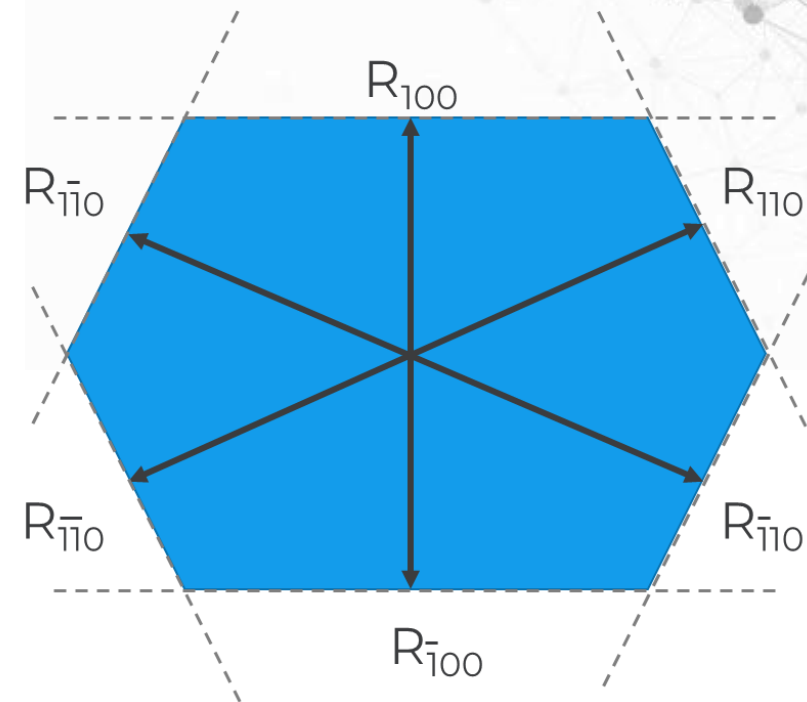
- *Show One*: Introduction to the CSD, CSD-Particle and Particle Informatics
- *Show One*: Case study by Prof. Elena Simone
- *Show One: Surface Analysis using CSD-Particle*
- *Try One*: Hands-on examples
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Which surface to analyse?

How do crystals grow?

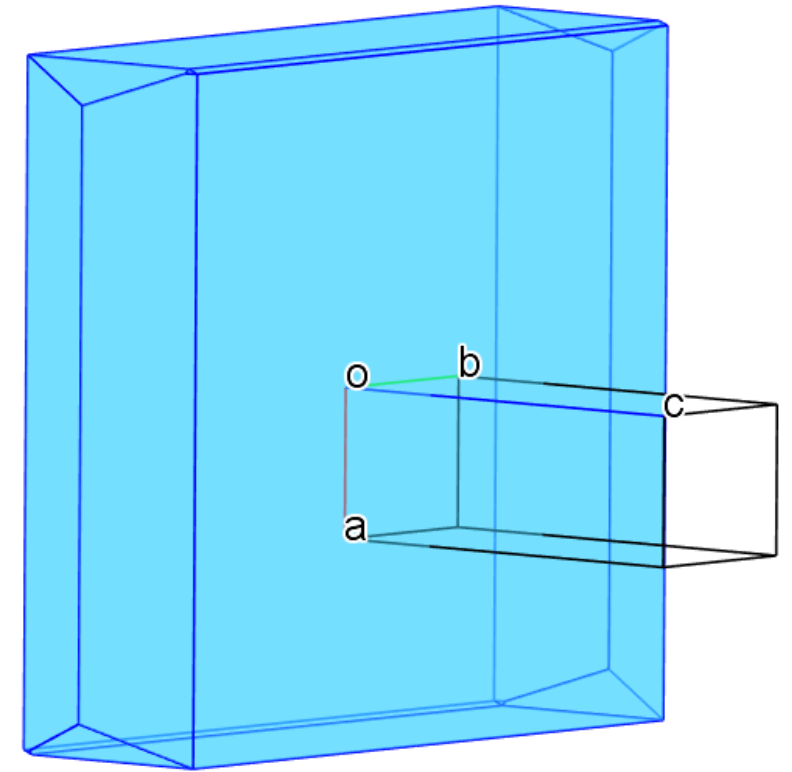
- Depends on **relative growth rates**
 - R_{hkl}
 - *Faster growing faces are smaller*
- Growth rates are dependent on many things:
 - Supersaturation
 - Solvents
 - Impurities

R = rate
 hkl = to indicate direction of growth



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.



BFDH = Bravais-
Friedel-Donnay-Harker

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

VisualHabit

- Uses a range of simple forcefields to calculate lattice, slice, and attachment energies.
- Integrated into Mercury and interfaces with other tools in the CSD-Particle suite.
- Developed through a collaboration with the University of Leeds supported by a Knowledge Transfer Partnership.



Innovate
UK

CCDC

Accessing morphologies in 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:

Morphology BFDH... Slip Planes... VisualHabit... Surface Analysis...

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

Crystal Structures Spacegroup

Tree View Multiple Structures Structures...

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

BFDH Morphology

The screenshot displays the Mercury software interface. The main window shows a 3D ball-and-stick model of a molecule centered within a light blue polyhedral morphology. The faces of the polyhedron are labeled with Miller indices: (-110), (-100), (-11-1), (-10-1), (010), (001), (01-1), (0-11), (00-1), (0-10), (101), (1-11), (100), and (1-10). A context menu is open over the 'CSD-Particle' object, with 'Morphology' selected, and a sub-menu showing 'BFDH...' and 'VisualHabit...'. The 'Morphology' dialog box is open, showing the following settings:

- Show Morphology
- Scale factor: 100 (with 'Auto scale' checked)
- Show (hkl) labels
- Draw faces: Colour (light blue), 0.5
- Shadows
- Draw edges: Colour (dark blue)
- Fill morphology with molecules

Buttons for 'Open...', 'Save...', 'Defaults', and 'OK' are visible. At the bottom left, the 'Display Options' dialog box is partially visible, showing options for 'Packing', 'Asymmetric Unit', 'Auto centre', 'Short Contact', 'H-Bond', 'User defined', 'Contacts...', 'More Info', and 'Powder...'. The 'Options' section includes 'Show hydrogens', 'Depth cue', 'Show cell axes', 'Z-Clipping', 'Label atoms', and 'Stereo'. A 'Tree View' checkbox is also present.

Display Options

Save and Load

Learn more on BFDH Morphology in the *Glossary* in the handout.

Accessing VisualHabit

The screenshot shows the Mercury software interface. The main window displays a crystal structure model with a habit polyhedron overlaid. The polyhedron is semi-transparent blue and has several faces labeled with Miller indices: (-100), (-11-1), (-10-1), (-1-10), (010), (001), (0-11), (01-1), (00-1), (0-10), (110), (101), (1-11), and (100). The structure is shown in a ball-and-stick representation. The interface includes a menu bar, a toolbar, and a structure navigator on the right.

The screenshot shows the 'CSD-Particle' menu with the following options: Morphology, Slip Planes..., Surface Analysis..., BFDH..., and VisualHabit... The 'VisualHabit...' option is highlighted in blue.

The screenshot shows the 'VisualHabit Morphology' dialog box. It has tabs for Calculation, Visualiser, Synthesis, and Surface. The 'Calculation' tab is active, showing 'Input' and 'Results' sections.

Input

Forcefield	Dreiding II
Limiting Radius (Angstrom)	30
Electrostatic Correction	Evjen

Results

Lattice Energy Results	
AABHTZ - Dreiding II results (in kJ mol ⁻¹)	
Total Lattice Energy	-163.706
Electrostatic Energy	-9.226
van der Waals Energy	-128.867
Hydrogen bonding energy	-25.613

Convergence

Limiting Radius (Å)	H-Bond Energy (kJ mol ⁻¹)	van der Waals Energy (kJ mol ⁻¹)
2	0.00	0.00
4	0.00	0.00
6	0.00	0.00
8	-32.22	-96.65
10	-32.22	-128.87
12	-32.22	-128.87
14	-32.22	-128.87
16	-32.22	-128.87
18	-32.22	-128.87
20	-32.22	-128.87
22	-32.22	-128.87
24	-32.22	-128.87
26	-32.22	-128.87
28	-32.22	-128.87
30	-32.22	-128.87

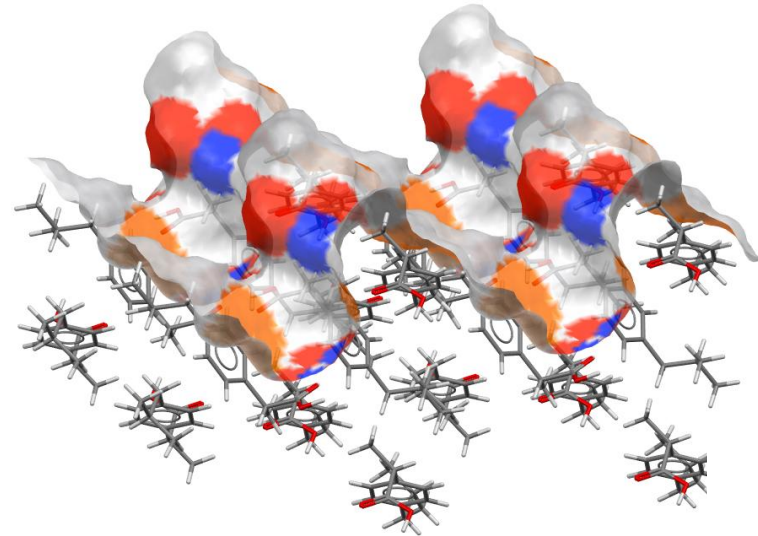
Calculation Converged ✓

Bonus: Experimental Habit Data Field

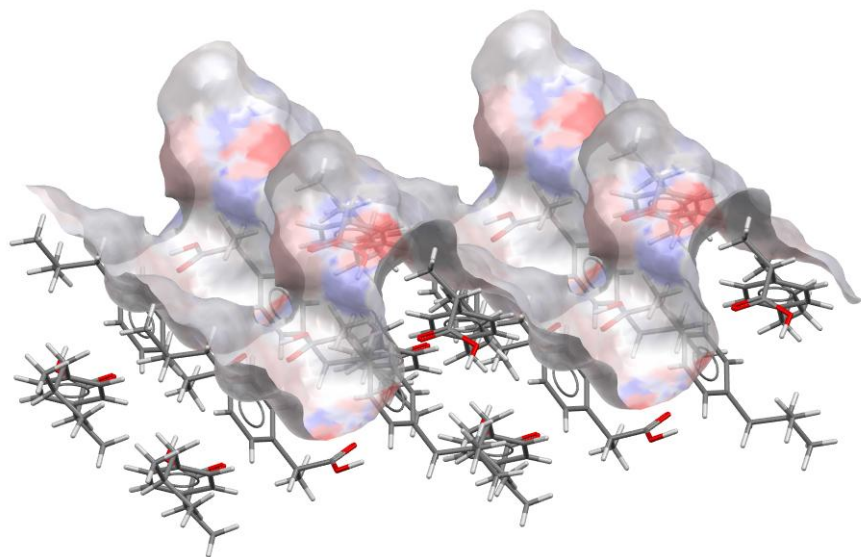
The image illustrates the process of adding experimental habit data to a structure record in a software application. It shows three overlapping windows:

- Structure Information...:** A menu on the left with 'Customise...' highlighted. A blue arrow points from this menu to the 'Customise' dialog.
- Customise:** A dialog box with two panes: 'Available Items (Right-click for options)' and 'Selected Items (Right-click for options)'.
 - The 'Available Items' pane lists various categories, with 'Crystal' expanded to show 'Habit' highlighted. A blue box highlights the 'Habit' item, and a blue arrow points from it to the 'Add >>' button.
 - The 'Selected Items' pane shows a list of fields including 'Habit', 'Identifier', 'Literature Reference', 'Formula', 'Compound Name', 'Synonym', 'Space Group', 'Cell Length', 'Cell Angles', 'Cell Volume', 'Density (CCDC)', and 'Density (author)'. A blue arrow points from this pane to the 'ABABUD' structure information window.
- ABABUD:** A window showing structure information for 'ABABUD'. The 'Habit' field is highlighted in blue, and its value is 'block'. The window also displays other fields like 'Z, Z'', 'R-Factor (%)', 'Disorder', 'Polymorph', 'Powder Study', 'Reduced Cell Lengths', 'Reduced Cell Angles', 'Reduced Cell Volume', 'Bioactivity', and 'Remarks'.

