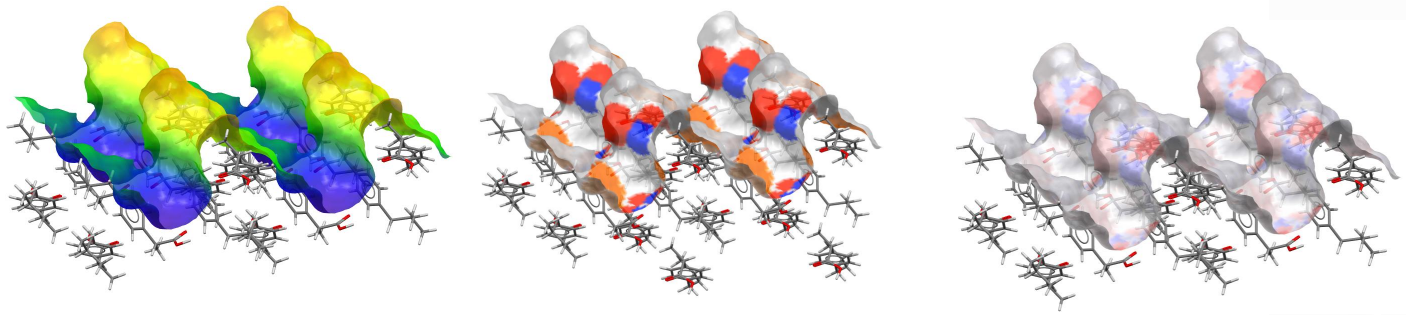

REC

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

CCDC Virtual Workshop

21st October 2025

CCDC
advancing structural science

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.

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Agenda

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

- *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

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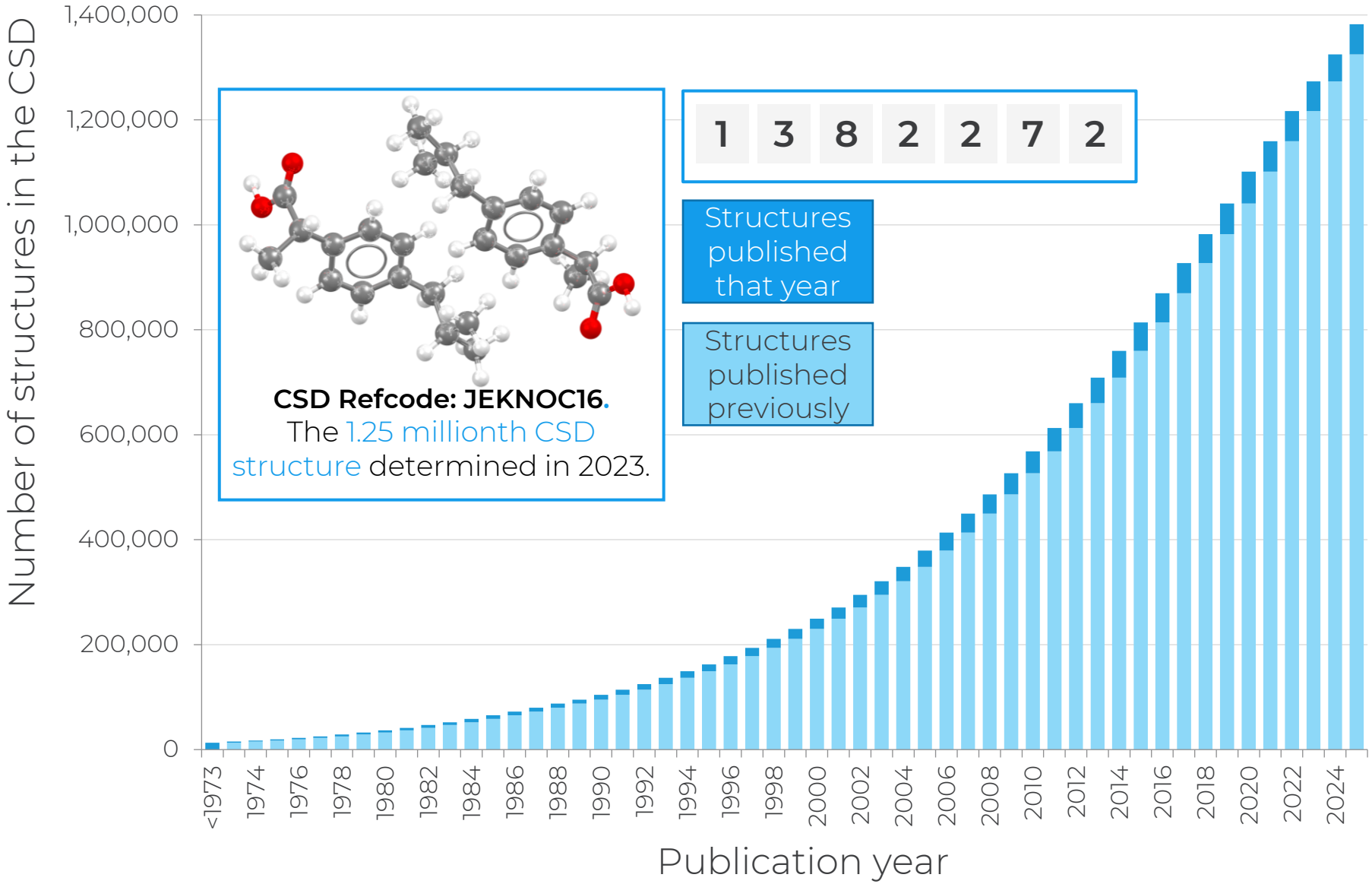
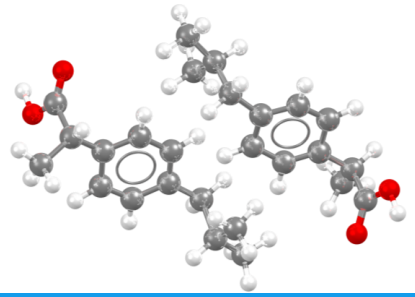
The Cambridge Structural Database



- 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

Refcode 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* refcode families

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

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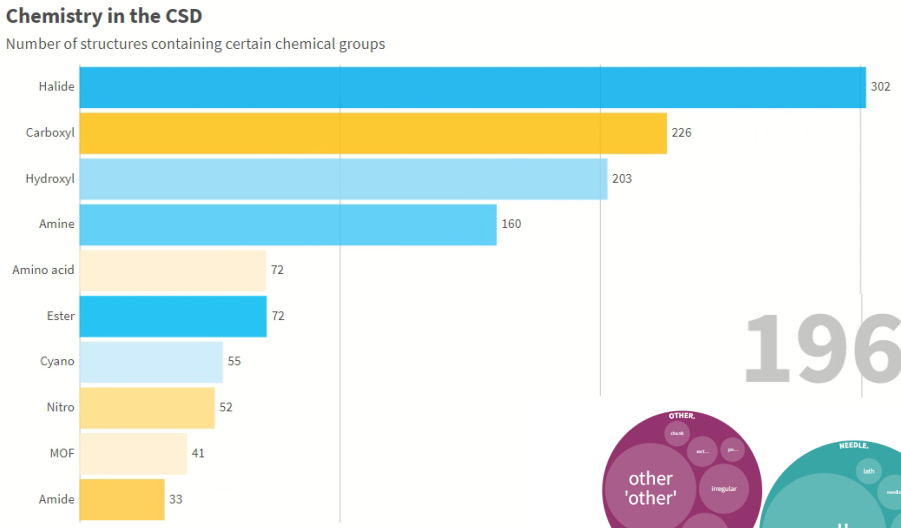
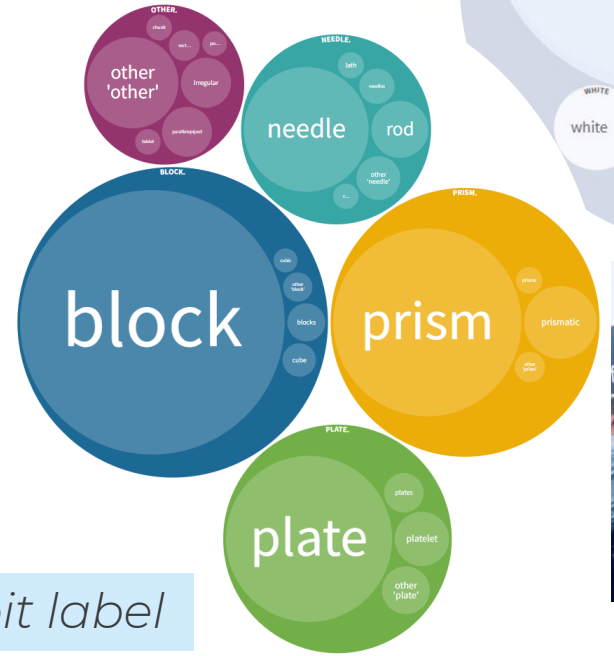
Statistics in the CSD



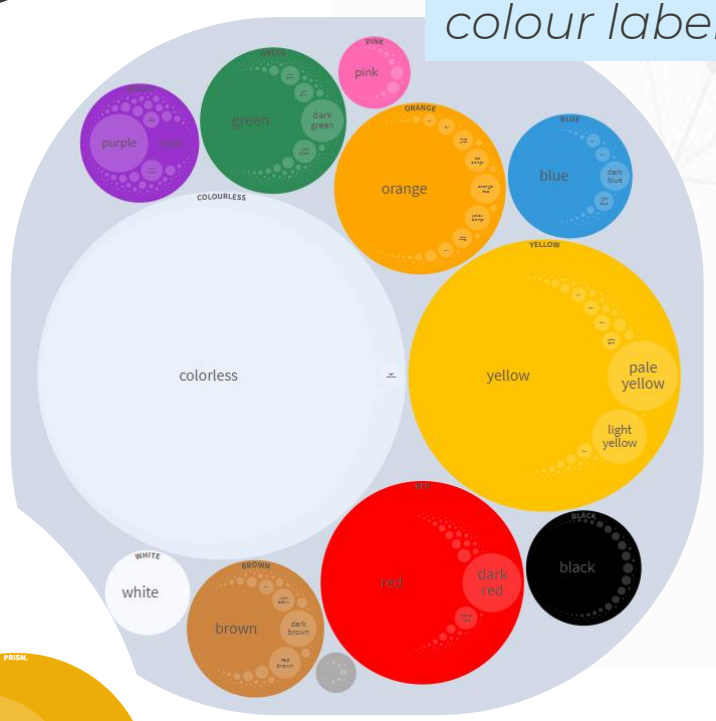
1965



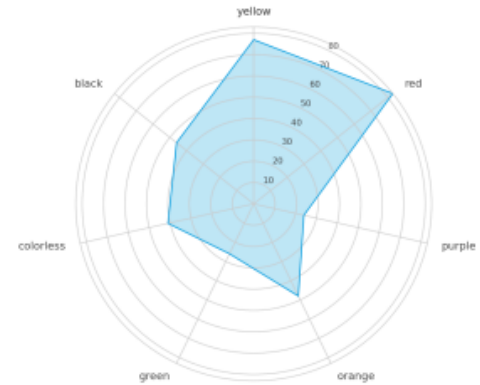
Data collected using the CSD Python API and graphs created with Flourish

habit label

colour label



From our #CSDLeaderboard at conferences!



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!

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The CSD Portfolio

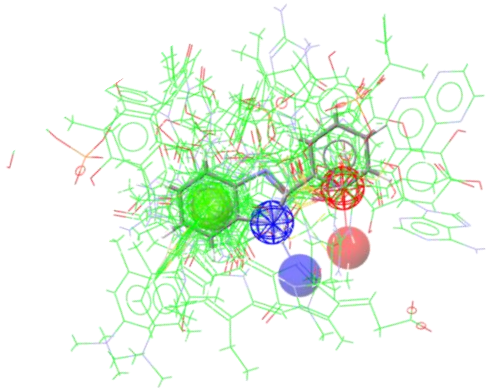
CSDEnterprise.

CSDCore.

Mercury

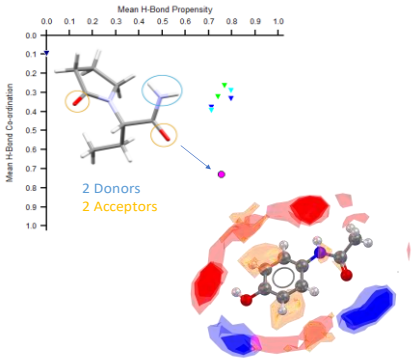
CSDDiscovery.