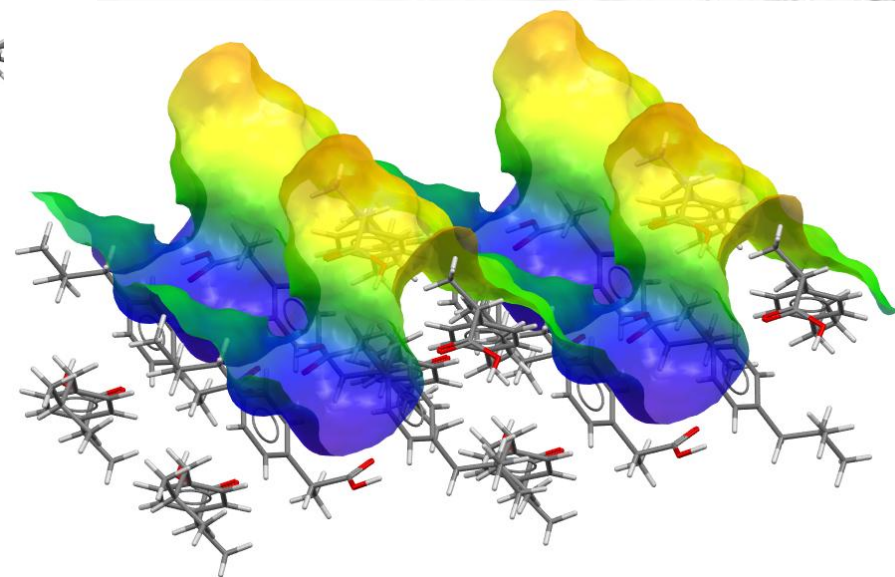
Surface Analysis



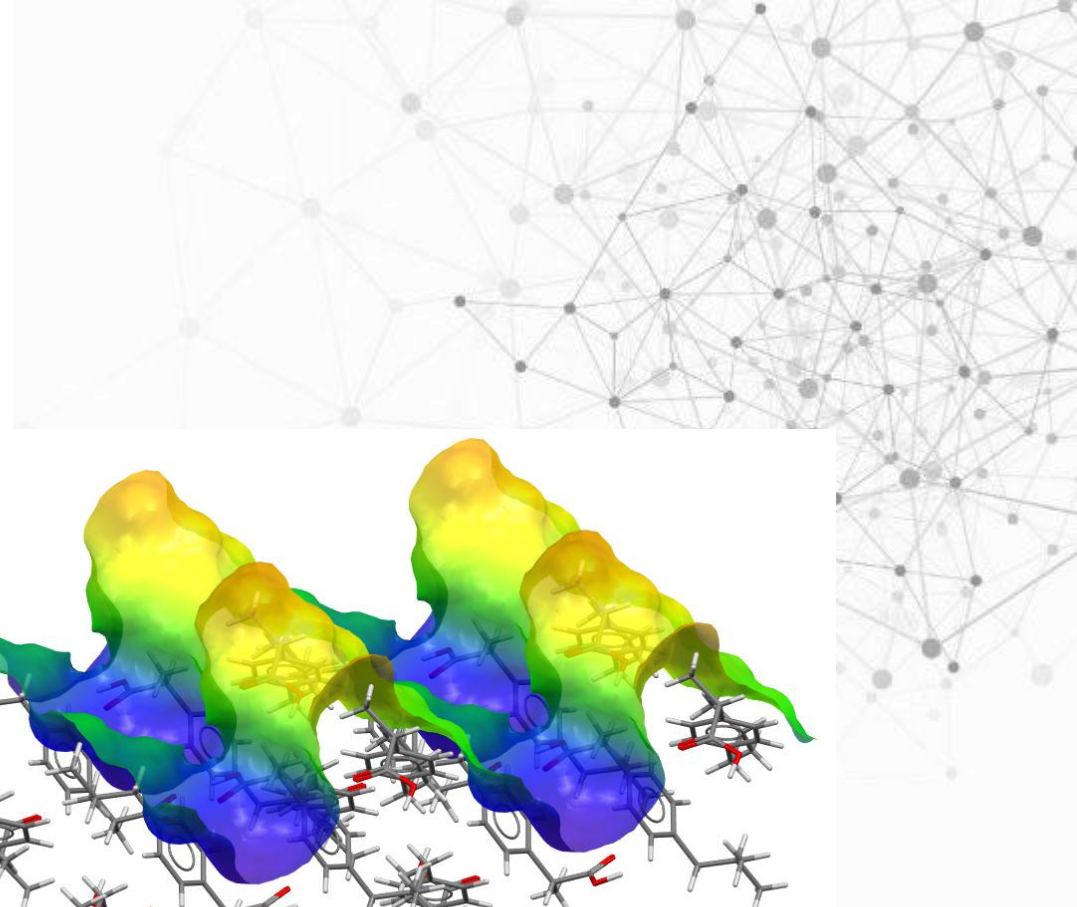
Surface Chemistry



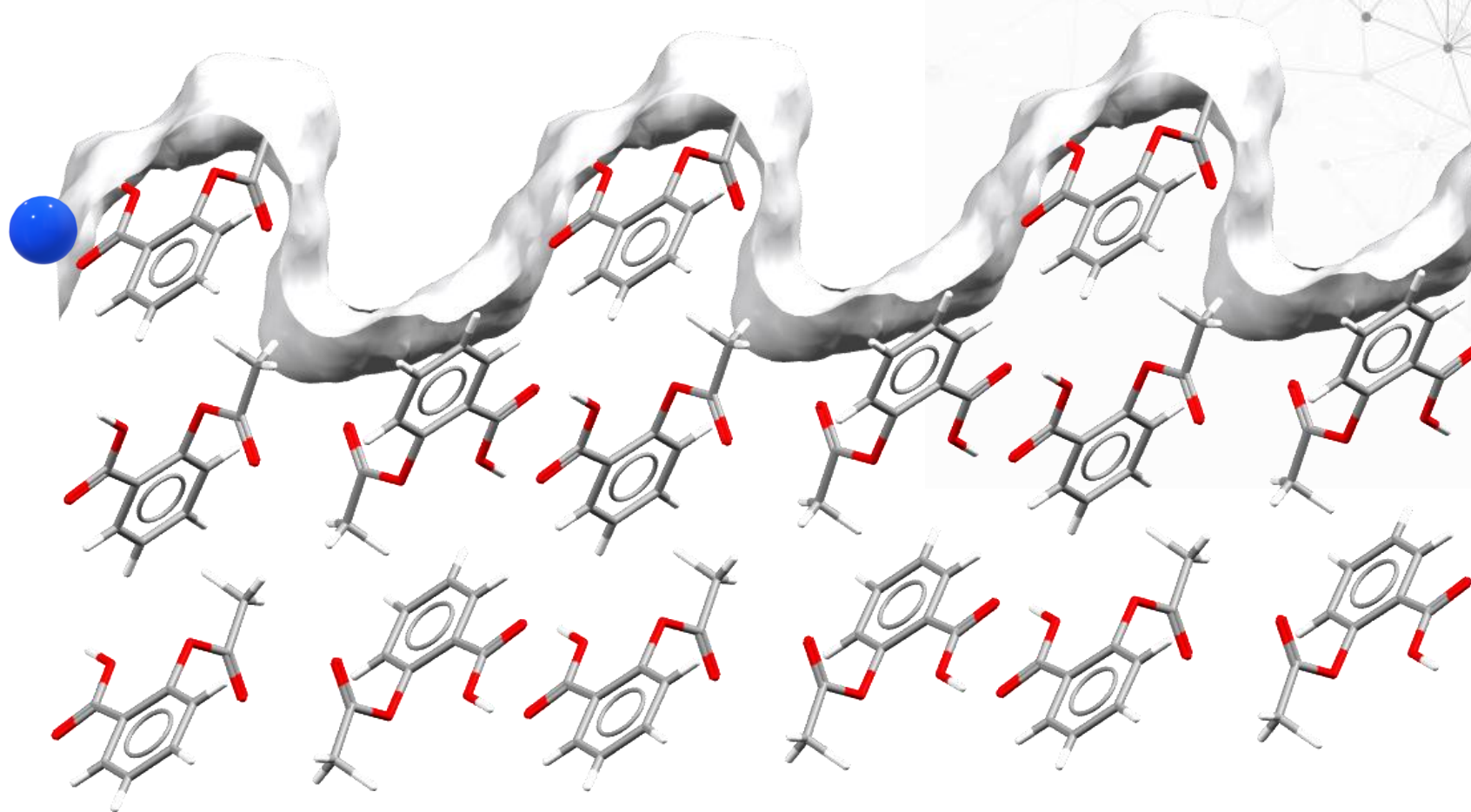
Surface Charge



Surface Roughness



Surface Analysis

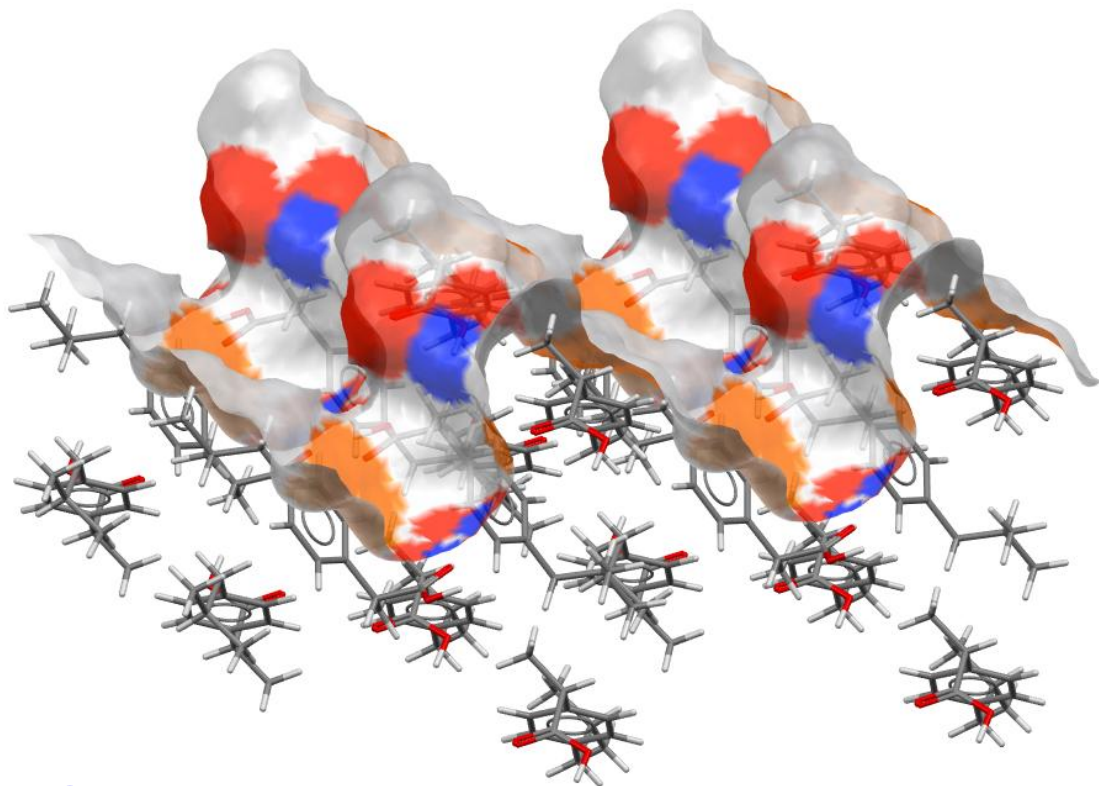


M. J. Bryant *et al.*, *Cryst. Growth Des.* (2019), 19, 9, 5258-5266

Alexandru A. Moldovan and Andrew G. P. Maloney *Crystal Growth & Design* 2024 24 (10), 4160-4169

CCDC

Surface Analysis



H-bond donor



H-bond acceptor

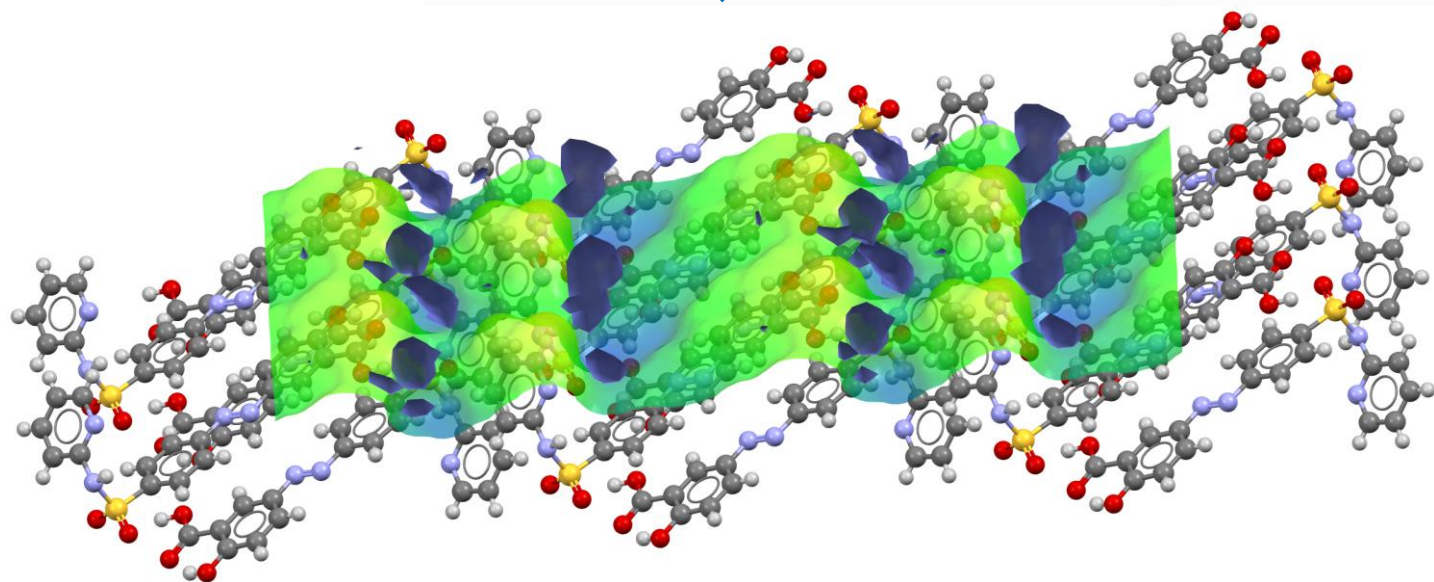
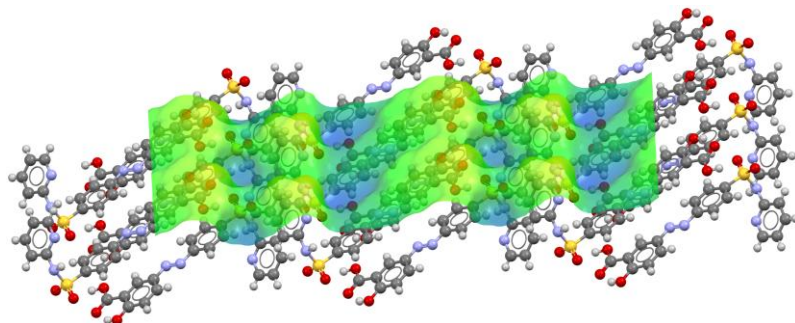
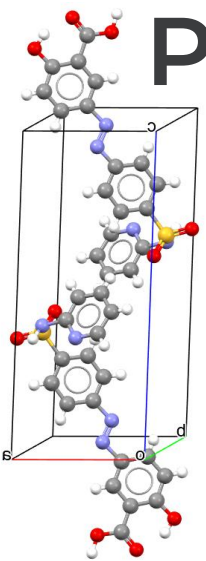


Aromatic bond

Descriptors

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

Particle Informatics



Descriptors

Physical

Chemical

Reticular Surface Area

Hydrogen Bond Donor/Acceptor Density

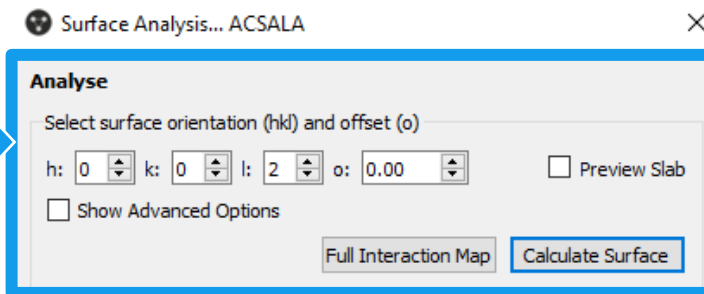
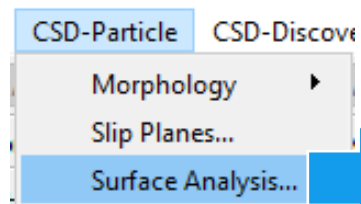
Rugosity

RMSD, Skewness, and Kurtosis

Aromatic Bond Density

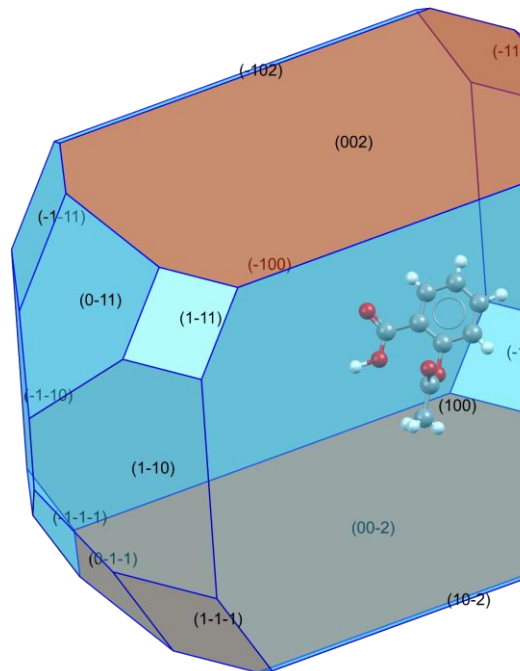
FIMs on Surface

CSD-Particle – Surface Analysis



Input

Extra TIP: also launch directly from VisualHabit



VisualHabit Morphology

Calculation Visualiser Synthons Surface

ACSALA - Gavezzotti Surface Results (in kJ mol⁻¹)