Design of new molecules



CSDMaterials.

Assessment of solid form stability and properties

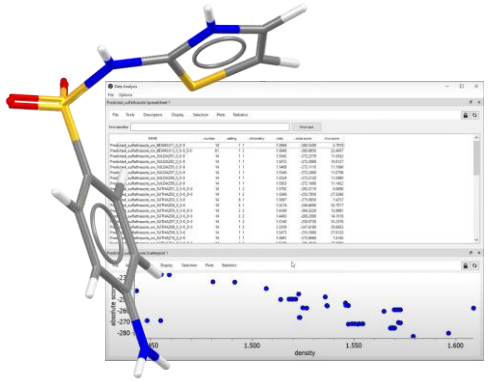


CSDParticle.

Anticipate particle properties and behaviour

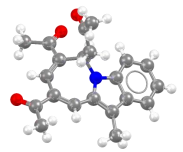
CSDTheory.

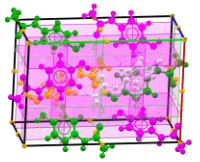
Generate solid form landscapes



CSDCommunity.

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





CSDU

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

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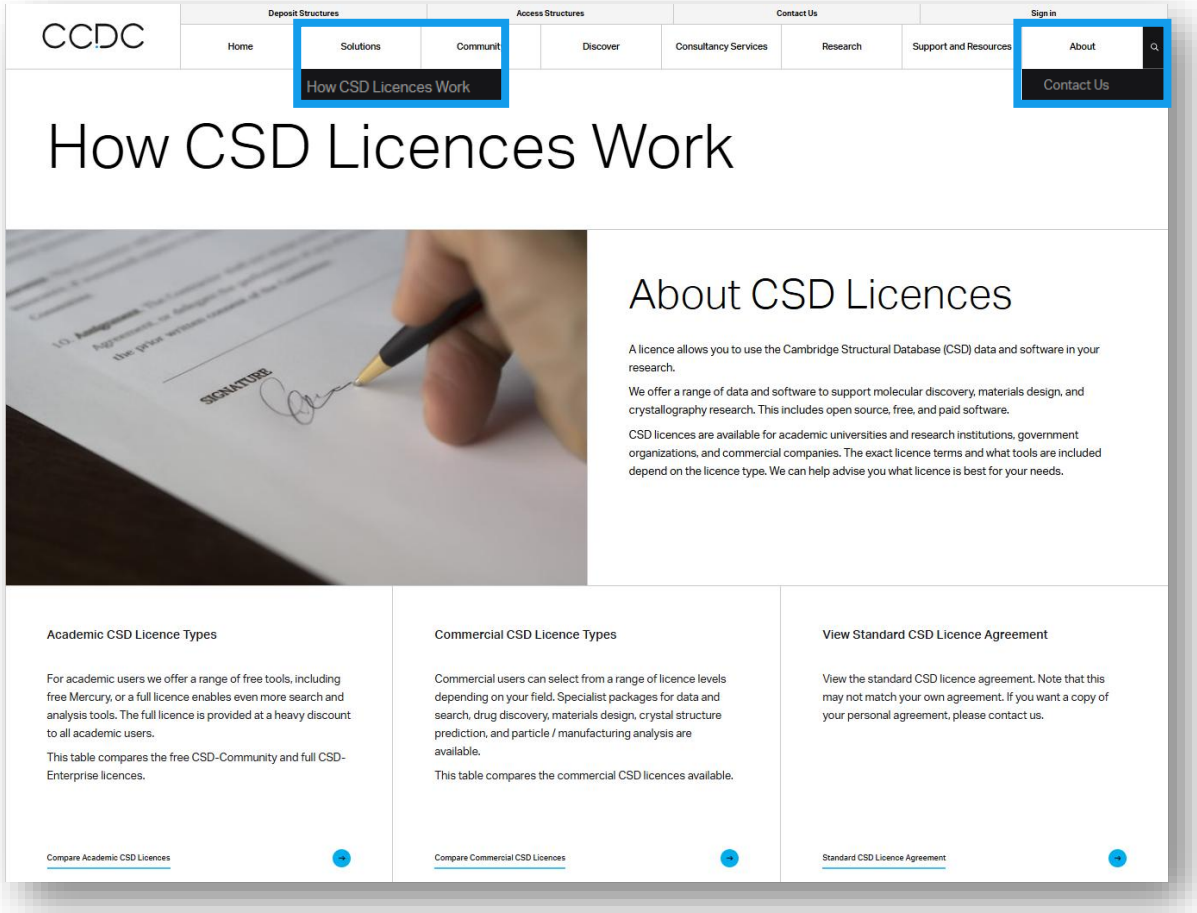
What can you do with a licence?



- **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

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- *Show One:* Case study by Prof. Elena Simone
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- *Try One:* Hands-on examples
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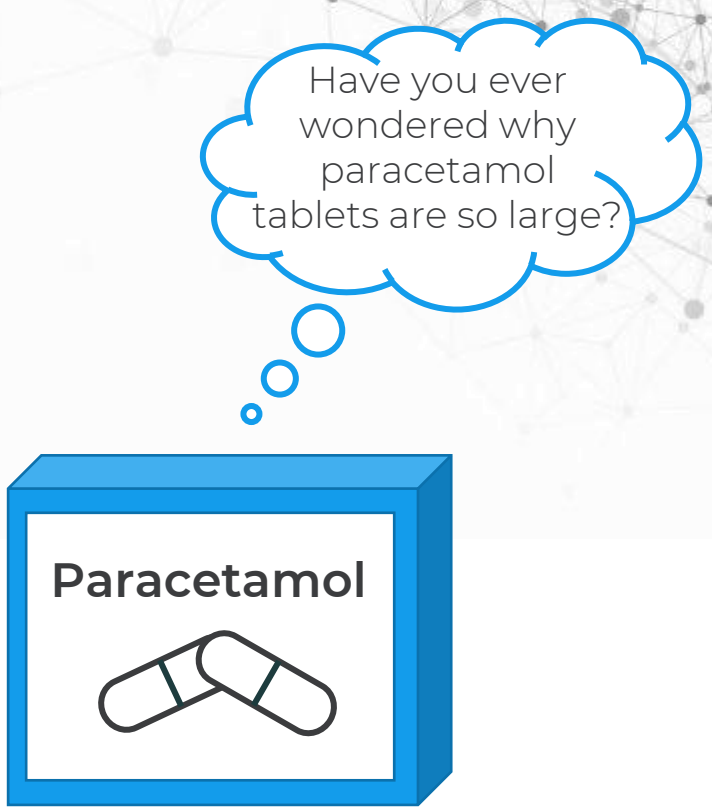
Why does particle shape matter?

- 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.



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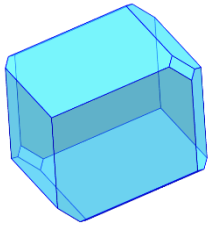
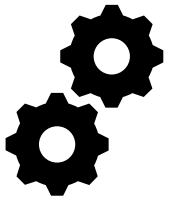
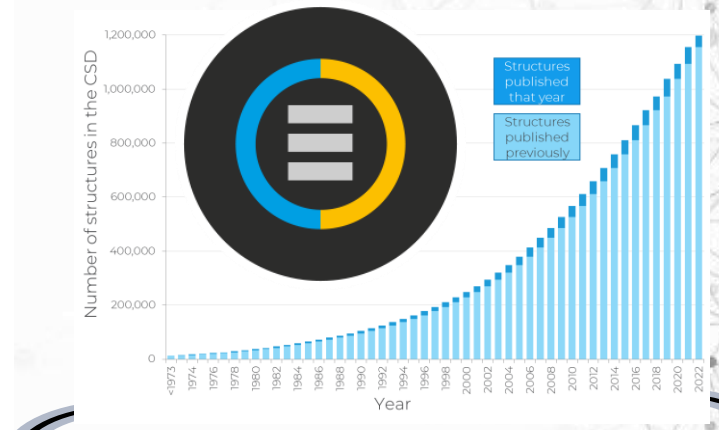
The field



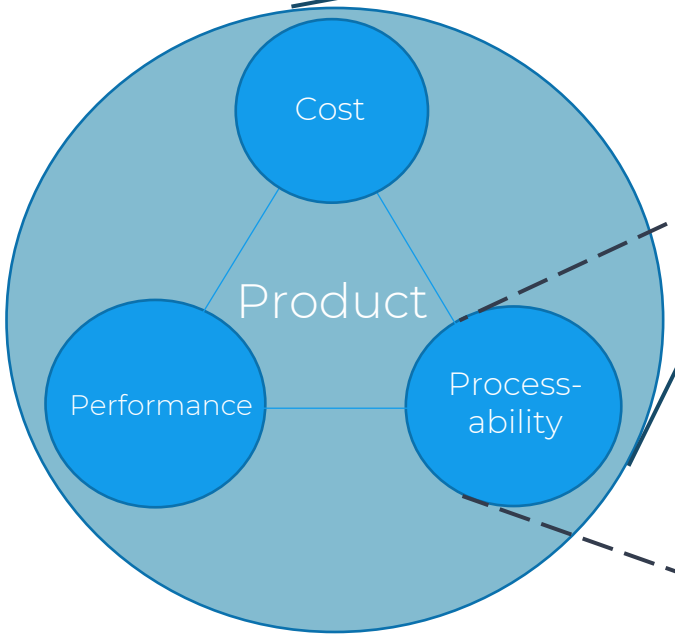
Particle

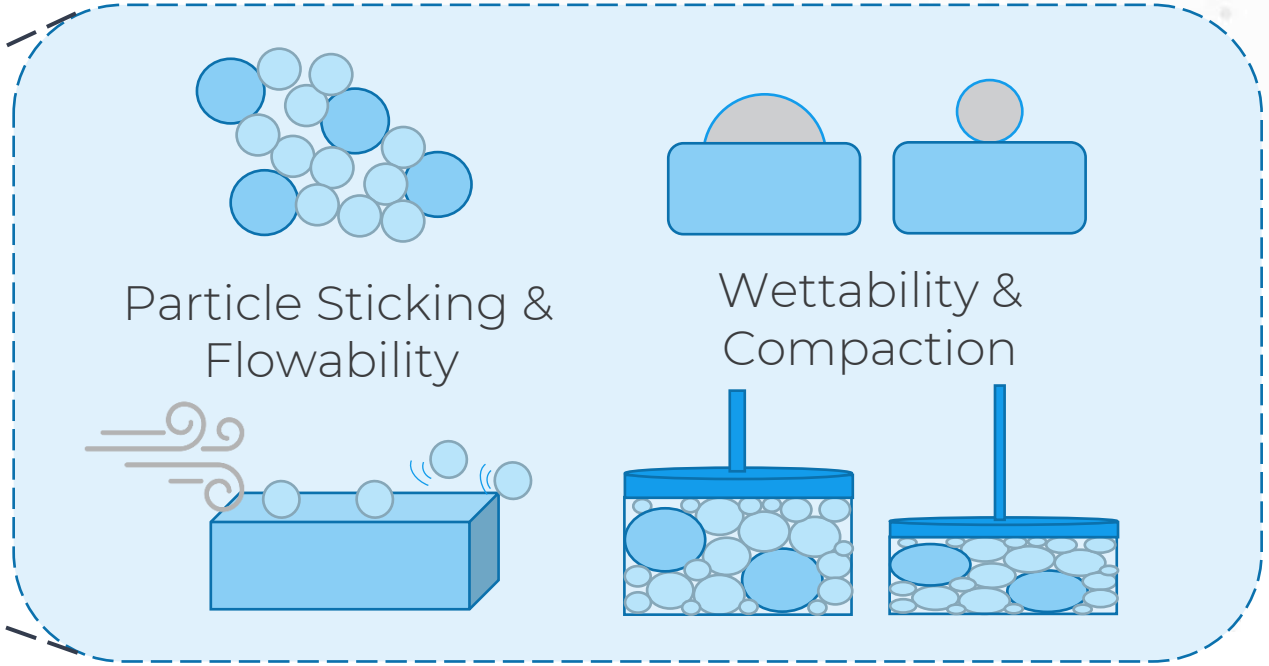


Product

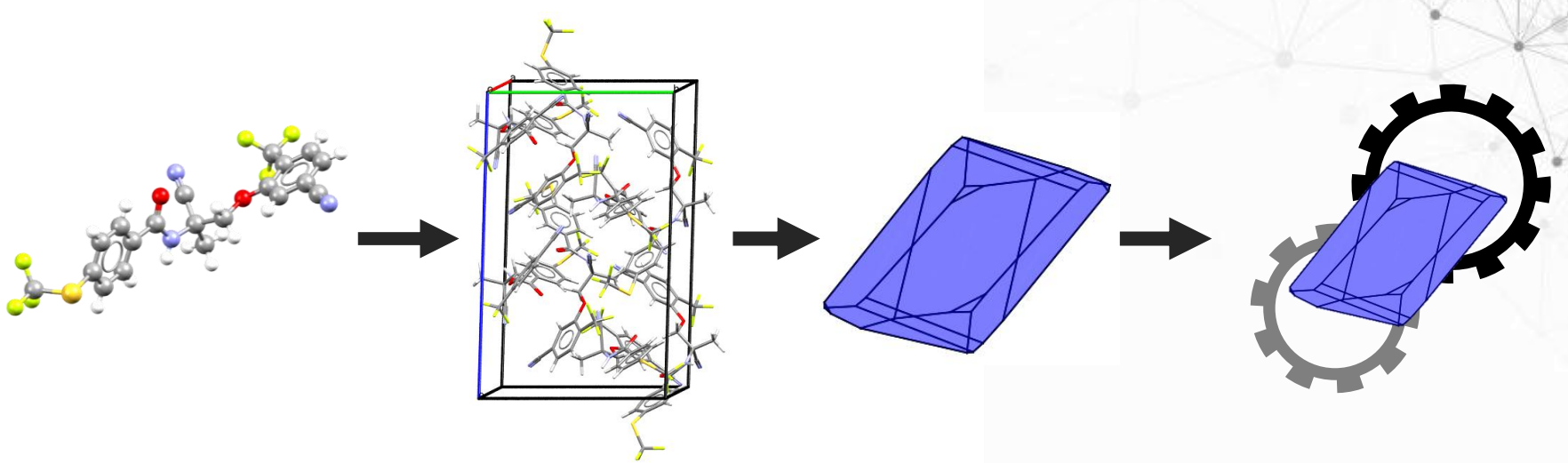


CSD





From solid form to particle properties



Molecule Form Particle Properties

Solid Form Informatics

Particle Informatics

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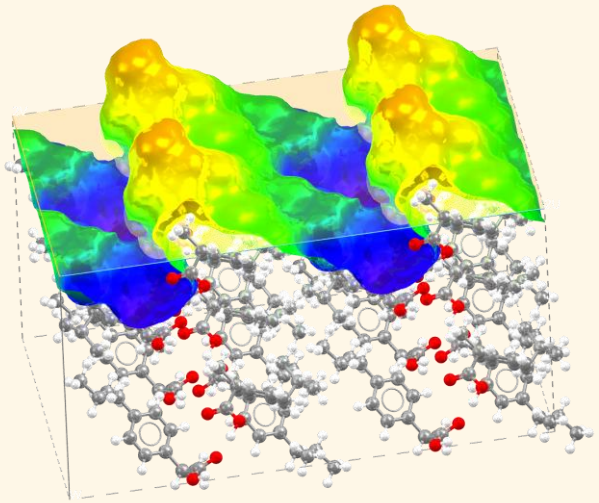
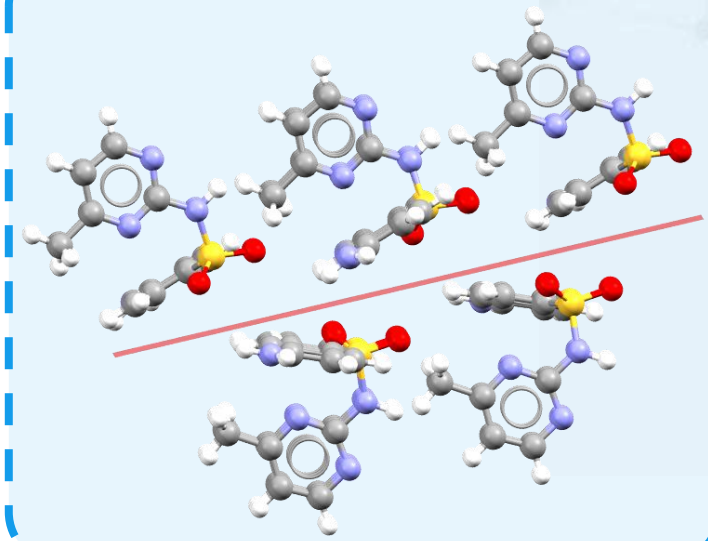
Analysing particle properties

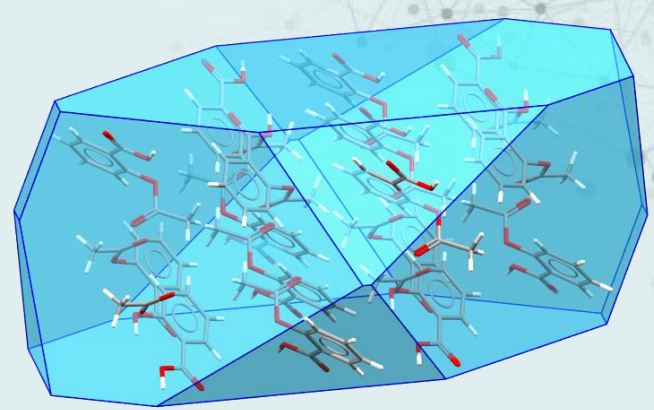
Surface Properties



Slip Planes



Morphology



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

M. J. Bryant *et al.*, *Cryst. Growth Des.* (2019), **19**, 9, 5258-5266. ISSN 1528-7483

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Prof. Elena Simone

Politecnico di Torino

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

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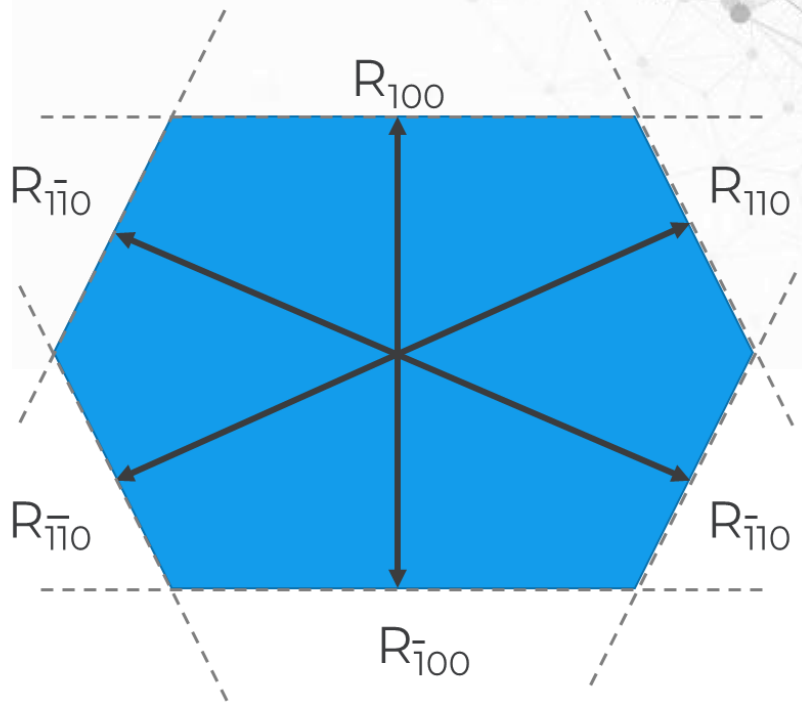
Which surface to analyse?

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



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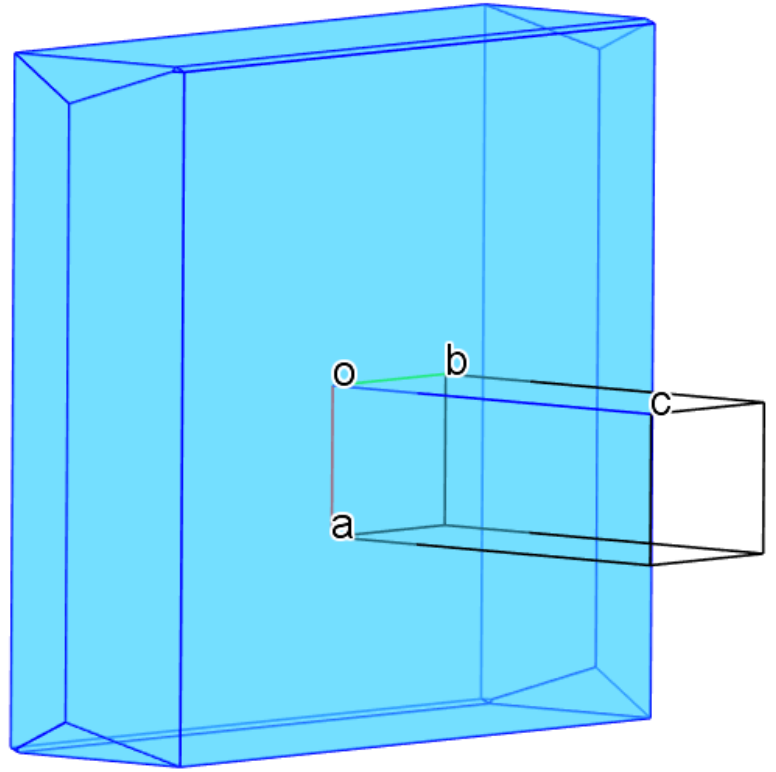
BFDH morphologies

- 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.G. Friedel *Bull. Soc. Franc. Miner.* (1907), 9, 326-455.
J.D. Donnay, D. Harker, *Amer. Min.* (1937), 22, 446-467.