Form	Offset	Electrostatic Energy	van der Waals Energy	Hydrogen Bond Energy	A ²
(1 0 0)	0.000	0.000	-36.906	0.000	-3
(0 0 2)	0.567	0.000	-47.721	0.000	-4
(1 1 0)	0.571	0.000	-69.984	0.000	-6
(0 1 1)	0.000	0.000	-74.223	0.000	-7
(1 1 -1)	0.520	0.000	-74.724	0.000	-7
(1 0 -2)	-1.585	0.000	-59.711	0.000	-5
(1 1 1)	1.000	0.000	-74.179	0.000	-7
(1 0 -4)	-1.126	0.000	-62.324	0.000	-6
(1 0 2)	0.000	0.000	-69.685	0.000	-6
(1 0 4)	0.000	0.000	-75.454	0.000	-7

Analyse Surface Export

Close

Results - ACSALA (002)[0.00]

Density Info (count/Å²)

H-Bond Acceptors: 0.079 Aromatic Bonds: 0.159

H-Bond Donors: 0.013 Unsatisfied H-Bond Donors: 0.013

Topology Info

Surface Area (Å²): 637.558 Projected Area (Å²): 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

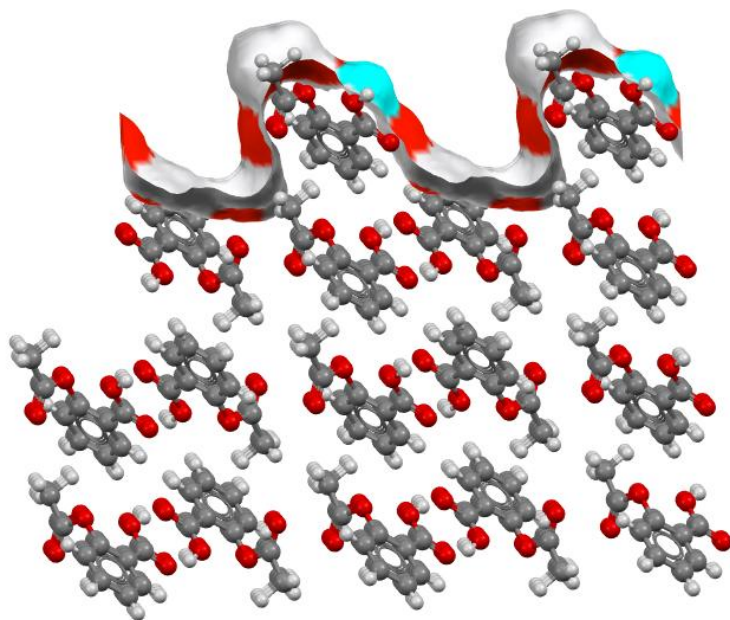
Charge H-Bond Acceptors

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

Results - ACSALA (002)[0.00]

Density Info (count/Å ²)	
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 ²): 637.558	Projected Area (Å ²): 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

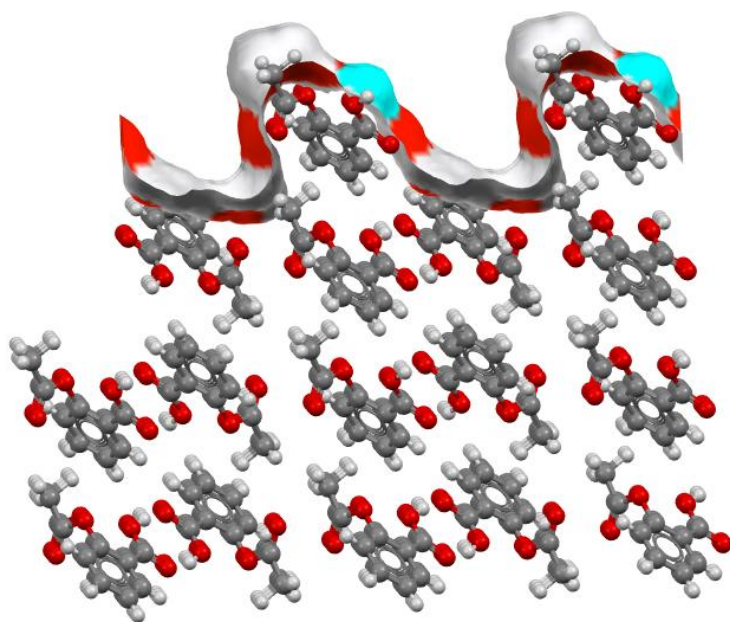
Aromatic H-Bond Donors

Unsatisfied H-Bond Donors

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/Å²)

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 ²): 637.558	Projected Area (Å ²): 301.991
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Display Options

Surface colouring: Atom Properties

Opacity: (%) 100

Periodic View Hide Molecules

Atom Properties

Charge H-Bond Acceptors

Aromatic H-Bond Donors

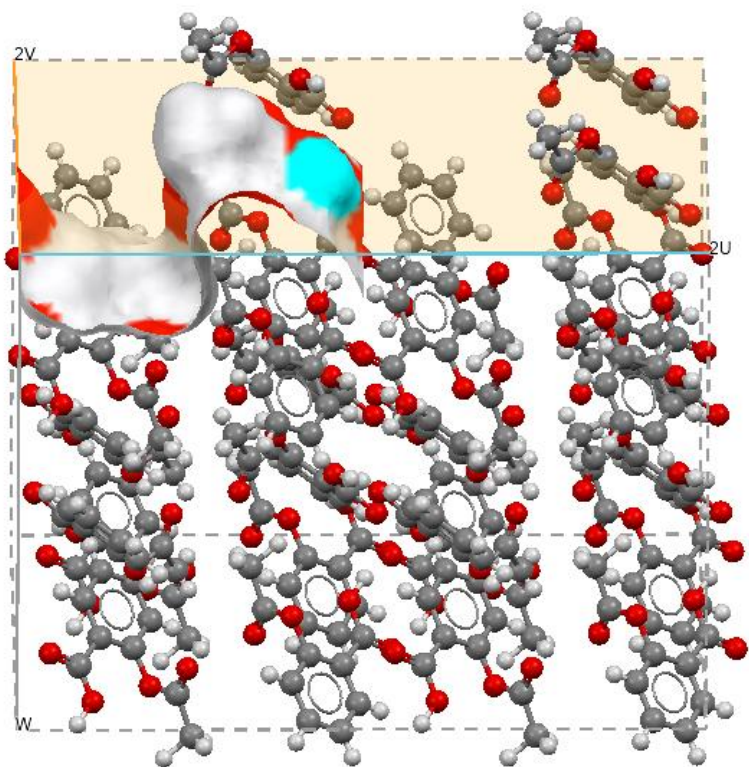
Unsatisfied H-Bond Donors

Reset Close

Display Options

CCDC

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

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/Å²)

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 ²): 159.389	Projected Area (Å ²): 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

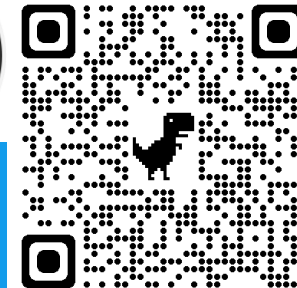
Atom Properties

<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

Advanced Options



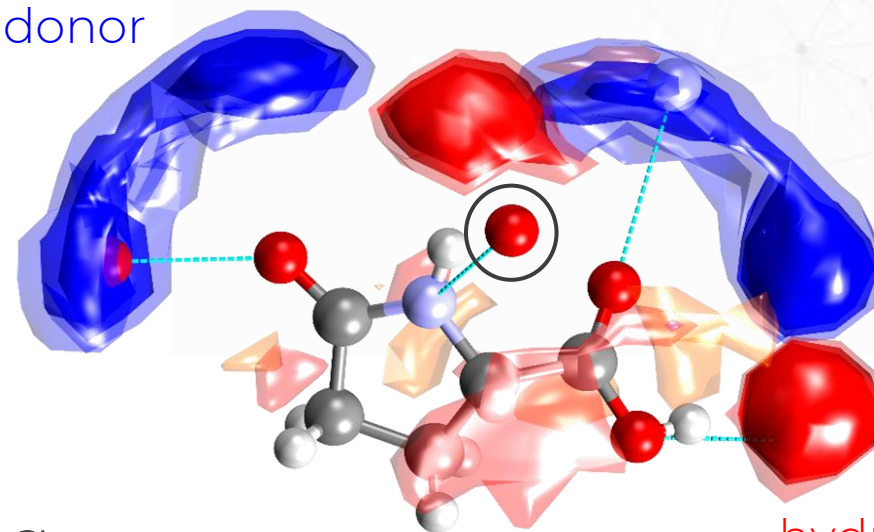
Learn about
FIMs in this
free online
CSDU course



Full Interaction Maps (FIMs)

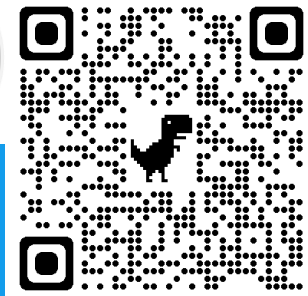
- Map **interaction preferences** around complete molecules in a crystal structure
- Visualise observed atom-atom contacts with respect to likely geometries in 3D space
- Identify interaction hot-spots around chemical groups
- The maps are built from the **knowledge in the CSD** by observing the relative position of interacting chemical groups

hydrogen-bond
donor



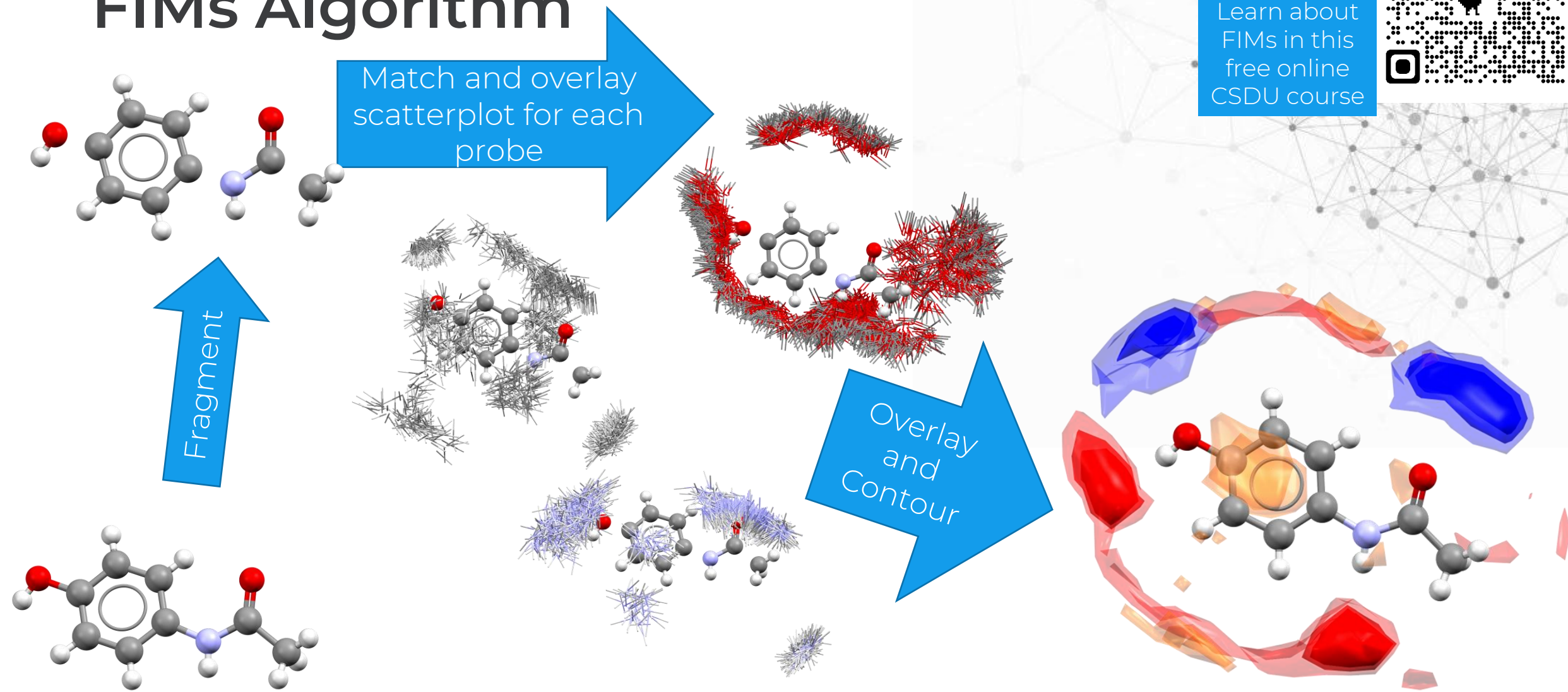
hydrophobic
interactions

hydrogen-bond
acceptor



Learn about FIMs in this free online CSDU course

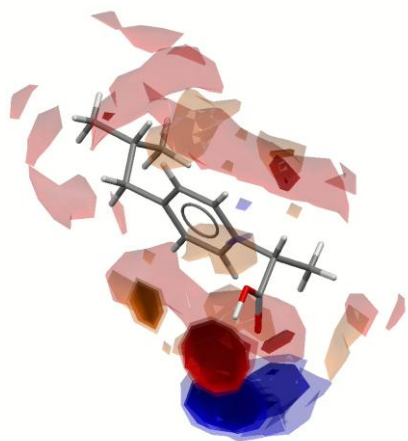
FIMs Algorithm



Wood P. A., et al. *CrystEngComm* (2013) 15, 65-72.