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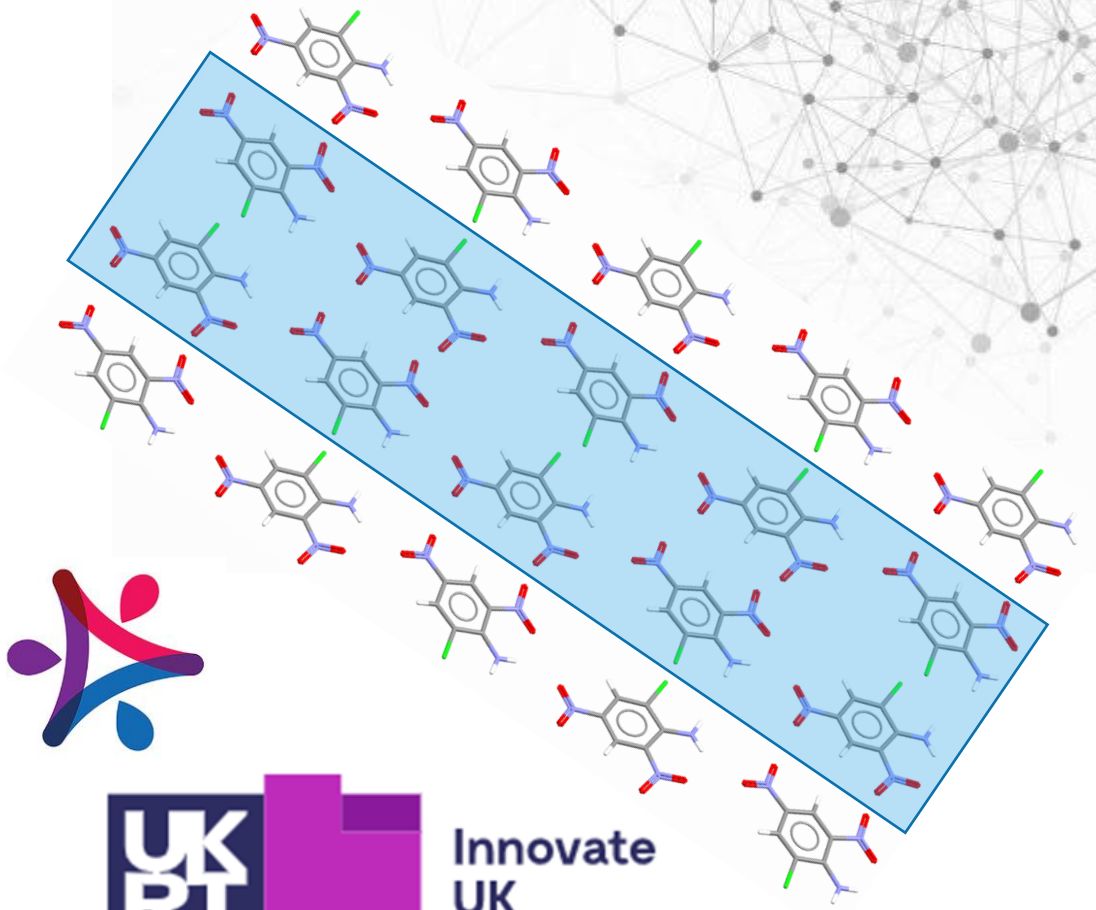
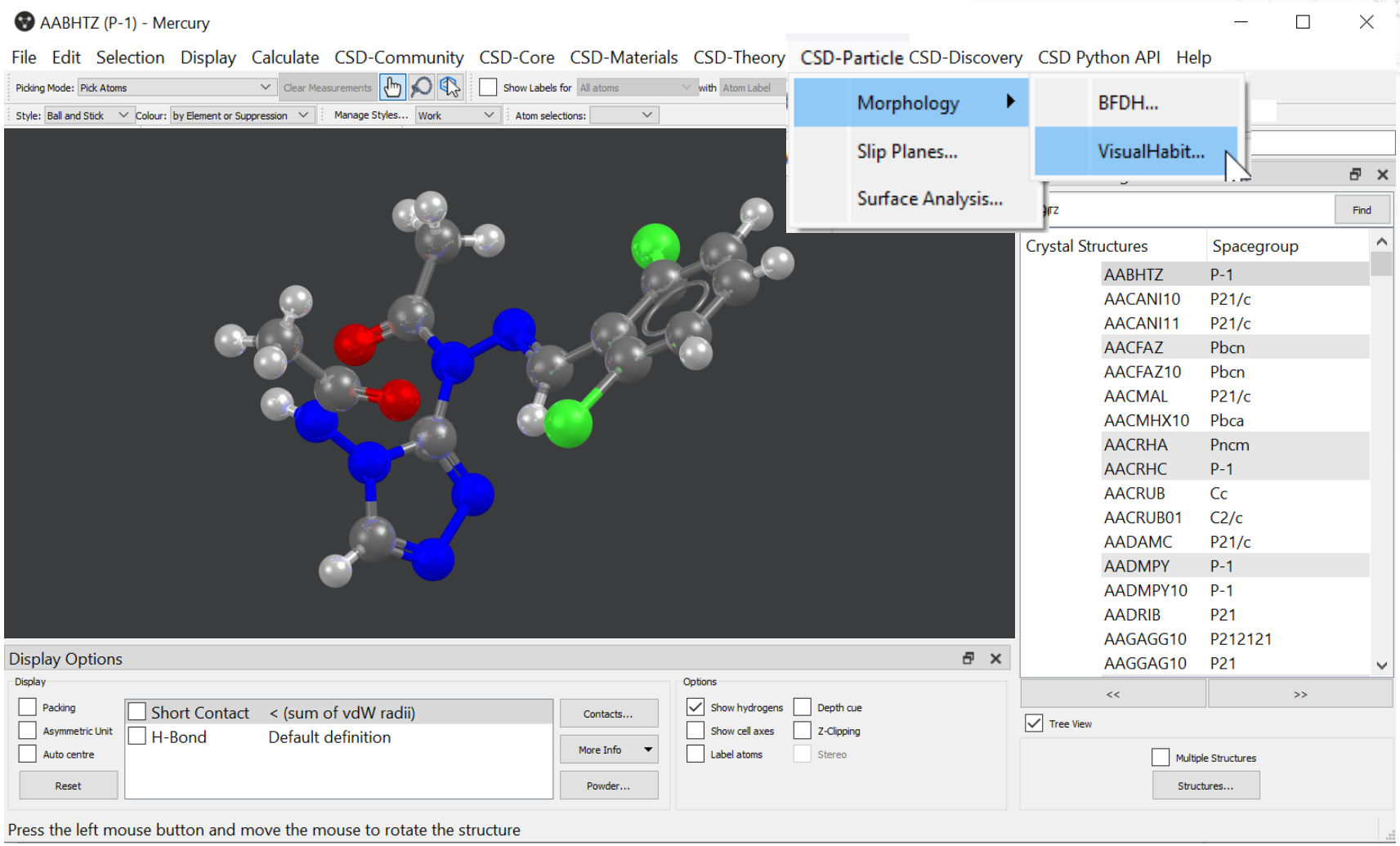
VisualHabit

- 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.

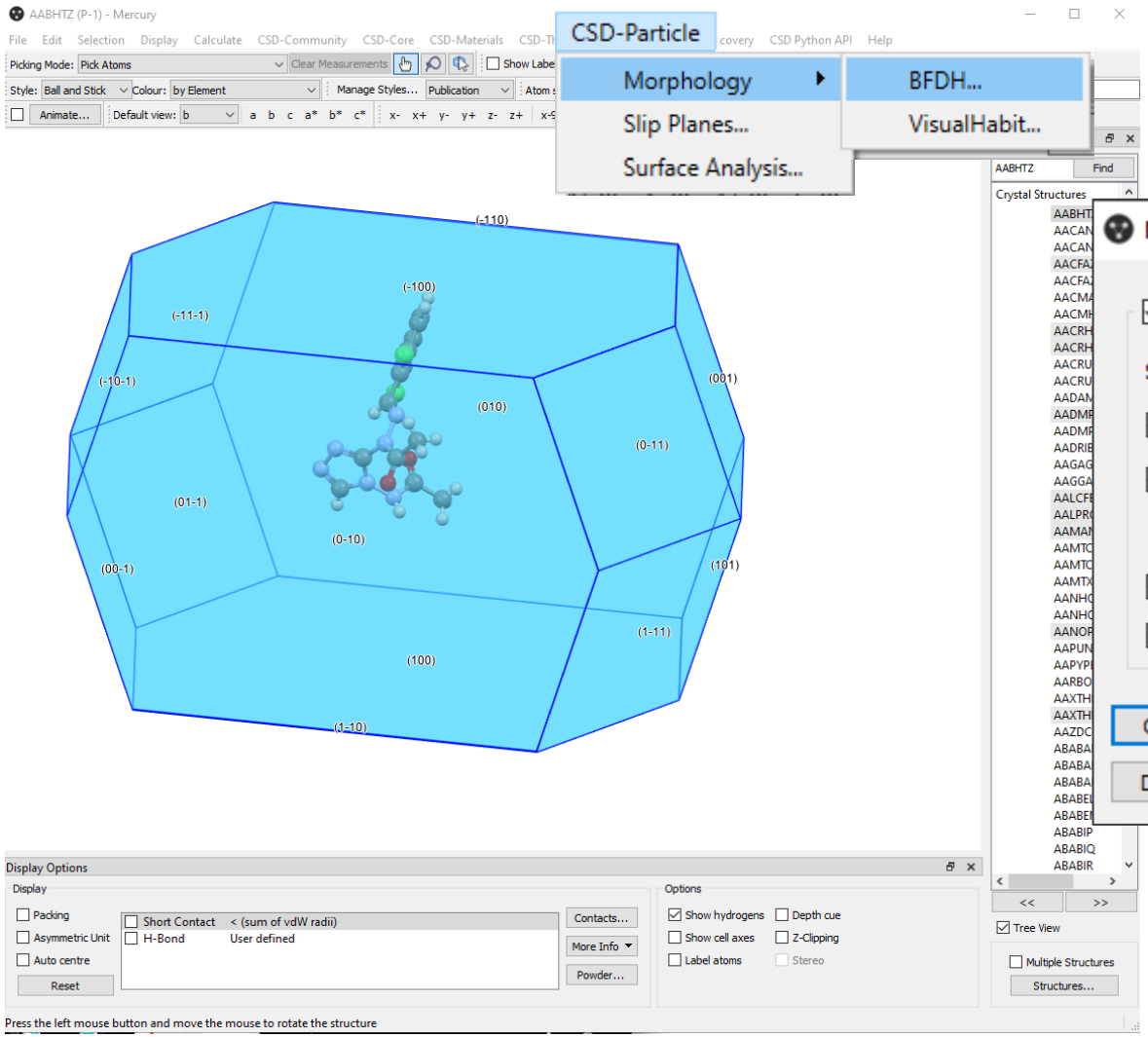


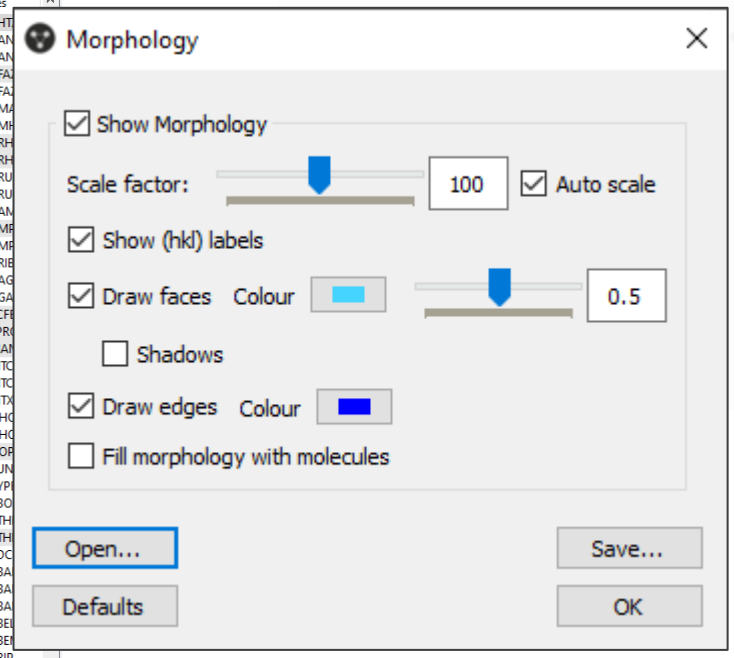
G. Clydesdale, R. Docherty, K. J. Roberts, *Comput. Phys. Commun.* 1991, 64 (2), 311–328. https://doi.org/10.1016/0010-4655(91)90040-R

Accessing morphologies in Mercury



BFDH Morphology





Display Options

Save and Load

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

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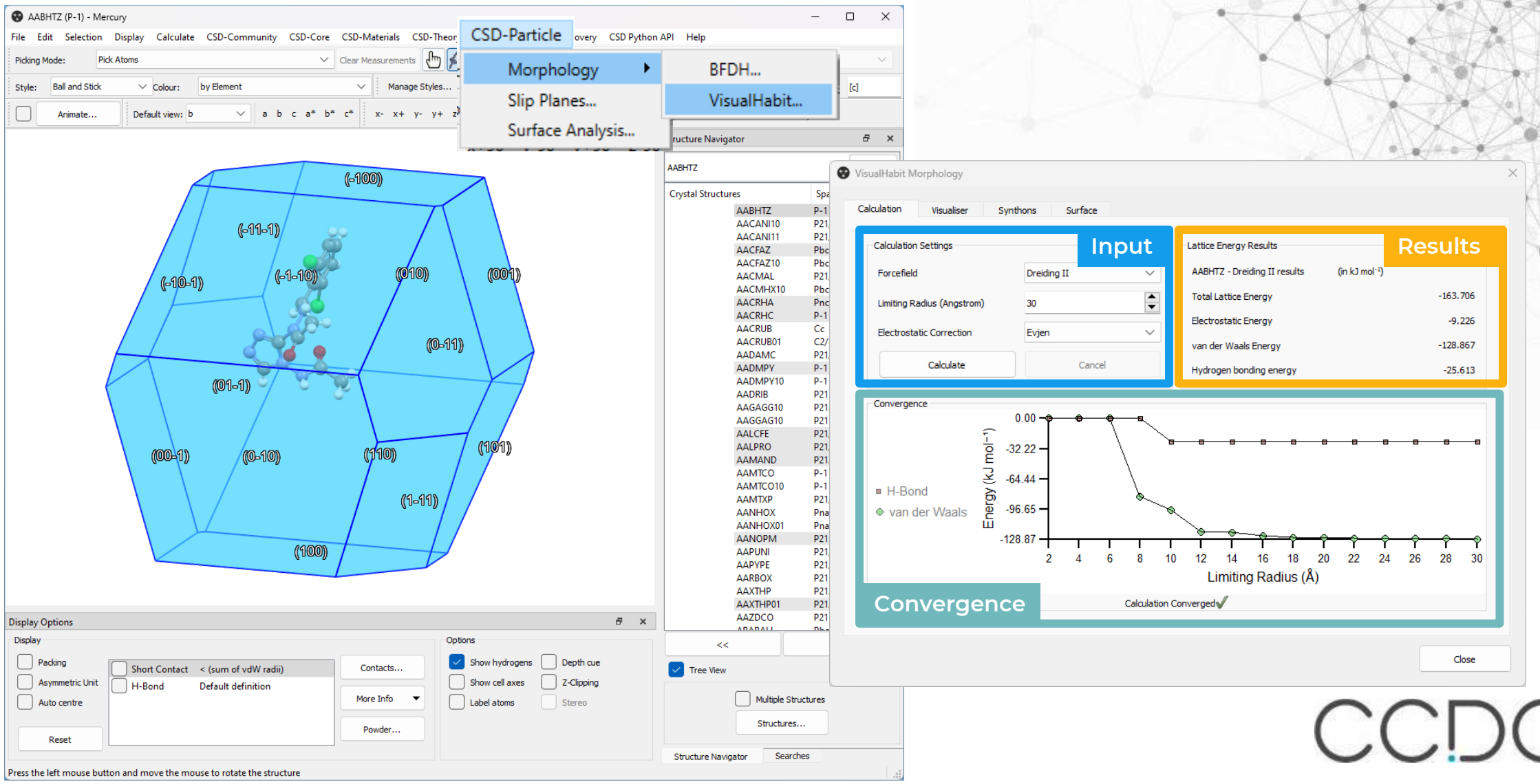
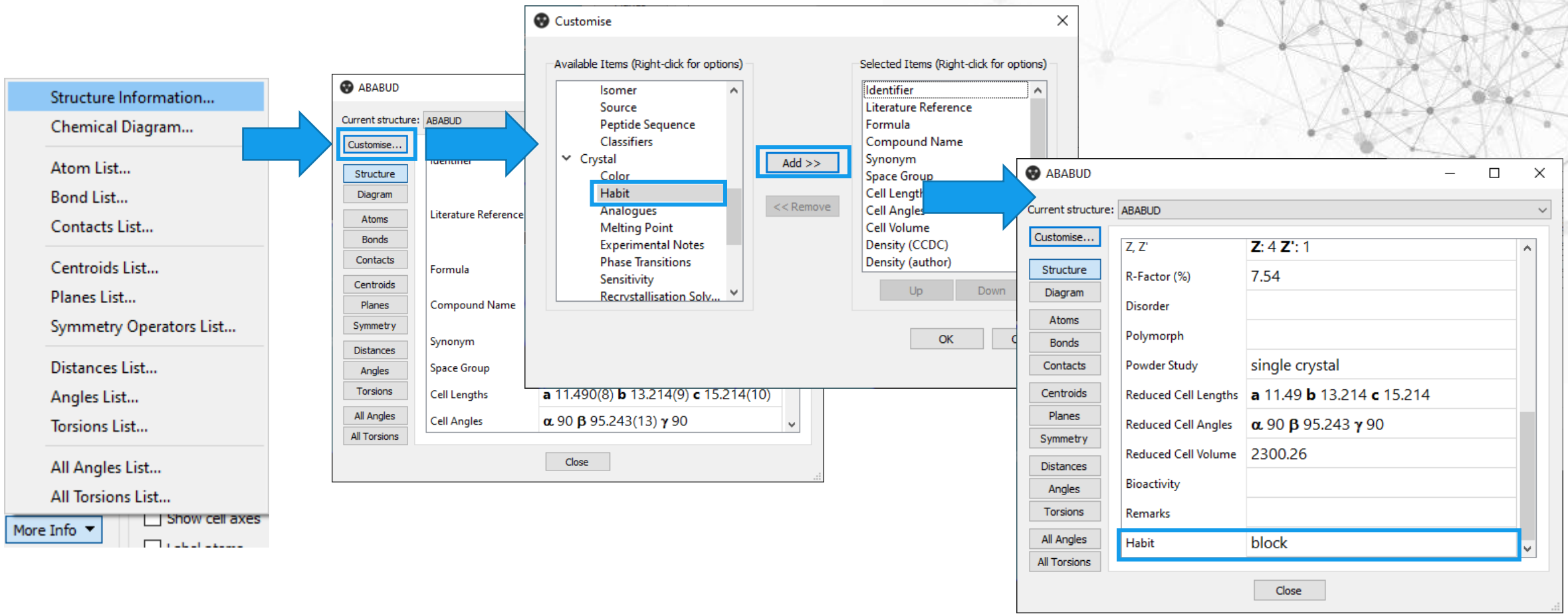
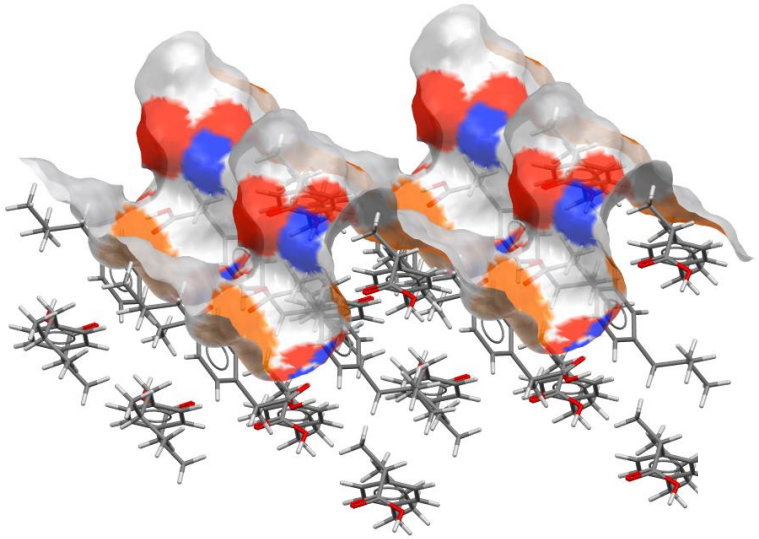
Accessing VisualHabit



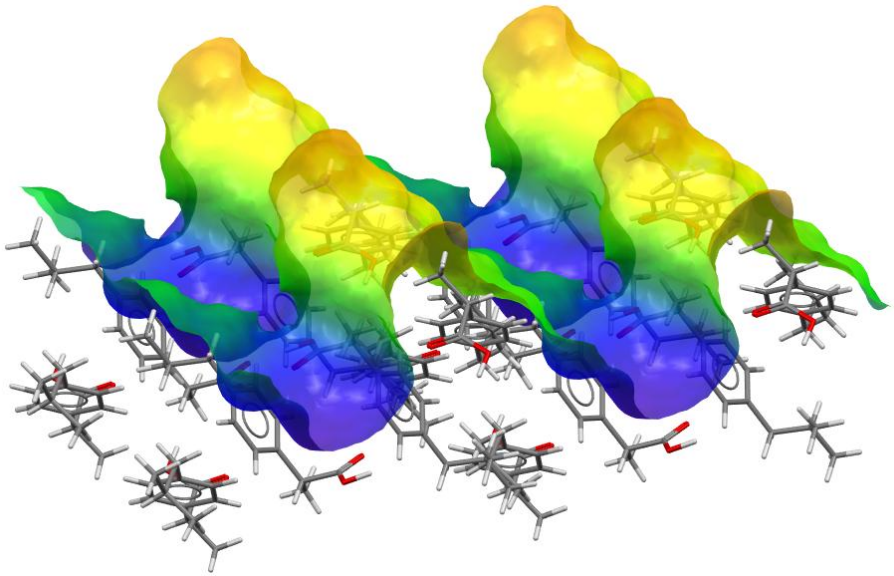
Bonus: Experimental Habit Data Field



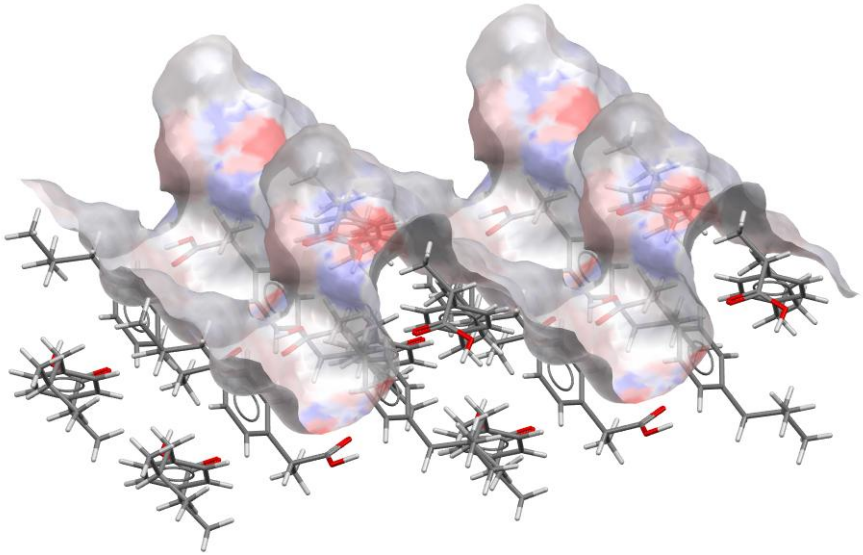


Surface Chemistry

Surface Analysis



Surface Roughness



Surface Charge

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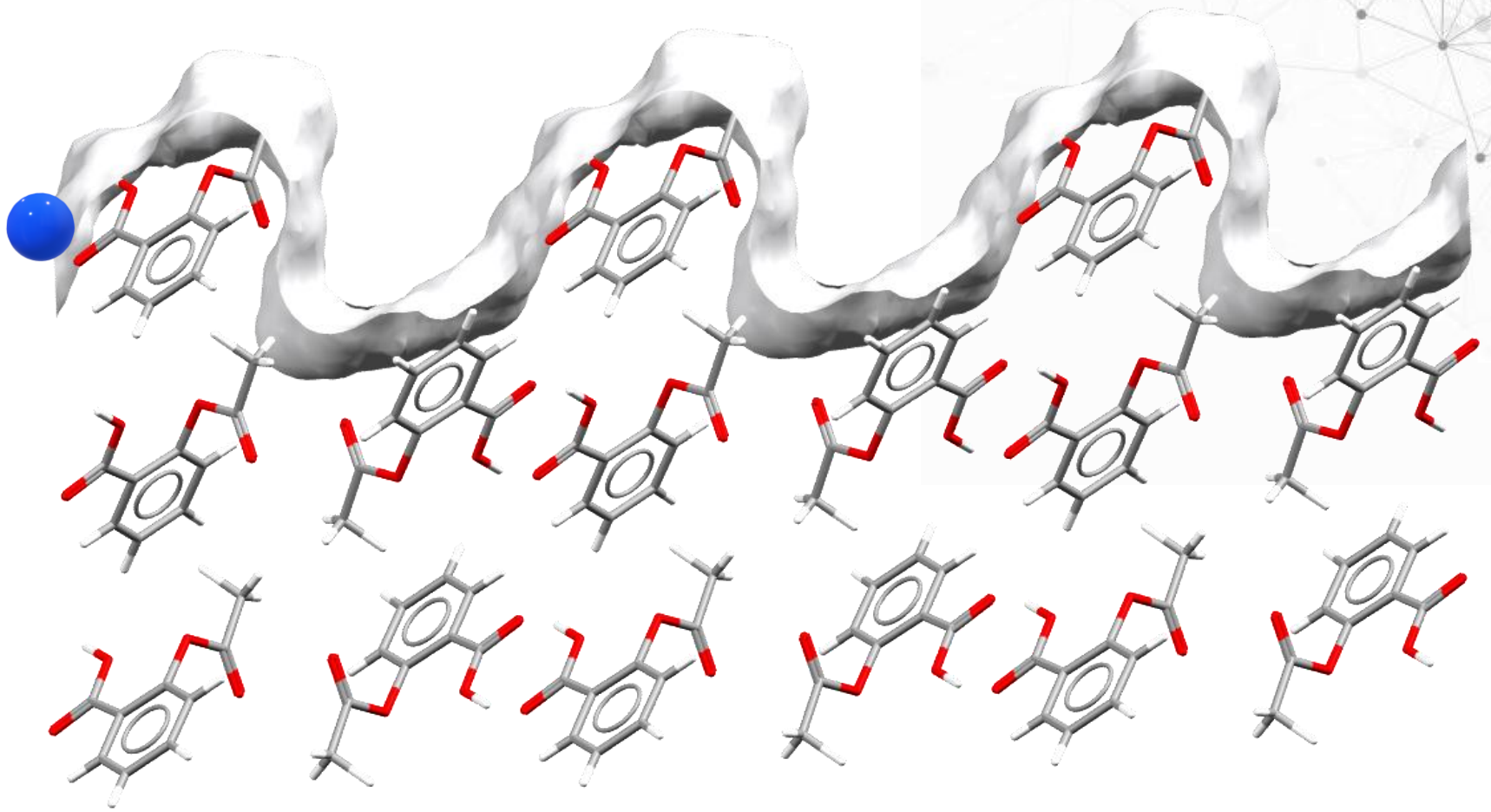
Surface Analysis