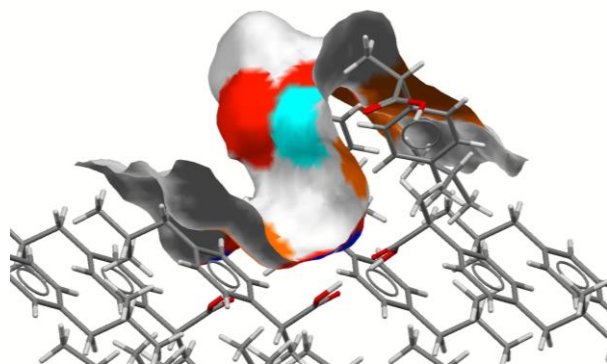


FIMs on Surface



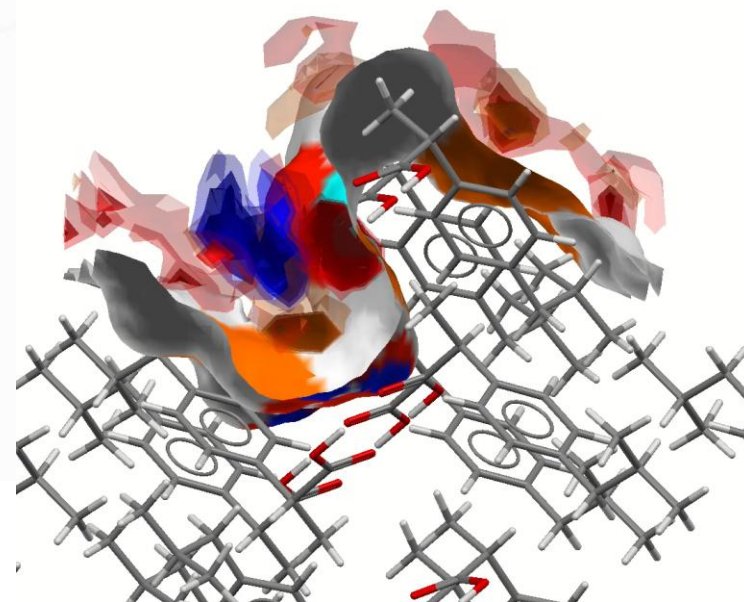
FIM

+



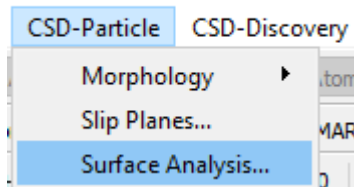
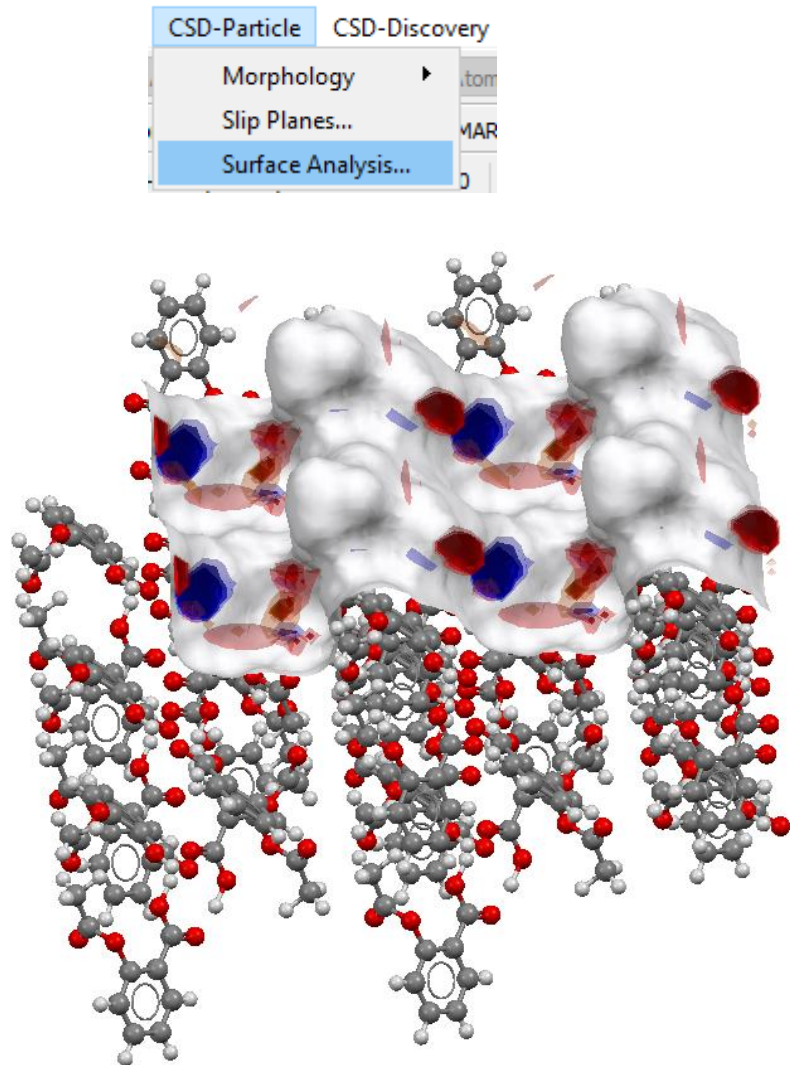
Surface

=



FIM on Surface

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

Full Interaction Map

Results - ACSALA (002)[0.00]

Density Info (count/Å²)

H-Bond Acceptors: 0.079	Aromatic Bonds: 0.159
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Topology Info

Surface Area (Å ²): 159.389	Projected Area (Å ²): 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

Charge H-Bond Acceptors

Aromatic H-Bond Donors

Unsatisfied H-Bond Donors

Full Interaction Map
on Surface

Full Interaction Maps on Surface

Options Maps Hotspots Log Files

Map Contour Levels

Display first contour with initial level of 2.0

Display second contour with initial level of 4.0

Display third contour with initial level of 6.0

Hotspots

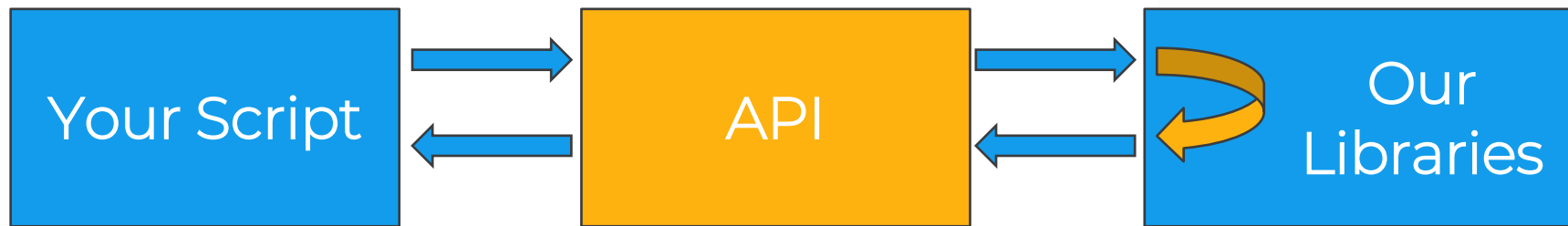
Generate hotspots in the map

Probe

<input checked="" type="checkbox"/> Uncharged NH Nitrogen	Colour
<input type="checkbox"/> Charged NH Nitrogen	
<input type="checkbox"/> RNH3 Nitrogen	
<input type="checkbox"/> Alcohol Oxygen	
<input checked="" type="checkbox"/> Carbonyl Oxygen	
<input type="checkbox"/> Water Oxygen	
<input type="checkbox"/> Oxygen Atom	
<input type="checkbox"/> Methyl Carbon	
<input checked="" type="checkbox"/> Aromatic CH Carbon	
<input type="checkbox"/> C-F Fluorine	
<input type="checkbox"/> C-Cl Chlorine	
<input type="checkbox"/> C-Br Bromine	
<input type="checkbox"/> C-I Iodine	

Accessible from the CSD Python API

- All CSD-Particle functionality is in the CSD Python API
- Carry out automated large-scale analysis
- Develop further methodologies utilising underlying data.

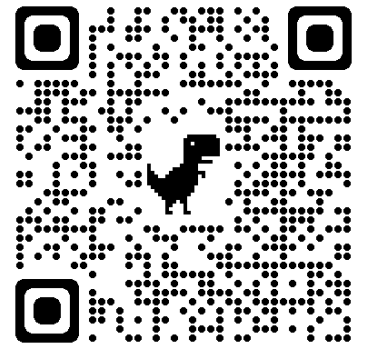


- Share your analysis via our code repository

<https://github.com/ccdc-opensource/csd-python-api-scripts>



Learn more about
our CSD Python API
in CSDU on-
demand course



CCDC

Mercury Overview

More advanced functionality to analyse and learn from structures

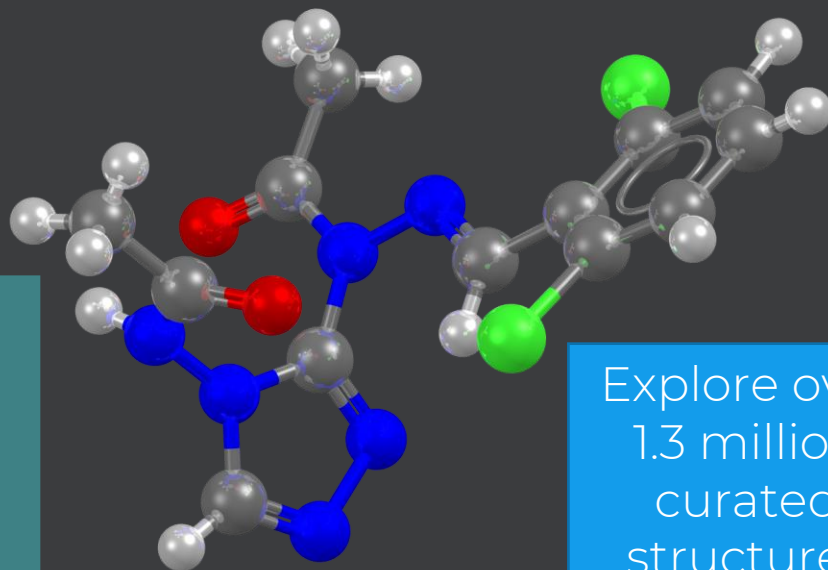
AABHTZ (P-1) - Mercury

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]



Display options to visualise and navigate structures

Explore over 1.3 million curated structures

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	Pnmc
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

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

Mercury Visualisation 101

Learn more in this free online CSDU course

Introduction

Mercury is the visualisation and analysis software of the Cambridge Structural Database (CSD). Mercury is used in investigating and analysing crystal structures with features that allow a user to generate packing diagrams, display and assess the strength of intermolecular interaction networks, calculate and display voids, create BFDH theoretical crystal morphologies and more (features availability subject to appropriate licenses). With Mercury you can visualise 3D structures from the CSD as well as your own. You can also produce high-quality publication-ready images, films for movies, and 3D print files.

Before beginning this workshop, ensure that you have installed Mercury. Please contact your site administrator or workshop host for further information.

Learning Outcomes

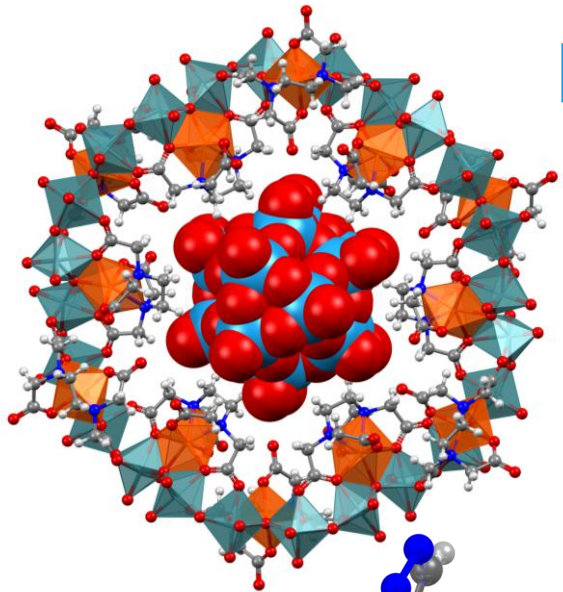
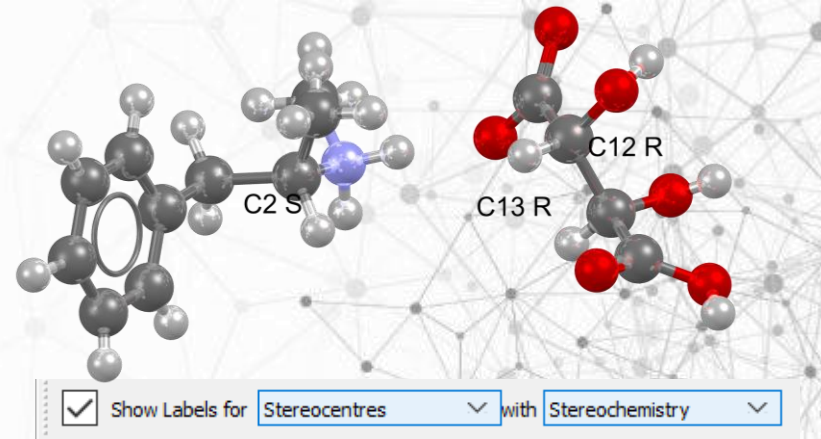
In this workshop we will learn about analysis tools in Mercury, specifically we will learn how to:

- Measure distances, angles and torsions.
- Calculate and display voids and planes.

Self-guided exercises

QR code linking to the exercises.

Lots of display and analysis options!

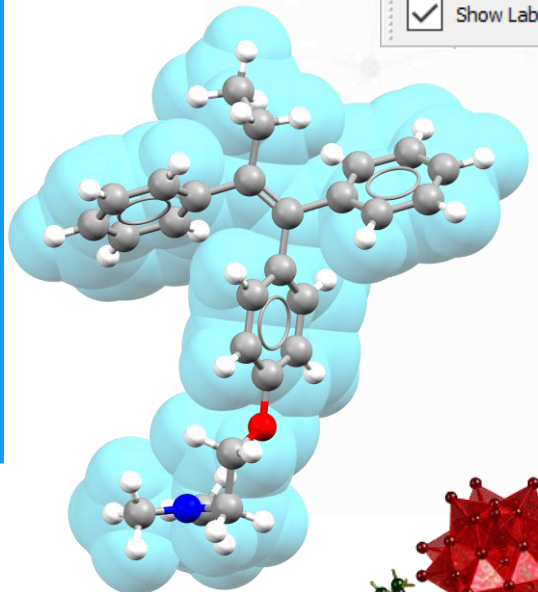


Display

- Styles ▶ Wireframe
- Labels ▶ Stick
- Colours ▶ Ball and stick
- Show/Hide ▶ Spacefill
- More Information ▶ Ellipsoid
- Symmetry Elements... ▶ Polyhedral
- Voids... ▶ Stick settings...
- Display Options... ▶ Ball and Stick settings...
- Manage Styles... ▶ Spacefill settings...
- View along ▶ Ellipsoid settings...
- Dial box... ▶ Polyhedral settings...
- Split ▶ Contact settings...
- Tools ▶ Measurement settings...

Calculate

- Centroids... selected atoms
- Planes...
- Packing/Slicing...**
- Contacts...
- Molecular Shell...
- Graph Sets...
- Powder Pattern...
- Structure Overlay...
- Molecule Overlay...



Watch the video on creating personalised styles



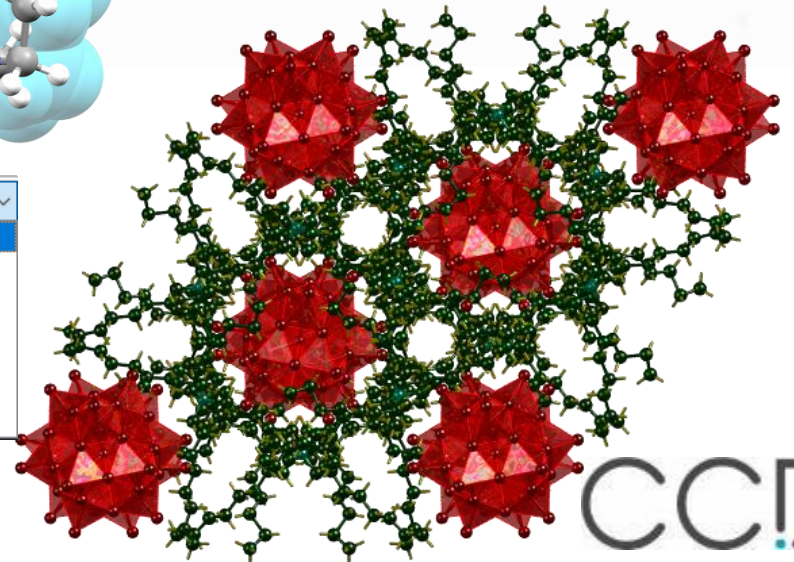
Include atoms

- ... that Fit
- ... in molecules whose Centroids fit
- ... in molecules where Any atom fits
- ... in molecules where All atoms fit
- ... in molecules which occupy Unique supercell positions

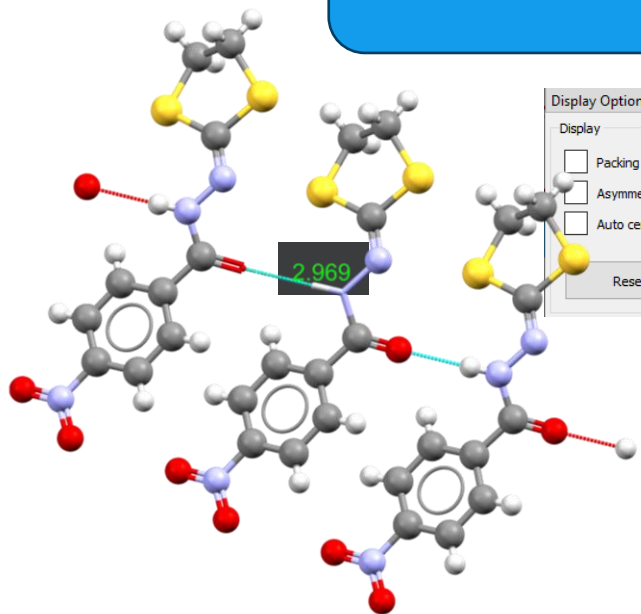
New

Colour: by Element or Suppression ▼

- by Element**
- by Symmetry equivalence
- by Atomic displacement
- by Symmetry operation
- by Gasteiger charge
- by Partial charge
- by Element or Suppression



Lots of display and analysis options!



Display Options

Display

Packing

Asymmetric Unit

Auto centre

Reset

Short Contact < (sum of vdW radii)

H-Bond Default definition

Contacts...

More Info

Powder...

Define H-bonds

Select options and click OK or Apply when done

Require hydrogen atom to be present

D-H...A angle >= 120.0 degrees

Donor atom types:

- all donors
- nitrogen
- metal bound N
- imine N
- aromatic (6-ring) N
- amide or thioamide N
- planar N
- pyramidal N
- ammonium.N.H34..._B.H4

Acceptor atom types:

- all acceptors
- metal bound N
- terminal N (cyano, etc.)
- aromatic (6-ring) N
- other 2-coordinate N
- 3-coordinate N
- unclassified N
- oxygen

WARNING: atom types may not be classified properly for non-Cambridge Structural Database structures

Contact distance range:

Actual distance VdW distance

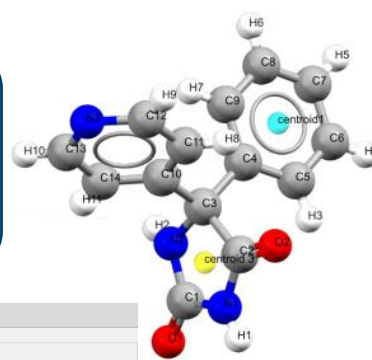
Minimum = sum of vdW radii minus 5.00

Maximum = sum of vdW radii plus 0.00

Intermolecular

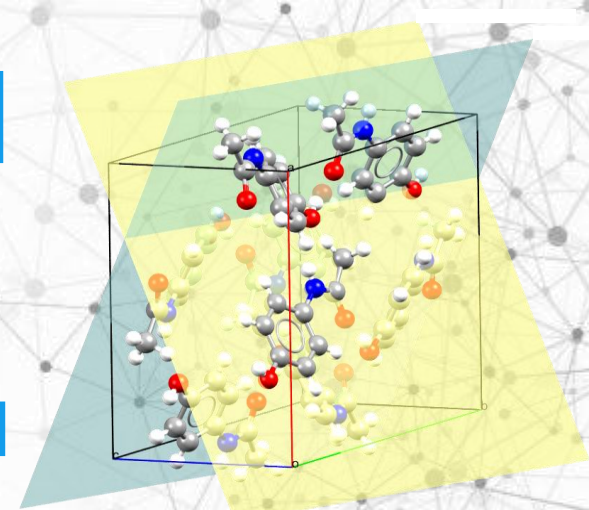
Intramolecular: Donor and Acceptor separated by > 3 bonds

Default Cancel Apply OK



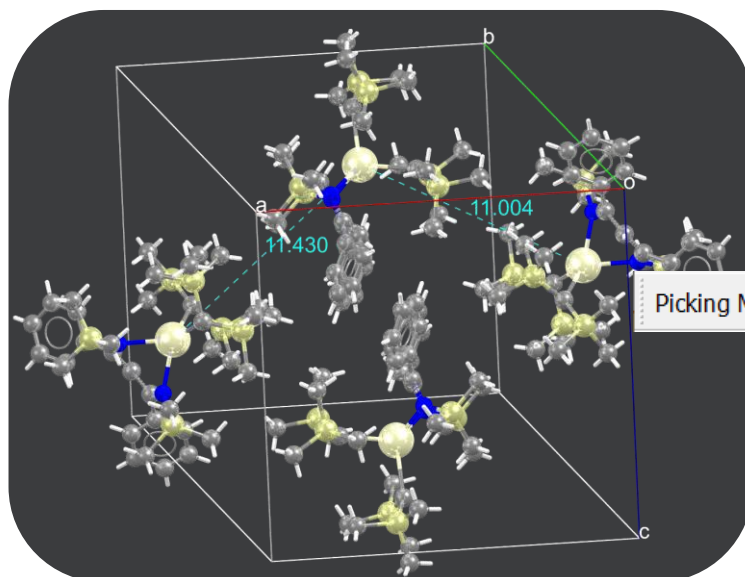
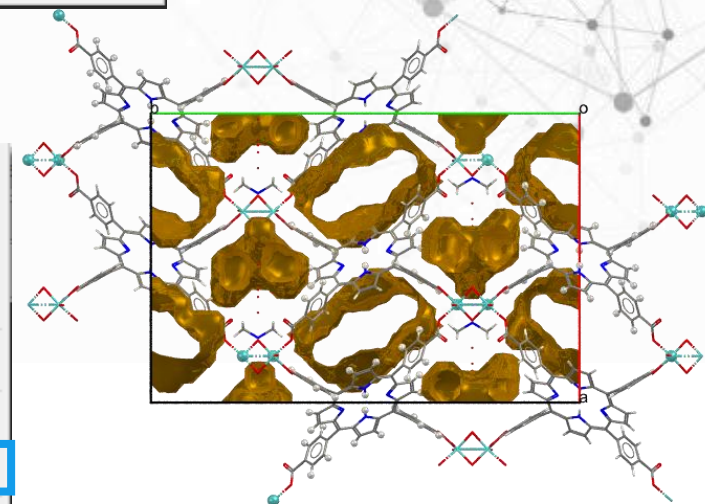
Calculate

- Centroids...
- Planes...
- Packing/Slicing...
- Contacts...
- Molecular Shell...
- Graph Sets...
- Powder Pattern...
- Pore Analyser...
- Structure Overlay...
- Molecule Overlay...

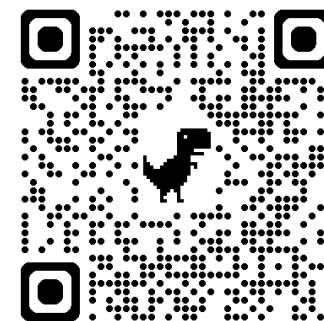


Display

- Styles
- Labels
- Colours
- Show/Hide
- More Information
- Symmetry Elements...
- Voids...
- Display Options...
- Manage Styles...
- View along
- Dial box...
- Splash screen
- Toolbars



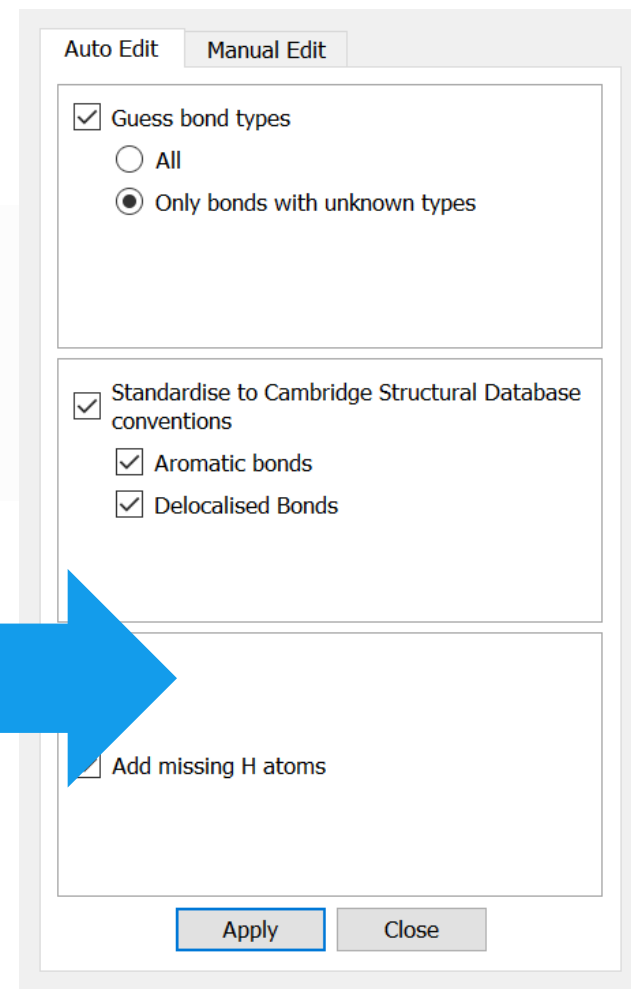
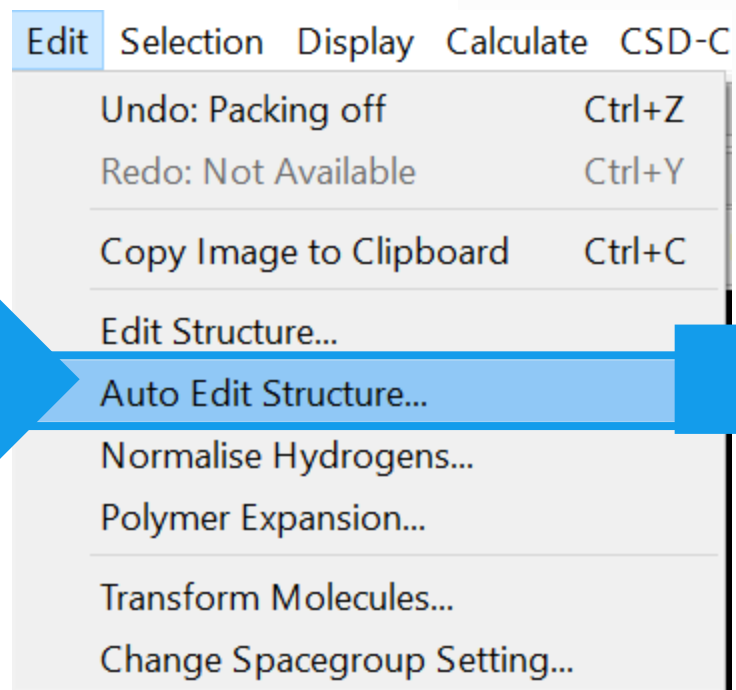
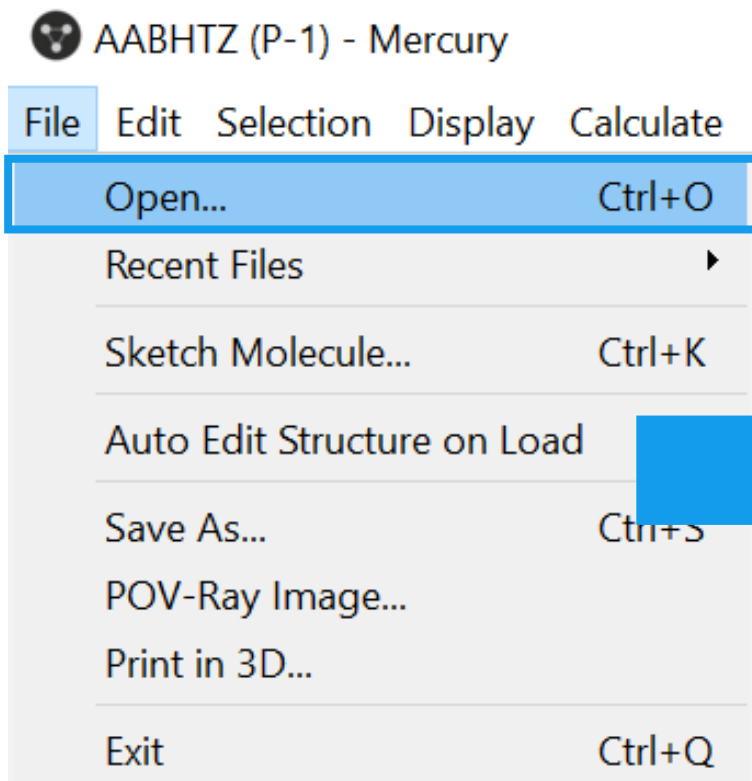
- Picking Mode:
- Pick Atoms
 - Pick Atoms
 - Lasso Atoms
 - Expand Contacts
 - Toggle Labels
 - Move Labels
 - Measure Distances
 - Measure Angles
 - Measure Torsions
 - Reveal Symmetry-Generated Molecules



Watch the video on using voids and other functionality for porous materials

Using your own file or from the web

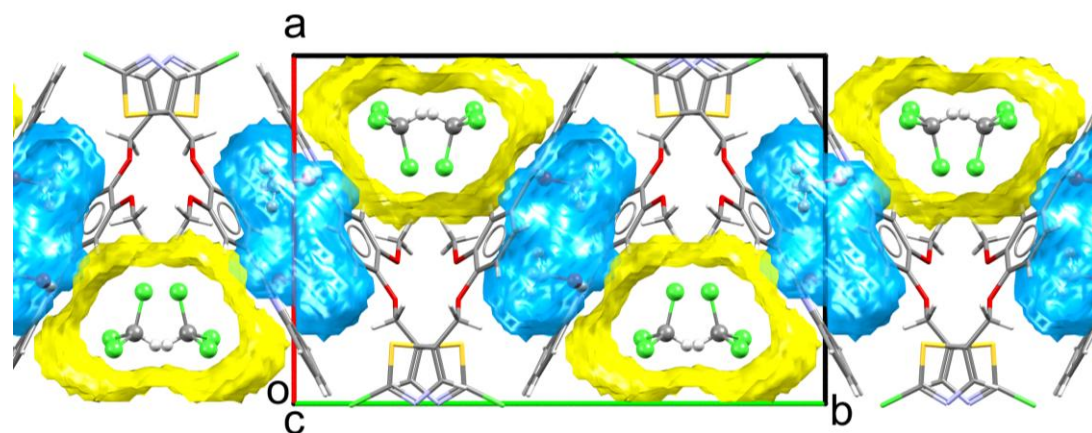
- File > Open – to open one of your own files for example a CIF
- Edit > Auto Edit Structure to assign bond types
- File > Auto Edit Structure on Load to automate



Solvate Analyser

- **Calculation** and **display** of the space occupied by each of the different solvent molecules
- Easy selection of solvent molecule(s)
- **Assessment** of any hydrogen bonding motifs to/from the solvents
- Obtain reports
- Works **with disorder feature** producing different results based on the disorder group selected

	1	2	3
Solvent	1	2	3
Formula	H2 O1	C2 H3 N1	C10 H8 N2
Volume (%)	2.9	3.7	6.0
Volume (Å ³)	54.31	69.35	113.97
Show Space	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Show Solvent	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Select Solvent	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Inside Colour	<input type="color"/>	<input type="color"/>	<input type="color"/>
Inside Opacity	<input type="range"/>	<input type="range"/>	<input type="range"/>
Outside Colour	<input type="color"/>	<input type="color"/>	<input type="color"/>
Outside Opacity	<input type="range"/>	<input type="range"/>	<input type="range"/>



Lost toolbars?