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

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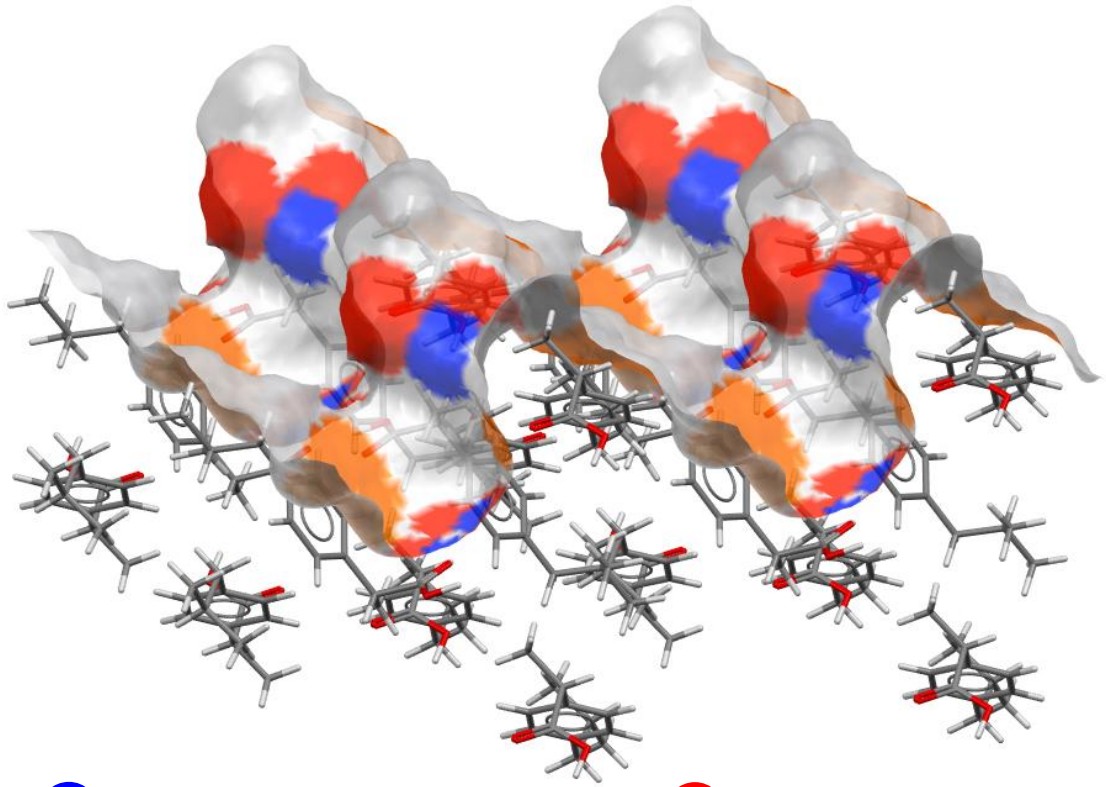
Surface Analysis



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

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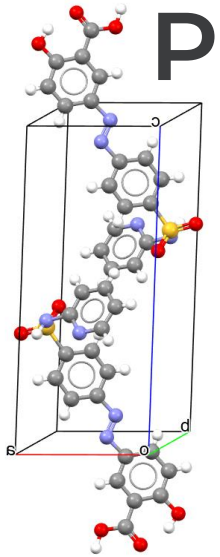
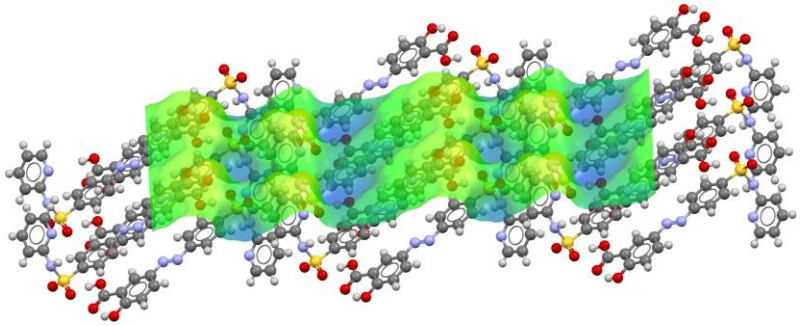
Particle Informatics





Descriptors	
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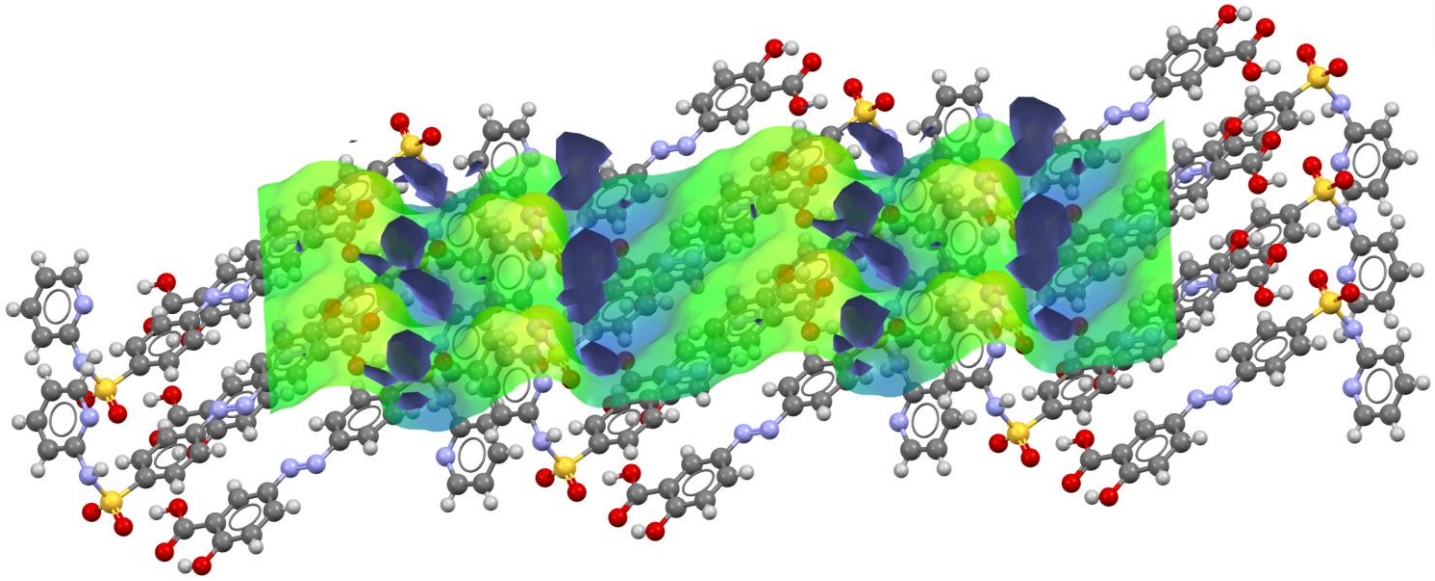
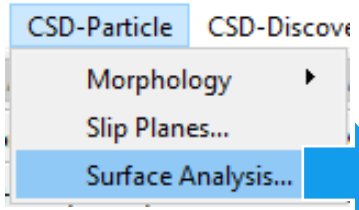
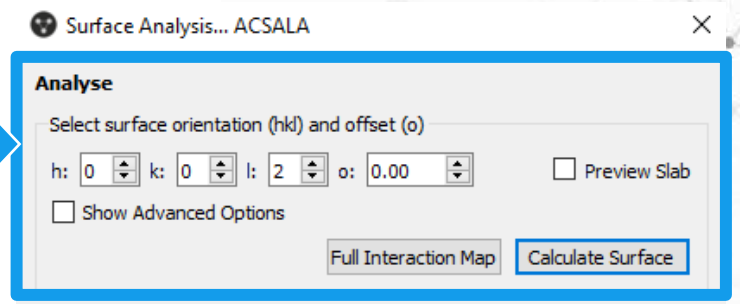
RMSD, Skewness, and Kurtosis	