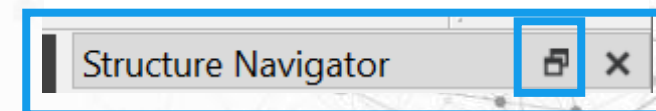
The screenshot shows the Mercury software interface. The 'Display' menu is open, listing various toolbars and options. A blue arrow points from the 'Structure Navigator' option in the menu to the 'Structure Navigator' toolbar, which is highlighted with a blue box. The toolbar contains a search input field with the placeholder text 'Type in a refcode' and a 'Find' button. Below the menu, the 'Structure Navigator' window is visible, displaying a list of crystal structures with columns for 'Crystal Structures' and 'Spacegr'. The list includes entries like 'AABHTZ P-1', 'AACANI10 P21/c', etc.

- Clear Measurements
- Show Labels for All atoms with
- Manage Styles... MyStyle
- Atom selections:
- Select by SMARTS:
- Display Options
- Graph Sets
- Intermolecular Potentials
- Searches
- Post Search Options
- Structure Navigator
- Picking Toolbar
- Labels
- Display
- Style Manager Toolbar
- Atom Selection Toolbar
- Select by SMARTS
- Animation Toolbar
- Crystal Orientation Operations
- Alignment and Orientation Operations

Crystal Structures	Spacegr
AABHTZ	P-1
AACANI10	P21/c
AACANI11	P21/c
AACFAZ	Pbcn
AACFAZ...	Pbcn
AACMAL	P21/c
AACMH...	Pbca
AACRHA	Pncm
AACRHC	P-1
AACRUB	Cc
AACRUB...	C2/c
AADAMC	P21/c
AADMPY	P-1
AADMP...	P-1
AADRIB	P21
AAGAG...	P212121
AAGGA...	P21
AALCFE	P21/c
AALDRO	P21/c

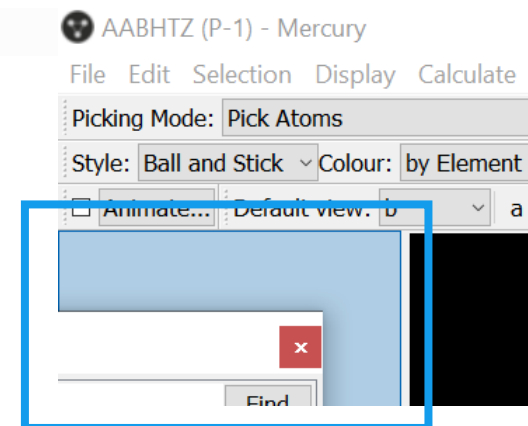
Extra Tip

Click on the resize icon or drag the top to pop the toolbar out.



Extra Tip

To pop the toolbar back in drag it to the area you want it.



AABHTZ (P-1) - Mercury

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

Picking Mode: Expand Contacts

Style: Ball and Stick Colour:

Animate... Default view

Measurements Show Labels for All atoms with Atom Label

Manage Styles... Publication Atom selections:

x+ y- y+ z- z+ x-90 x+90 y-90 y+90 z-90 z+90 ← → ↓ ↑ zoom- zoom+ Select by SMARTS: >>

Structure Navigator

AABHTZ Find

Crystal Structures

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
AADRIIB	P21
AAGAGG10	P212121
AAGGAG10	P21

- Centroids...
- Planes...
- Packing/Slicing...**
- Contacts...
- Molecular Shell...
- Graph Sets...
- Powder Pattern...



Packing and Slicing

Packing

Show cell axes

Label cell axes

Pack a: 0.0 1.0 + 0.5

b: 0.0 1.0 + 0.5

c: 0.0 1.0 + 0.5

2x2x2

3x3x3

Reset

Include atoms

- ... that Fit
- ... in molecules whose Centroids fit
- ... in molecules where Any atom fits
- ... in molecules where All atoms fit
- ... in molecules which occupy Unique supercell positions

New in 2025.1!

Display Options

Display

- Packing**
- Asymmetric Unit
- Auto centre
- Short Contact < (sum of vdW radii)
- H-Bond Default definition

Reset

Options

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

Contacts...

More Info

Powder...

Click on a red contact to see the whole molecule

Reset button: a friend!

HXACAN (Pcab) - Mercury

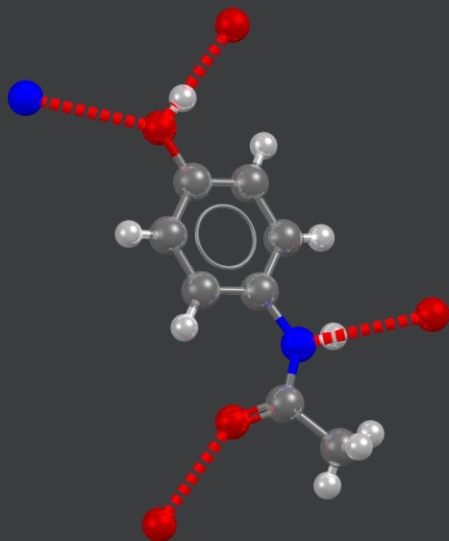
File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Discovery CSD Python API Help

Picking Mode: Expand Contacts Clear Measurements Show Labels for All atoms with Atom Label

Style: Ball and Stick Colour: by Element Manage Styles... Publication 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 Select by SMARTS:

Visualising hydrogen bonds



Structure Navigator

HXACAN Find

Crystal Structures

Define H-bonds

Select options and click OK or Apply when done

Require hydrogen atom to be present

D-H...A angle >= 120.0 degrees

Donor atom types:

- all donors
- nitrogen
 - metal bound N
 - imine N
 - aromatic (6-ring) N
 - amide or thioamide N

Acceptor atom types:

- all acceptors
- nitrogen
 - metal bound N
 - terminal N (cyano, etc.)
 - aromatic (6-ring) N
 - other 2-coordinate N
 - 3-coordinate N
 - unclassified N

Distance: 5.00

Separator separated by > 3 bonds

Default Cancel Apply OK

Click on "Default definition" to change the default H-bond definition

Display Options

Display

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

Options

- Show hydrogens
- Show cell axes
- Label atoms

Reset Contacts... More Info Powder...

Click on a red contact to see the whole molecule

HXACAN (Pcab) - Mercury

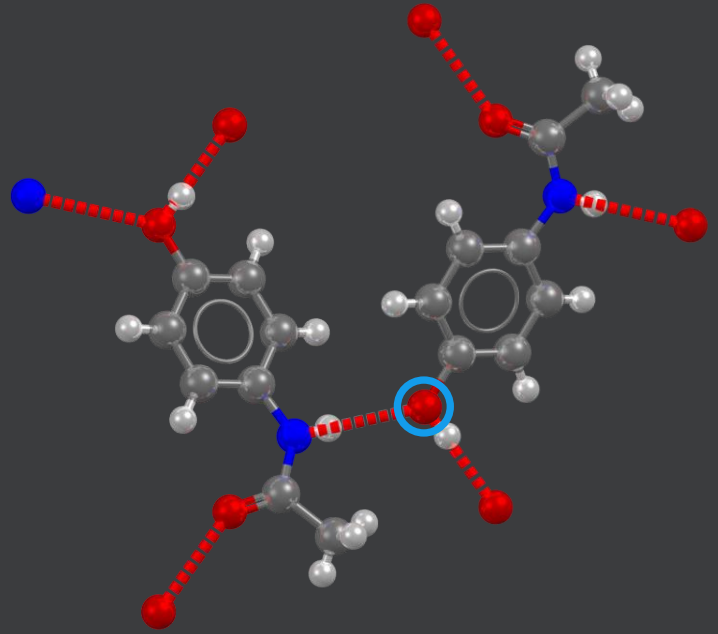
File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Discovery CSD Python API Help

Picking Mode: Expand Contacts Clear Measurements Show Labels for All atoms with Atom Label

Style: Ball and Stick Colour: by Element Manage Styles... Publication 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 Select by SMARTS: >>

Left click on the atoms at the end of the dashed lines (known as hanging contacts) to expand the network



- Selection
- Styles
- Colours
- Labels
- Show/Hide
- Contacts**
- Delete this Molecule
- Rotation Centre
- IsoStar Interactions Check...

Right click on hanging contacts to see more advanced options including delete hanging contacts

Structure Navigator

HXACAN Find

Crystal Structures

- Expand All
- Expand Contact
- Expand Contacts from this Atom
- Expand Contacts from this Molecule**
- Find Contacts from this Atom
- Find Contacts from this Molecule
- Delete Hanging Contacts
- Delete Contact
- Delete Contacts from this Atom
- Delete Contacts from this Molecule
- Delete this Molecule
- Reset Contacts

Display Options

Tip - Change H-bond thickness by Display>Styles>Contact settings...

Tip - Change H-bond colours by Display>Colours>Contacts...>colour by distance>All contacts

Click on a red contact to see the whole molecule






We will make the recording available to you in the next few days.

Agenda

- *Show One*: Introduction to the CSD, CSD-Particle and Particle Informatics
- *Show One*: Case study by Prof. Elena Simone
- *Show One*: Surface Analysis using CSD-Particle
- *Try One*: Hands-on examples
- *Explore More*: [Case studies, tips](#), quiz and summary
- *Extra time*: More time for hands on and Q&A



After the session you can earn a completion certificate for today by taking our test.

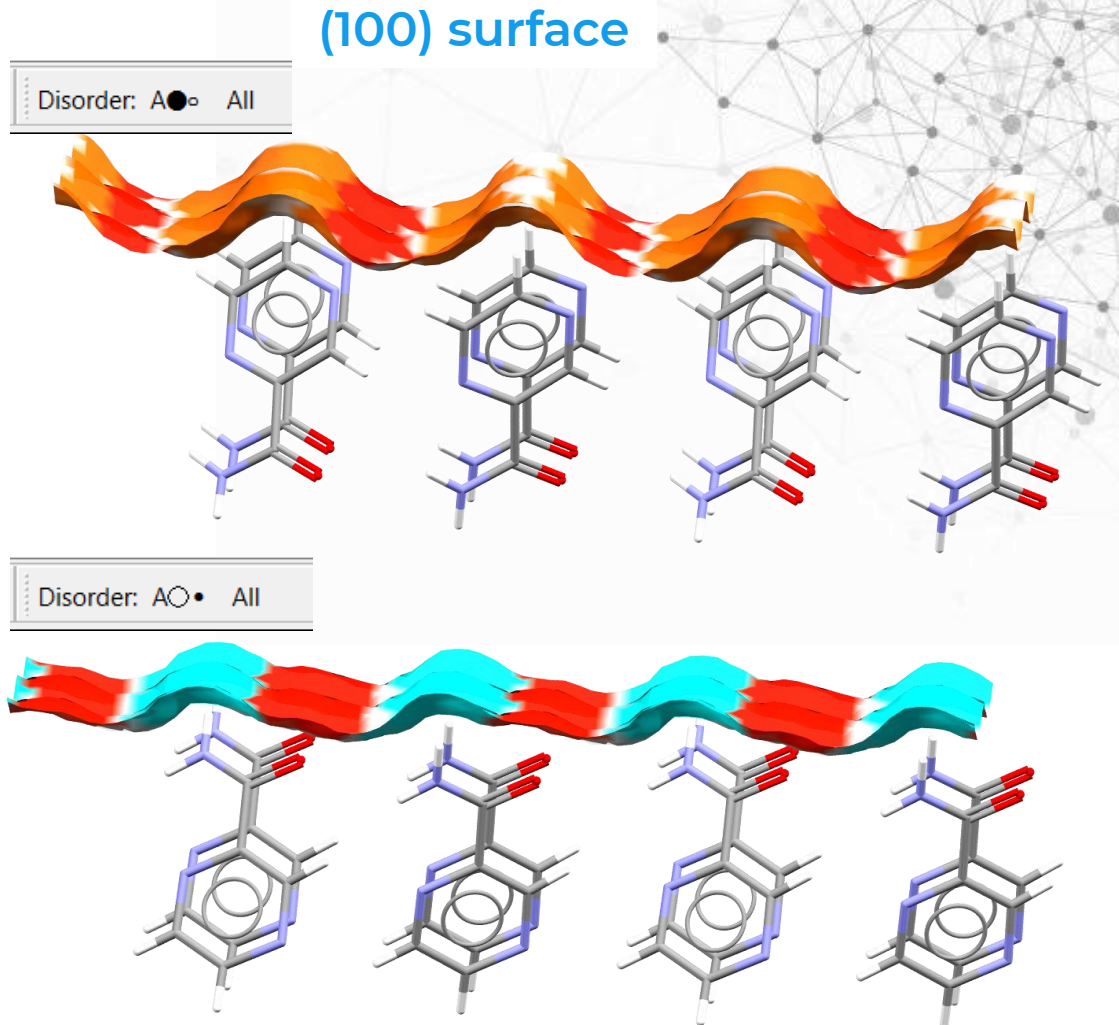
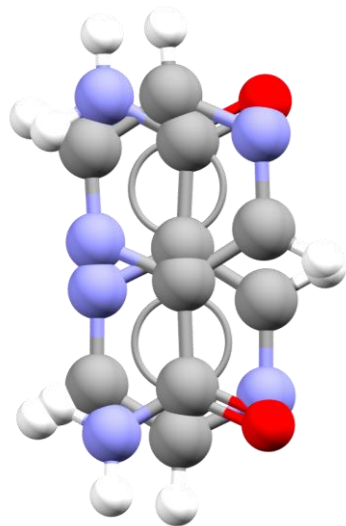


CCDC

Using Surface Analysis with disordered structures

- Visualise the different **disorder models**
- Works **in combination** with other functionality in Mercury

CSD refcode:
PYZIN19



We learnt more about disorder in the previous Virtual Workshop!

Calculating planes

Calculate CSD-Community

- Centroids...
- Planes...
- Packing/Slicing...
- Contacts...
- Molecular Shell...
- Graph Sets...
- Powder Pattern...
- Pore Analyser...
- Structure Overlay...
- Molecule Overlay...