FIMs on Surface



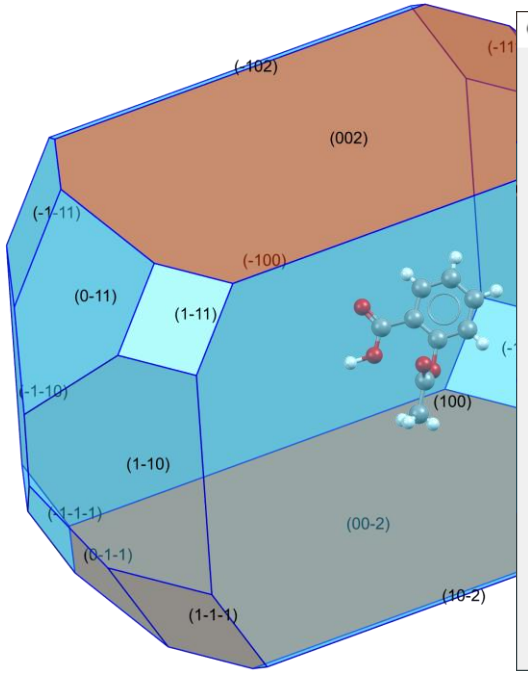
CSD-Particle – Surface Analysis

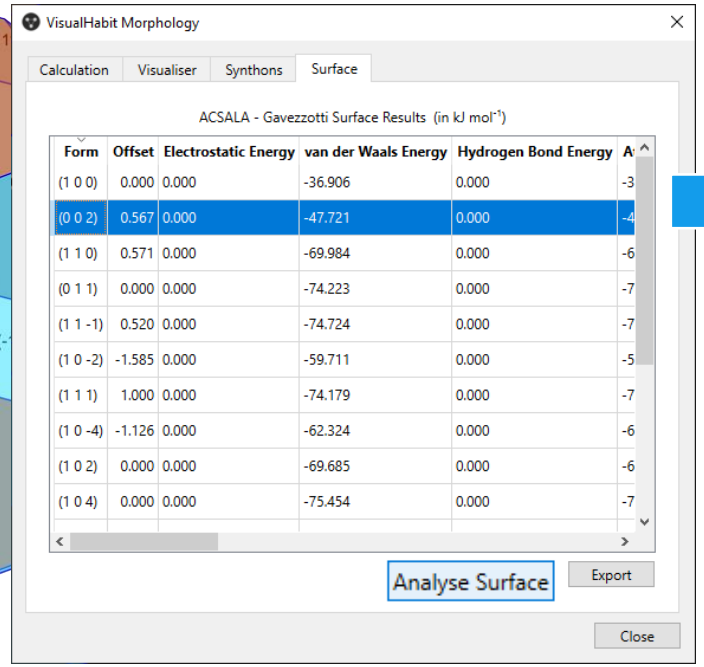


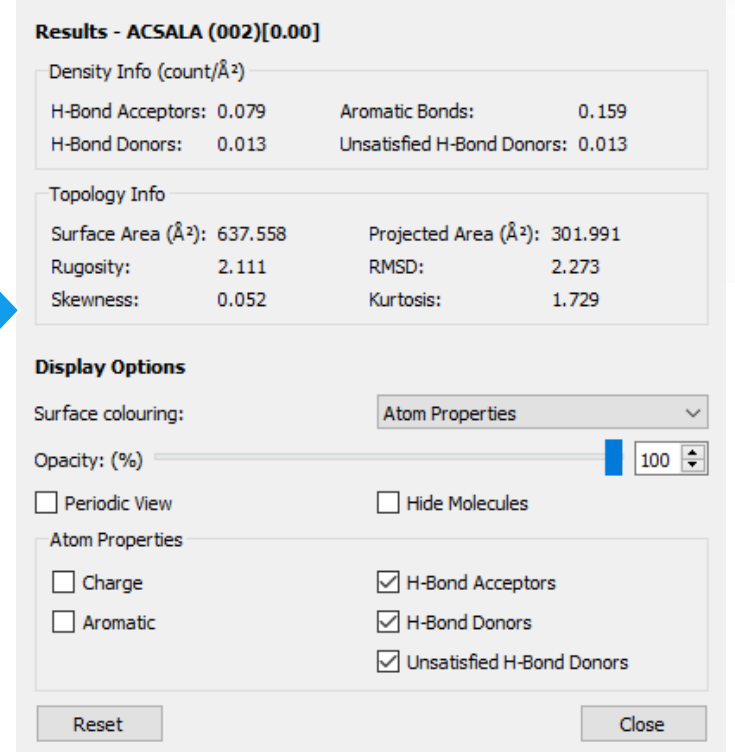


Input

Extra TIP: also launch directly from VisualHabit

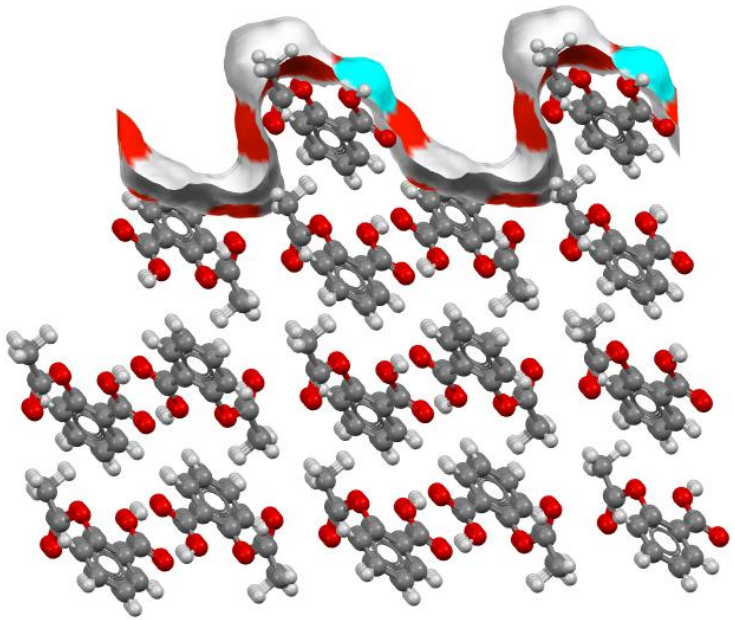






CCDC

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

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 (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

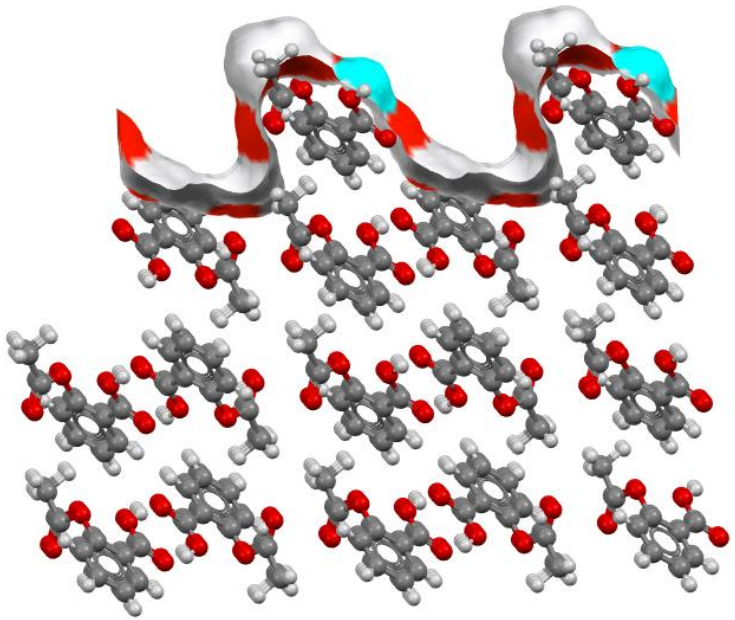
Unsatisfied H-Bond Donors

Reset Close

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]

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Aromatic H-Bond Donors

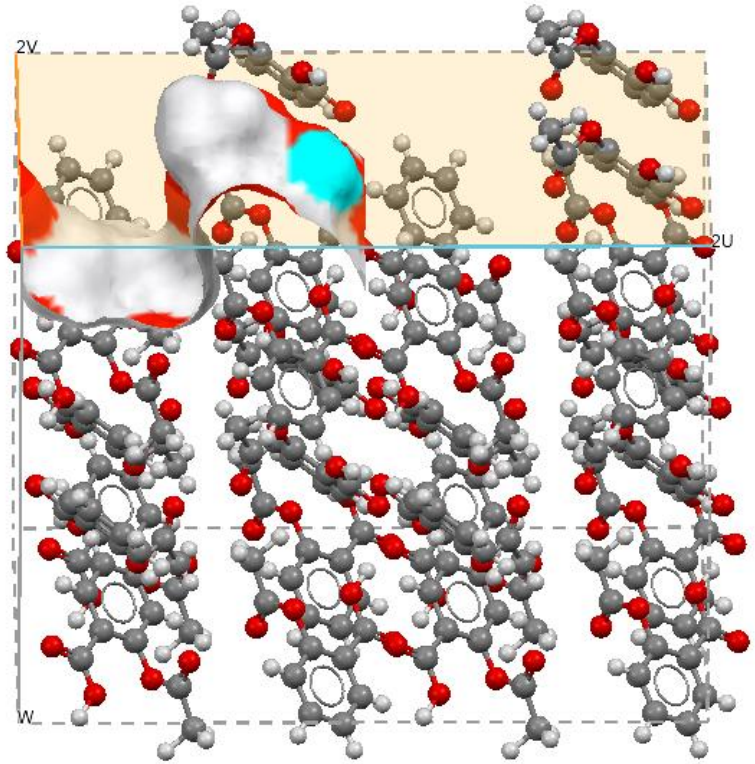
Unsatisfied H-Bond Donors

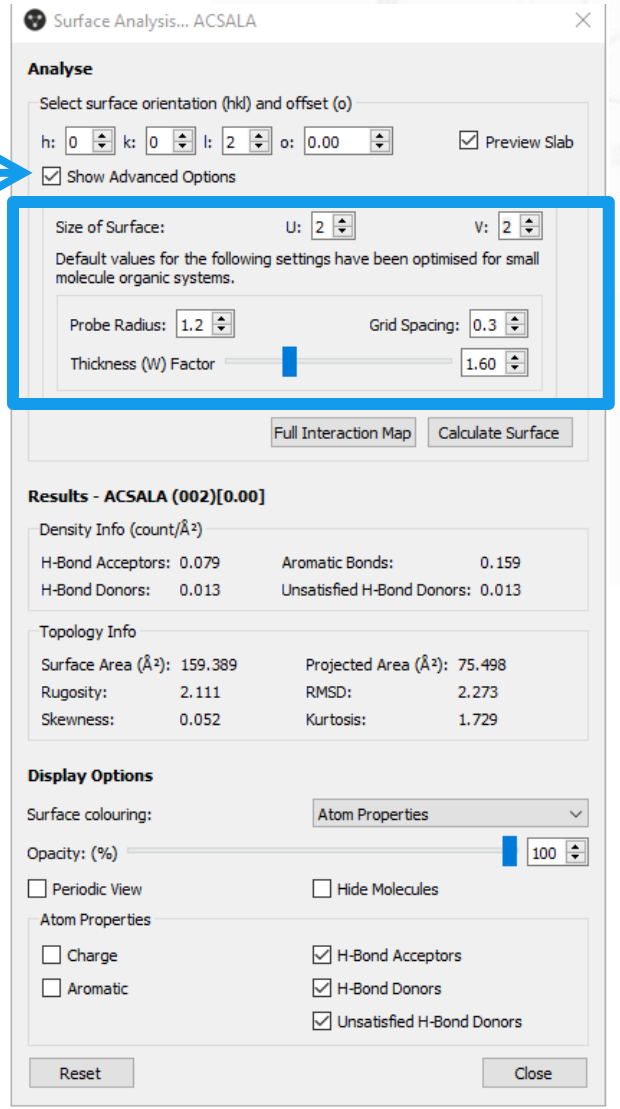
Reset Close

Display Options

CCDC

CSD-Particle – Surface Analysis





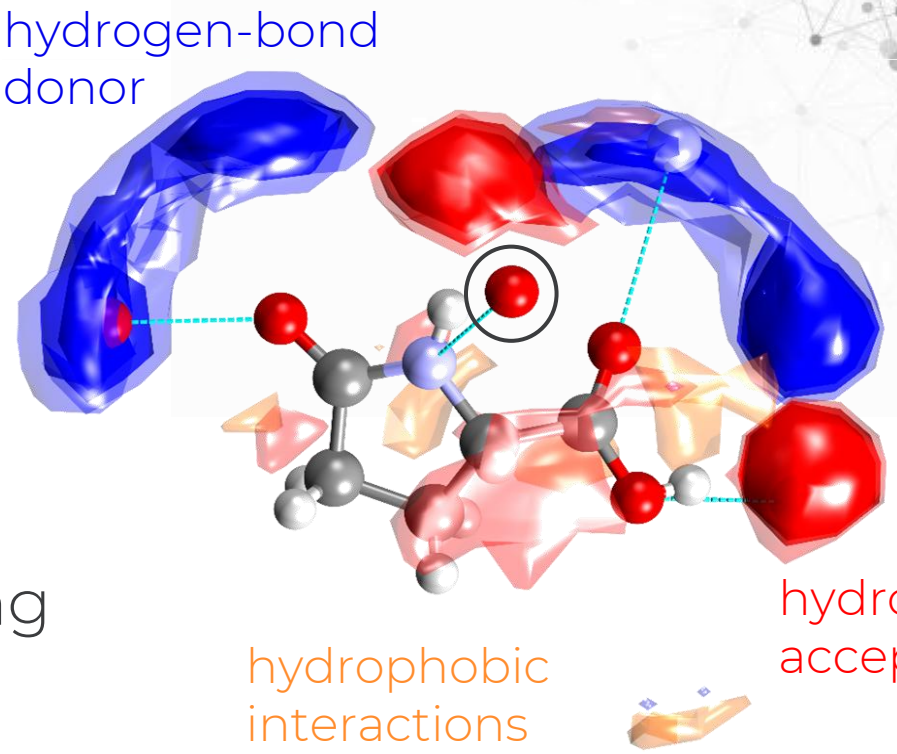
Advanced Options

CCDC

Full Interaction Maps (FIMs)

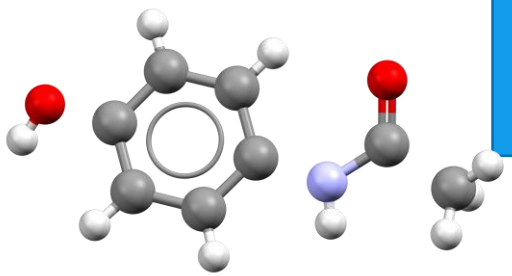
Learn about FIMs in this free online CSDU course