Planes

Pick an object from the list below, or in the graphics window, or right-click on a list item

New Plane... Edit... Close

Plane Properties

Mean plane hkl

Select at least three atoms to calculate least squares plane:

Pick atom to select:

- Picked atom
- Picked molecule
- Ring

Or select:

- All
- Non-hydrogen
- Hydrogen

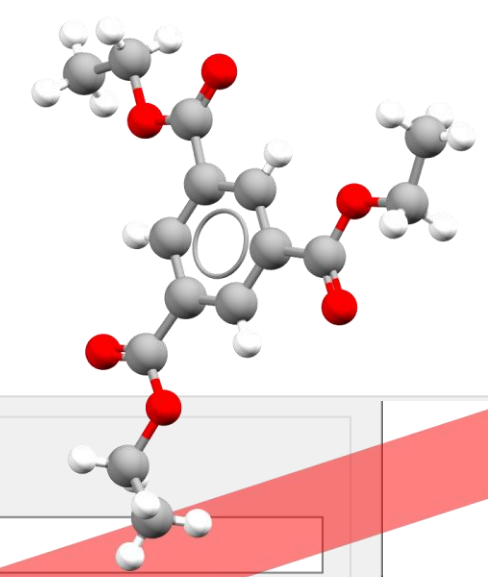
Plane Properties

Mean plane hkl

Create Miller plane:

Miller indices

h: k: l:

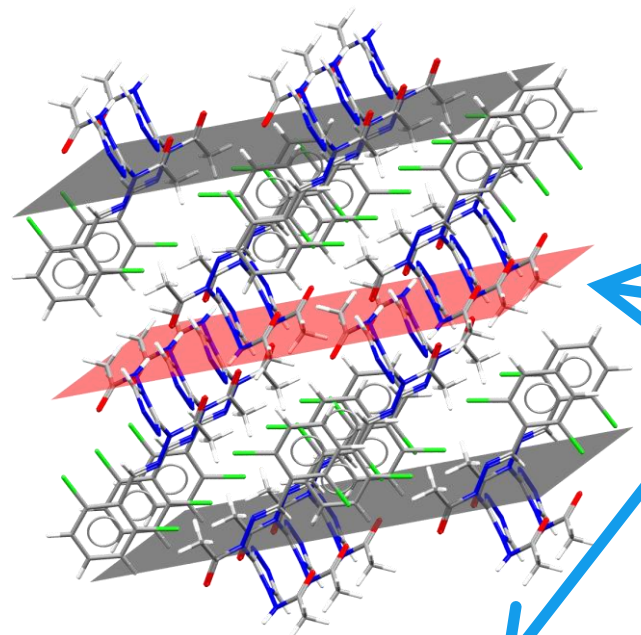


Plane Properties

- Show
- Label - Transparent
- Colour:

OK Cancel

Slicing



Packing and Slicing

Packing: Include atoms:

Slicing

Show slice

Select plane: ■ (100) BFDH relative area: 0.181

Show plane

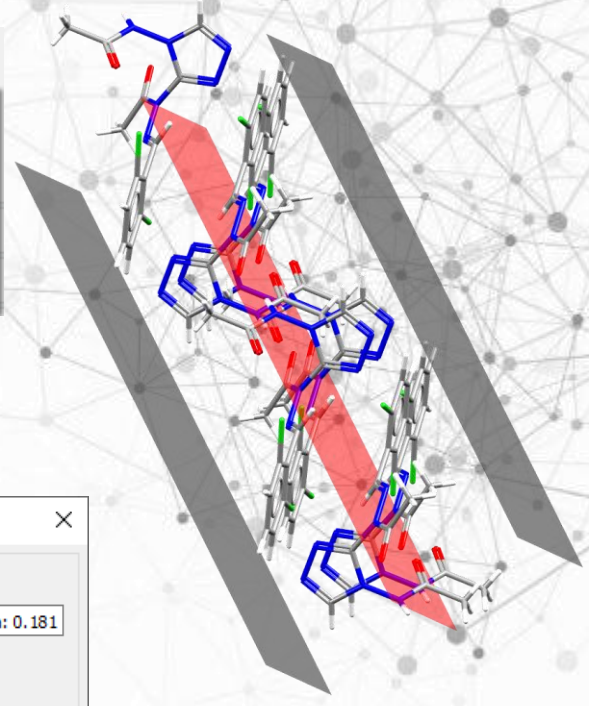
Show bounds

Depth:

Area:

Displacement:

- Select plane:
- (100) BFDH relative area: 0.181
 - (100) BFDH relative area: 0.181
 - (-100) BFDH relative area: 0.181
 - (0-10) BFDH relative area: 0.159
 - (010) BFDH relative area: 0.159
 - (001) BFDH relative area: 0.043
 - (00-1) BFDH relative area: 0.043
 - (-10-1) BFDH relative area: 0.043
 - (101) BFDH relative area: 0.043
 - (-11-1) BFDH relative area: 0.036
 - (1-11) BFDH relative area: 0.036



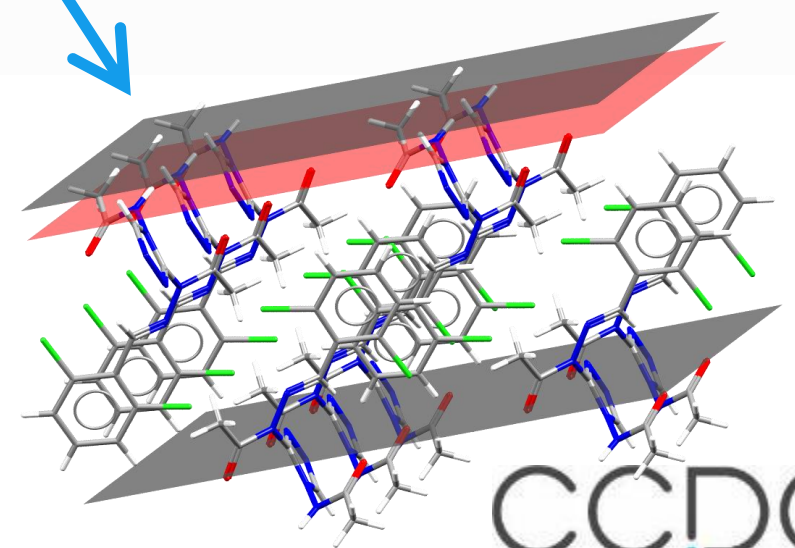
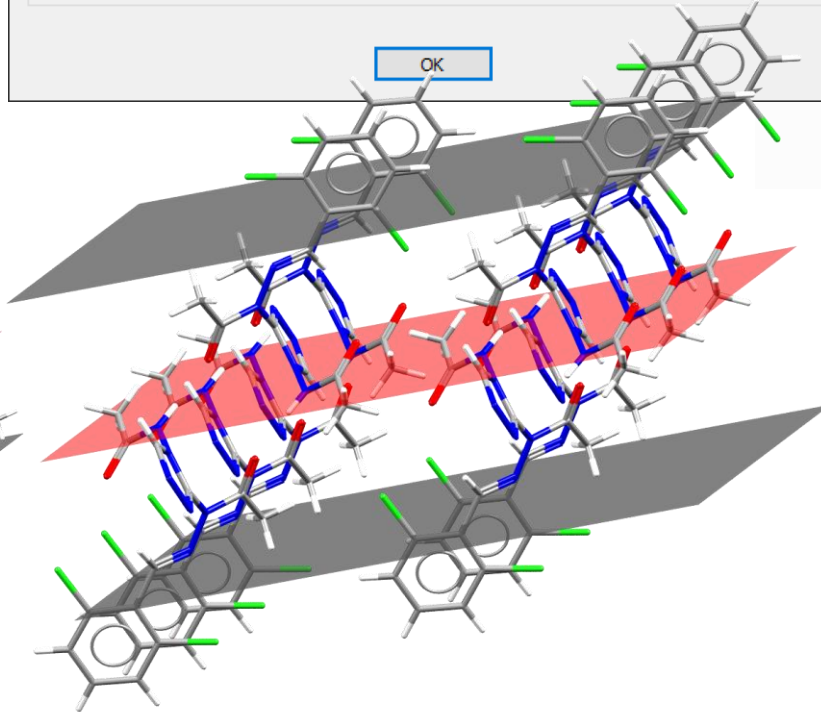
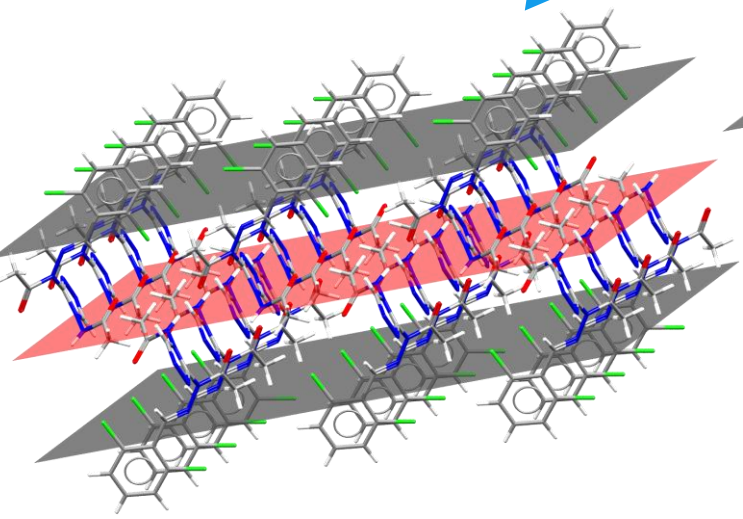
Properties

Show

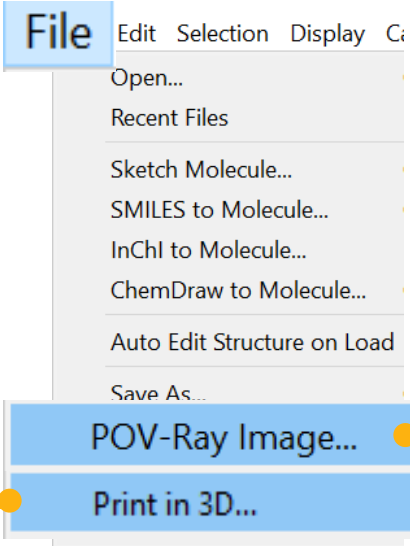
Label

Transparent

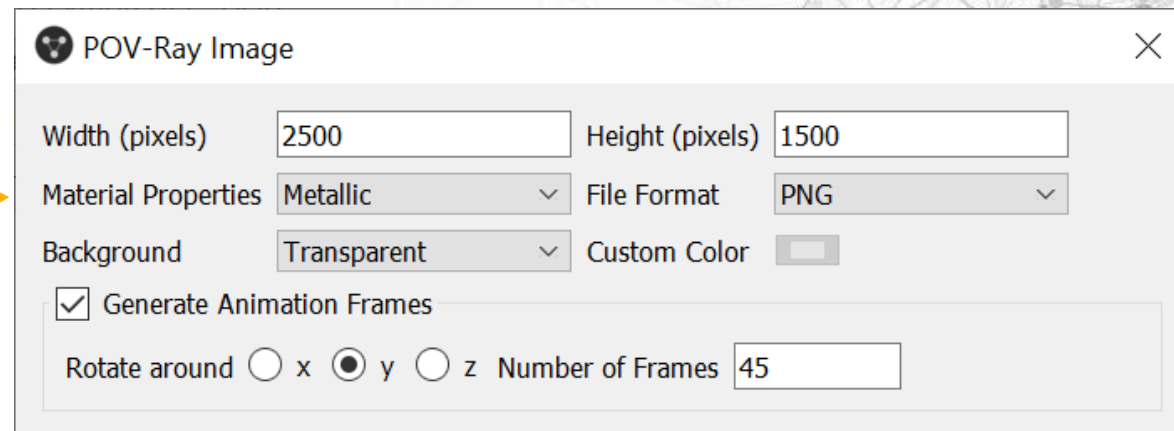
Colour: ■



Features for effective visualization

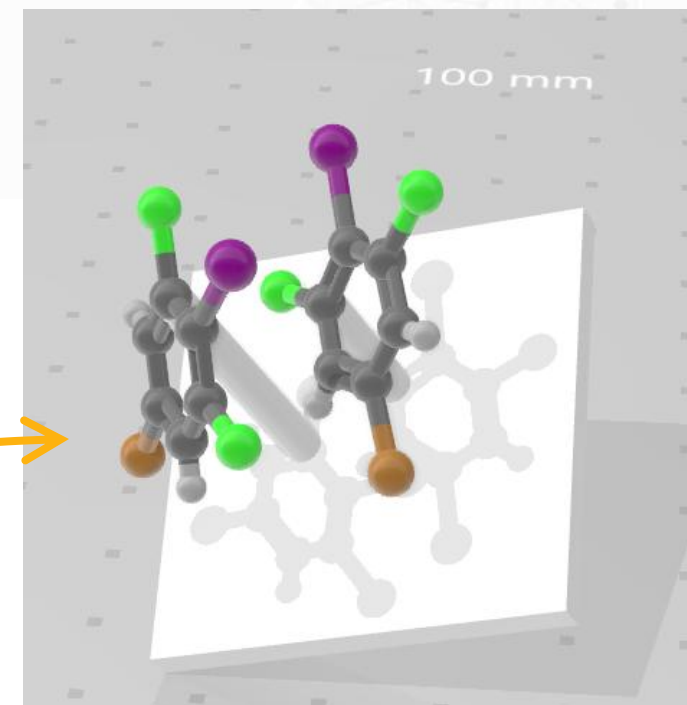
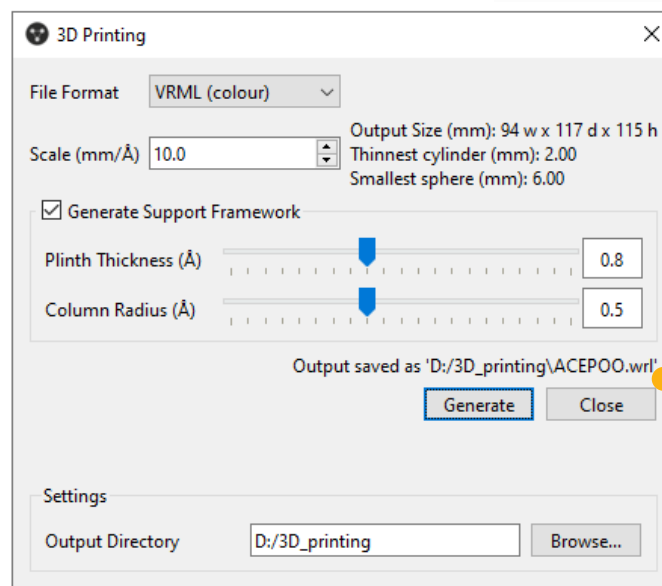
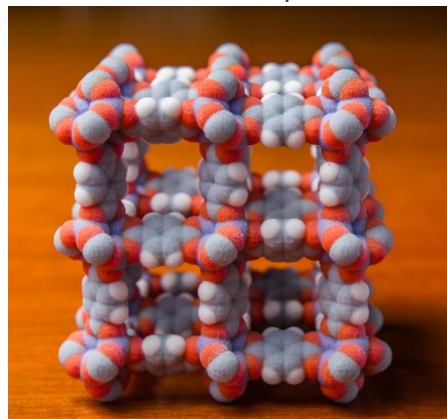


- Create high resolution images and frames for video or gifs

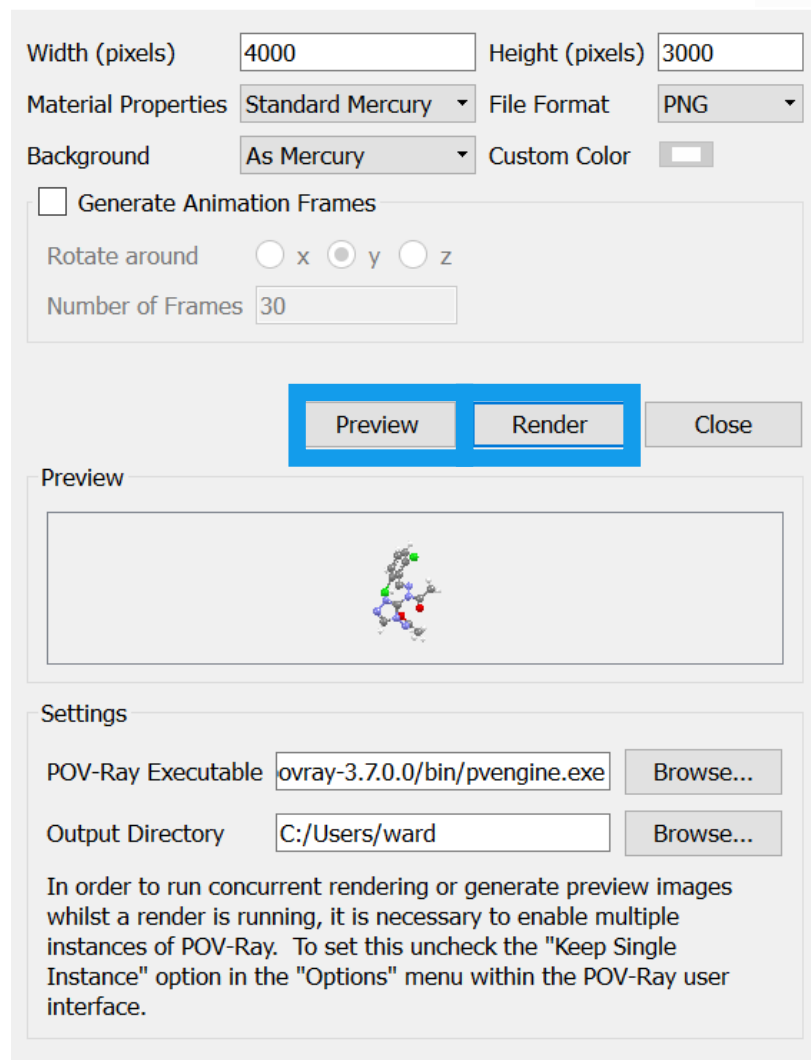
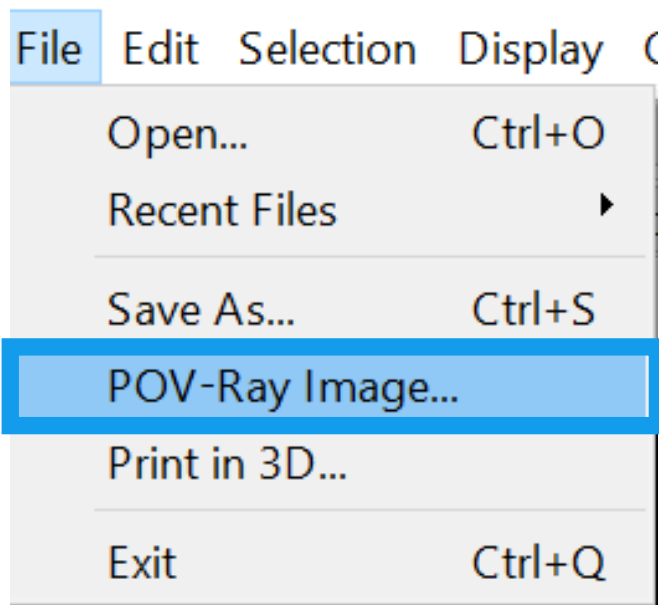


- Create files for 3D print

Example of 3D printed structure of CSD Refcode SAHYIK



Generating high quality images



File > POV-Ray Image

Change Resolution

Width = 4000

Height = 3000

Change 'Material Properties' to 'Metallic'

Set 'Background' to 'Transparent'

Press 'Preview'

Optimising display settings

Surface Analysis... AHIHAC

Analyse

Select surface orientation (hkl) and offset (o)
h: 0 k: 1 l: 1 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: 0.30
Thickness (W) Factor: 2.00

Results - AHIHAC (011)[0.00]

Density Info (count/Å³)

H-Bond Acceptors: 0.077	Aromatic Bonds: 0.173
H-Bond Donors: 0.129	Unsatisfied H-Bond Donors: 0.113

Topology Info

Surface Area (Å ²): 4109.980	Projected Area (Å ²): 992.165
Rugosity: 4.142	RMSD: 4.128
Skewness: -0.040	Kurtosis: 1.774

Display Options

Surface colouring: Atom Properties

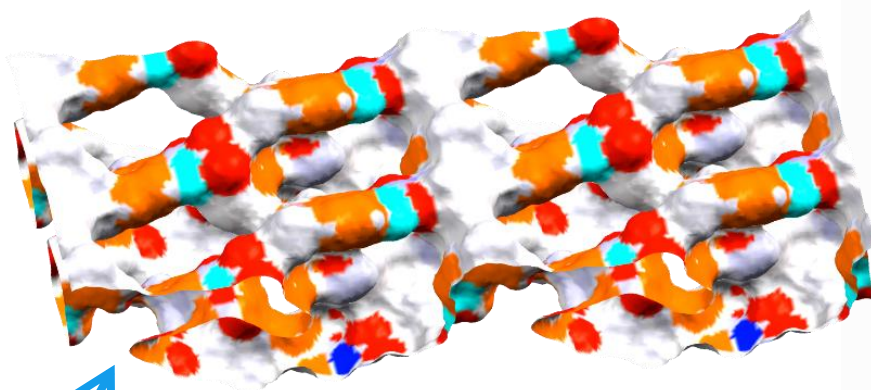
Opacity: (%) 100

Periodic View Hide Molecules

Atom Properties

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

AHIHAC (011)[0.00] – default settings



Display Calculate CSD-Community

Styles Labels Colours Show/Hide More Information Symmetry Elements Voids... **Display Options...** Manage Styles... View along Dial box... Splash screen Toolbars

Display Options

Background Depth Cueing Labels **Lighting** Clipping Box-Clipping

Light 1	Light 2	Light 3	Light 4
<input checked="" type="checkbox"/> Enabled			
Diffuse colour: [grey]			
Specular colour: [white]			
Position: x: 1 y: 1 z: 1			

Ambient Light

Enabled Diffuse ambient colour: [black]

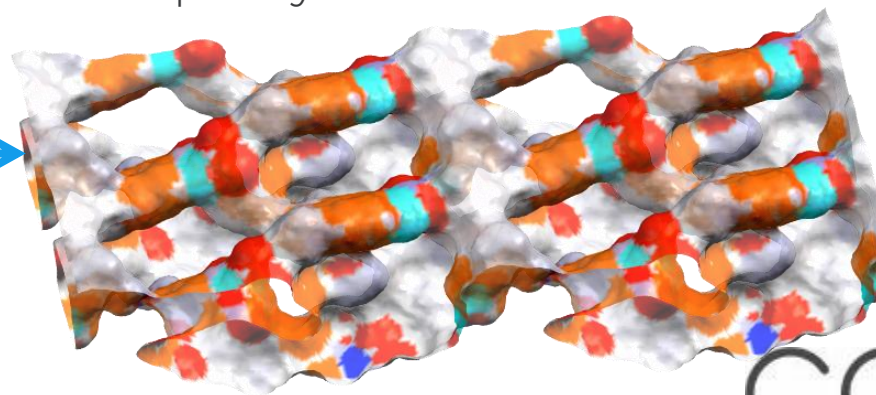
Turn ambient light off

Surface opacity at 70%

Display Options

Surface colouring: Atom Properties

Opacity: (%) 70




A wealth of structures, stories and possibilities.


CSD one million special issue

- 33 articles from industry and academia

**1 million structures.
stories.
possibilities.**



Cambridge Structural Database, CSD



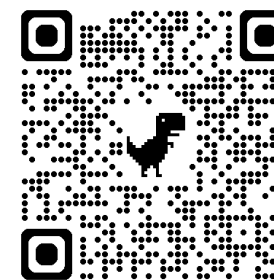
CCDC
advancing structural science

Legacy and Future Impact of the Cambridge Structural Database: A Tribute to Dr. Olga Kennard - special issue

- 29 articles from industry and academia



**CRYSTAL GROWTH
& DESIGN**

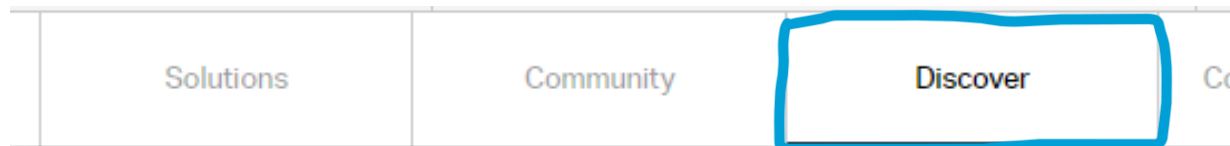


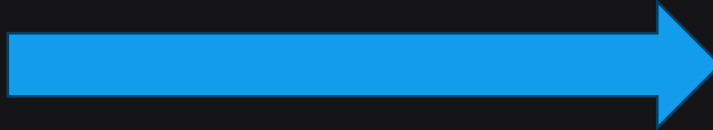

The CSD - A wealth of knowledge gained from a million structures. *CrystEngComm*, 2020,22, 7131-77502

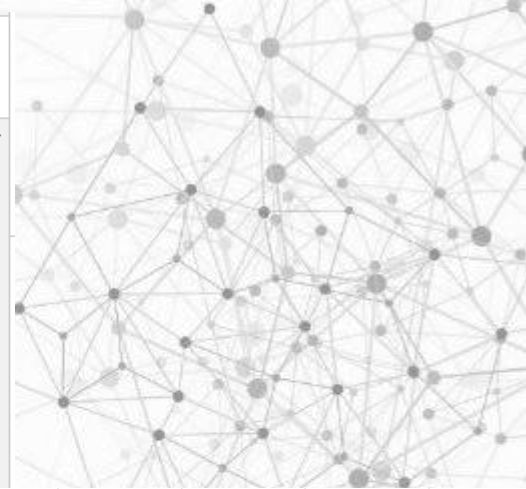
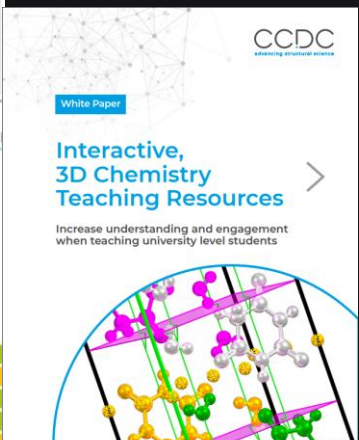


The CSD. C.R.Groom, I.J.Bruno, M.P.Lightfoot and S.C.Ward, *Acta Cryst.* (2016). B72, 171-179 DOI: 10.1107/S2052520616003954

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More case studies



- Discover All
- Case Studies** 
- Webinars
- White Papers** 
- Blogs
- News
- Events
- Newsletter



Tags

- Organometallics
- Organic Crystallography
- Organometallic Complexes
- Organometallic Ligands
- Partnerships
- People
- Pharmaceutical
- Pharmaceutical Discover
- Pharmaceuticals
- Pharmacophore
- Pipeline Pilot
- Polymorph**
- Poster
- Science Communication
- Science Stories
- Scientific Research
- SCXRD
- Semiconductors
- SMARTS
- Smiles
- Software
- Solid Form**
- Solid Form Informatics**

Unlocking Solid Form Innovation in CSD-Materials

Blog Hydrogen Bond Mercury Solid Form Stability

Investigating Solid Form Stability: Understanding Hydrogen Bond Propensity in Mercury


Blog CSD Landscape Generator CSD-Theory Polymorph Solid Form Informatics

How to Generate a Solid Form Landscape without a Crystal Structure with CSD Landscape Generator

Blog CSD-Materials Solid Form Informatics

How to Analyse Hydro

Blog CSD-Materials Drug Development Matwall



ase
res

How to cite the tools seen today

- **Surface Analysis**

Surface Analysis—From Crystal Structures to Particle Properties
Alexandru A. Moldovan and Andrew G. P. Maloney
Cryst. Growth Des. 2024, 24, 10, 4160–4169
<https://doi.org/10.1021/acs.cgd.4c00259>

- **Mercury**

Mercury 4.0: from visualization to analysis, design and prediction
C. F. Macrae, I. Sovago, S. J. Cottrell, P. T. A. Galek, P. McCabe, E.
Pidcock, M. Platings, G. P. Shields, J. S. Stevens, M. Towler and P. A.
Wood, *J. Appl. Cryst.*, **53**, 226-235, 2020
[\[DOI: 10.1107/S1600576719014092\]](https://doi.org/10.1107/S1600576719014092)

- **CSD**

The Cambridge Structural Database
C. R. Groom, I. J. Bruno, M. P. Lightfoot and S. C. Ward, *Acta Cryst.*
(2016). B72, 171-179
[DOI: 10.1107/S2052520616003954](https://doi.org/10.1107/S2052520616003954)



More reference
papers for
CSD-Particle



More reference
papers for
CSD Software

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What we have learnt

- ✓ Become familiar with the CSD
- ✓ How to use Mercury for Particle Informatics studies.
- ✓ How to use the Surface Analysis tool.
- ✓ How to calculate Full Interaction Maps on surfaces.
- ✓ How you can best use Mercury and CSD-Particle in your workflows.
- ✓ About recent advances and improvements in CSD-Particle tools.

Want to explore more?

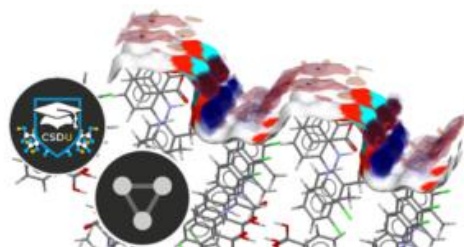
Training and learning

- Covering use cases with guided examples.
- Including examples from today as well as other CSD Software.



CSDU

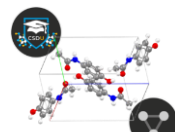
Learn on demand with free online training courses



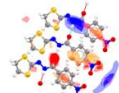
- Free
- Completion certificate upon passing a final test.
- In-depth review of today's topics and more software.



CSD
Python
API



Basics of
Mercury



Full
Interaction
Maps

Self-guided workshops

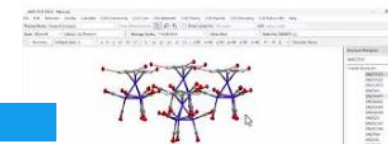


And more!

Videos



YouTube
channel



How to: Explore molecules and create eye-catching graphics with Mercury



How to: Build and combine searches in ConQuest

Want to explore more?

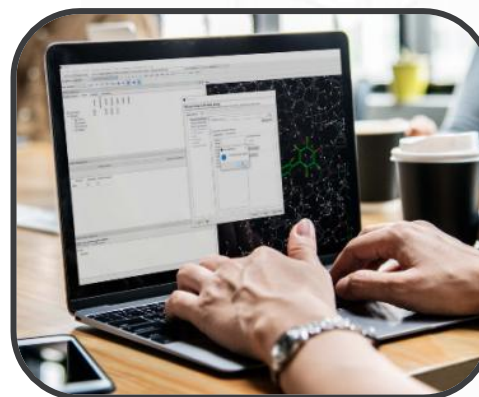
CCDC Virtual Workshops

- **4th November** – How to Use the Docking Software **GOLD** to Perform **Virtual Screening** Simulations

CCDC Webinars

- **13th November** - Using general purpose **force fields** in solid form studies
- **20th November, Panel** – **Frontiers in MOFs: Creating Real-World Solutions with MOFs**

Check our Events online for more virtual and in person events.



Frontiers in
MOFs
CCDC **60** YEARS
advancing structural science

WEBINAR

Creating Real-World Solutions with MOFs

Panel discussion with experts from academia and industry.

20th November, 3pm GMT [REGISTER](#)



Using General Purpose Force Fields in Solid Form Studies

Lily Hunnisett
Computational Solid-State Scientist, CCDC

Thursday, 13th November
15:00 (GMT)/ 10:00 (EST)



Technical and scientific support

Getting set up
Technical support
Scientific questions



Contact our support team
<https://support.ccdc.cam.ac.uk/support/tickets/new>

License queries
Renewals
Find out license contacts



Visit the **FAQs** on the website
<https://support.ccdc.cam.ac.uk/support/solutions>



See the documentation in **Support and Resources** on our website
<https://www.ccdc.cam.ac.uk/support-and-resources/>



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admin@ccdc.cam.ac.uk