- 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

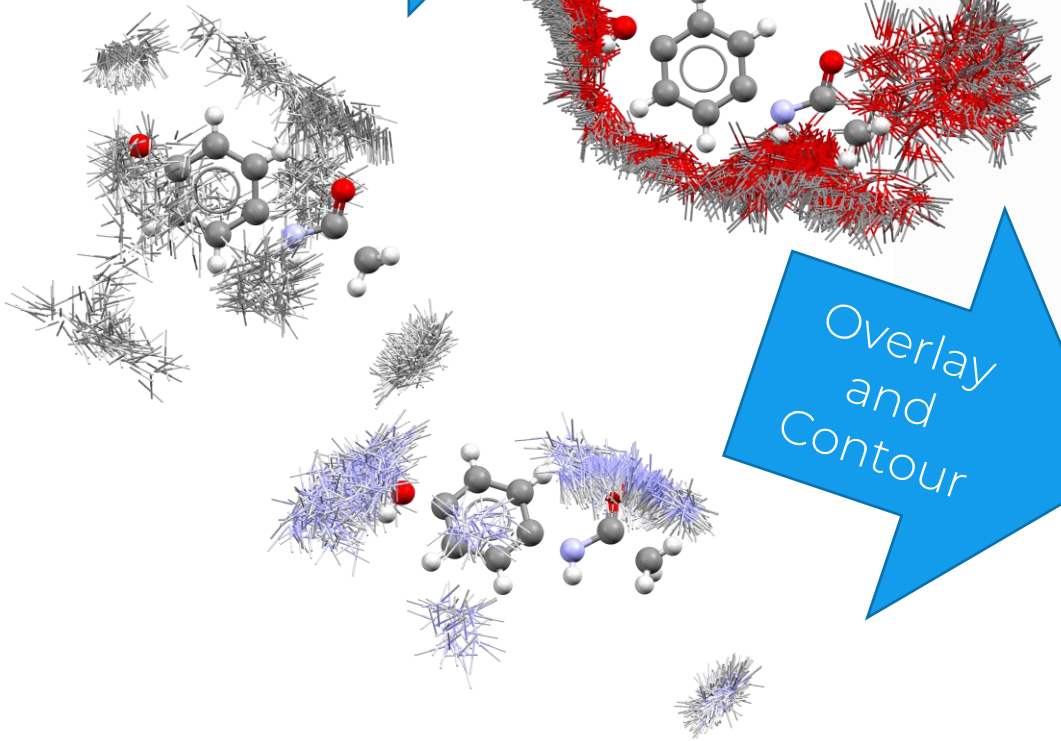


CCDC

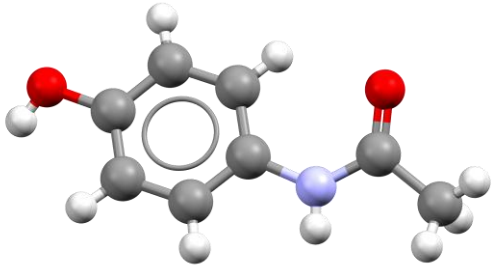
FIMs Algorithm



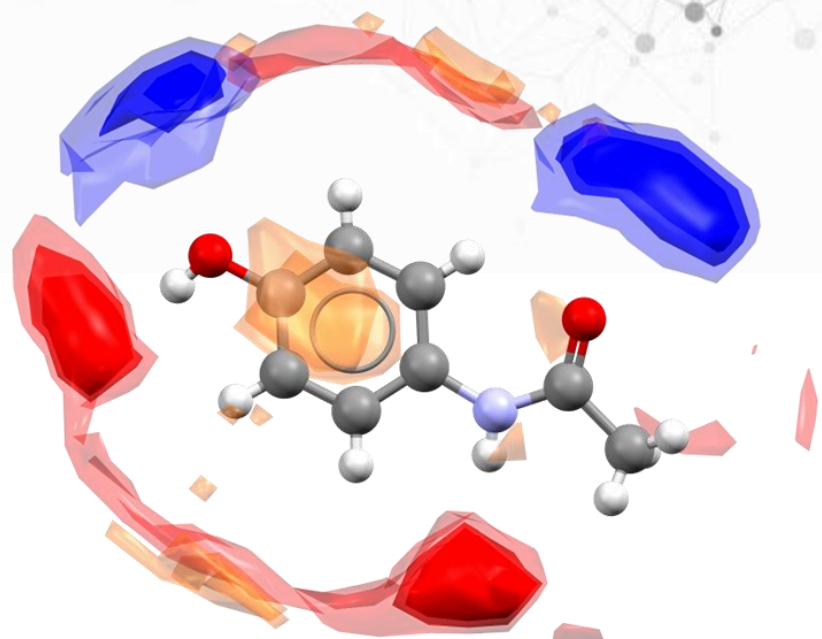
Match and overlay scatterplot for each probe



Fragment



Overlay and Contour

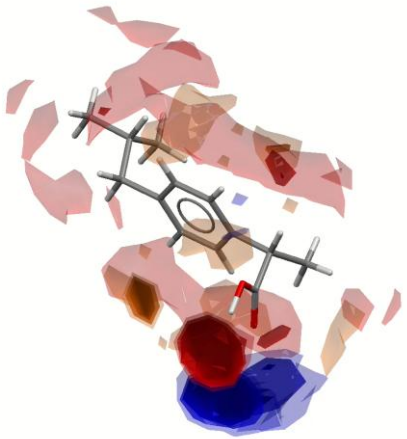


Learn about FIMs in this free online CSDU course

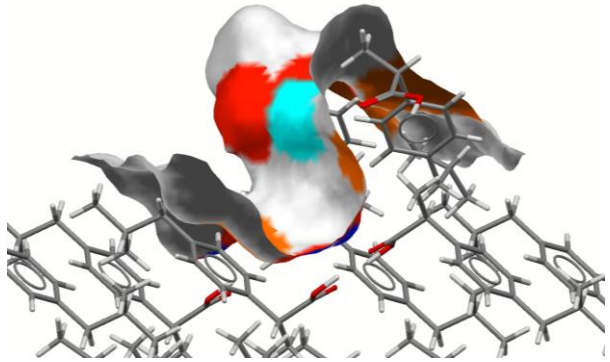
Wood P. A., *et al. CrystEngComm* (2013) **15**, 65-72.

CCDC

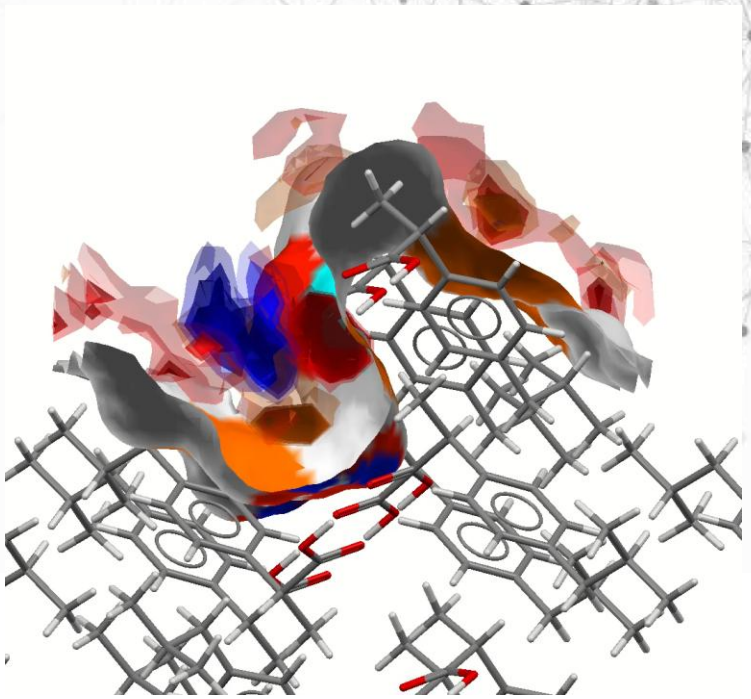
FIMs on Surface



FIM



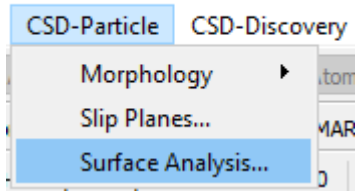
Surface

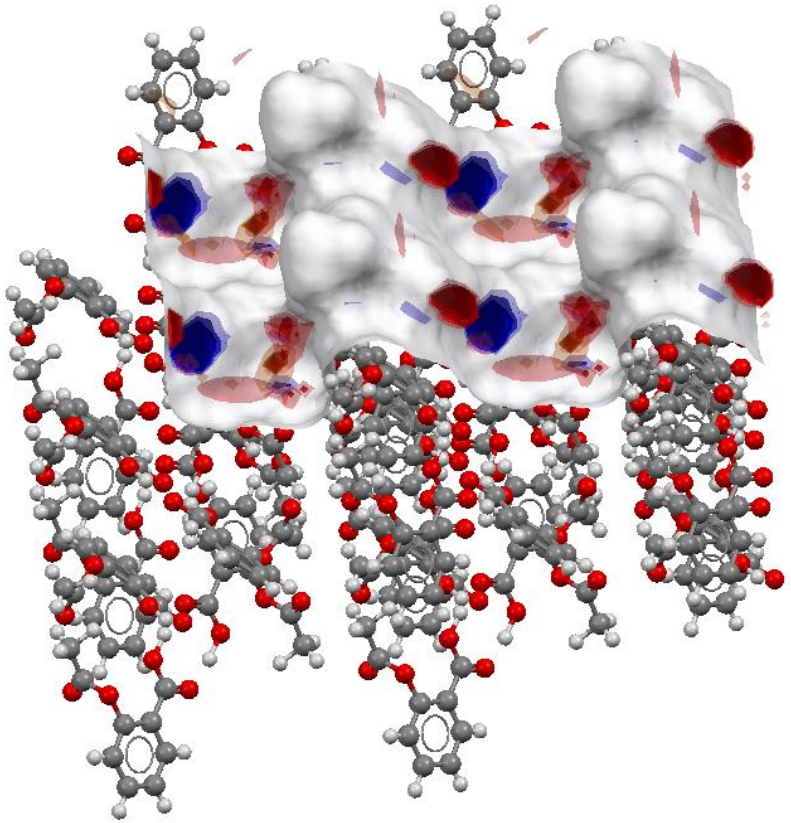


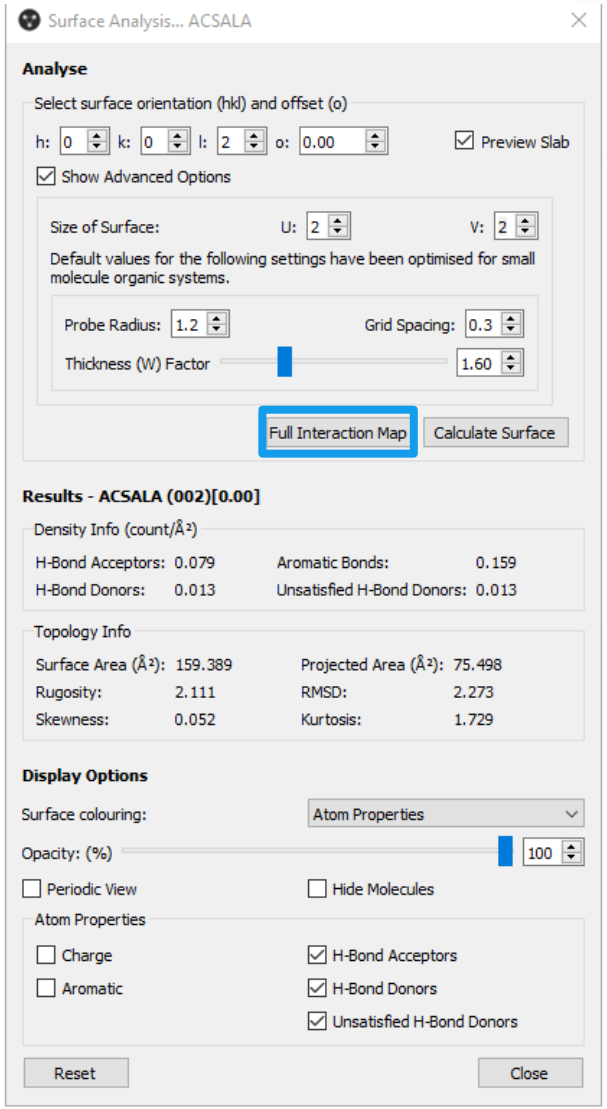
FIM on Surface

CCDC

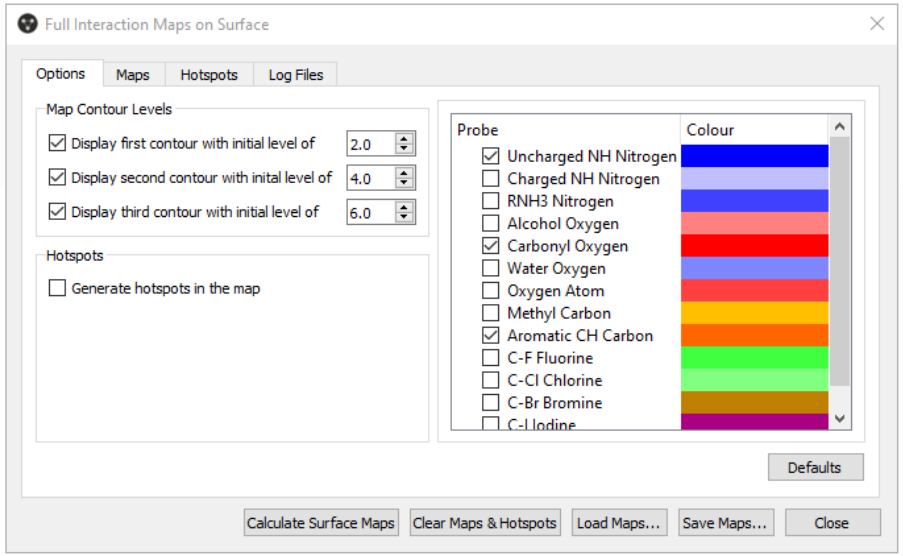
CSD-Particle – FIMs on Surface







Full Interaction Map on Surface



CCDC

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

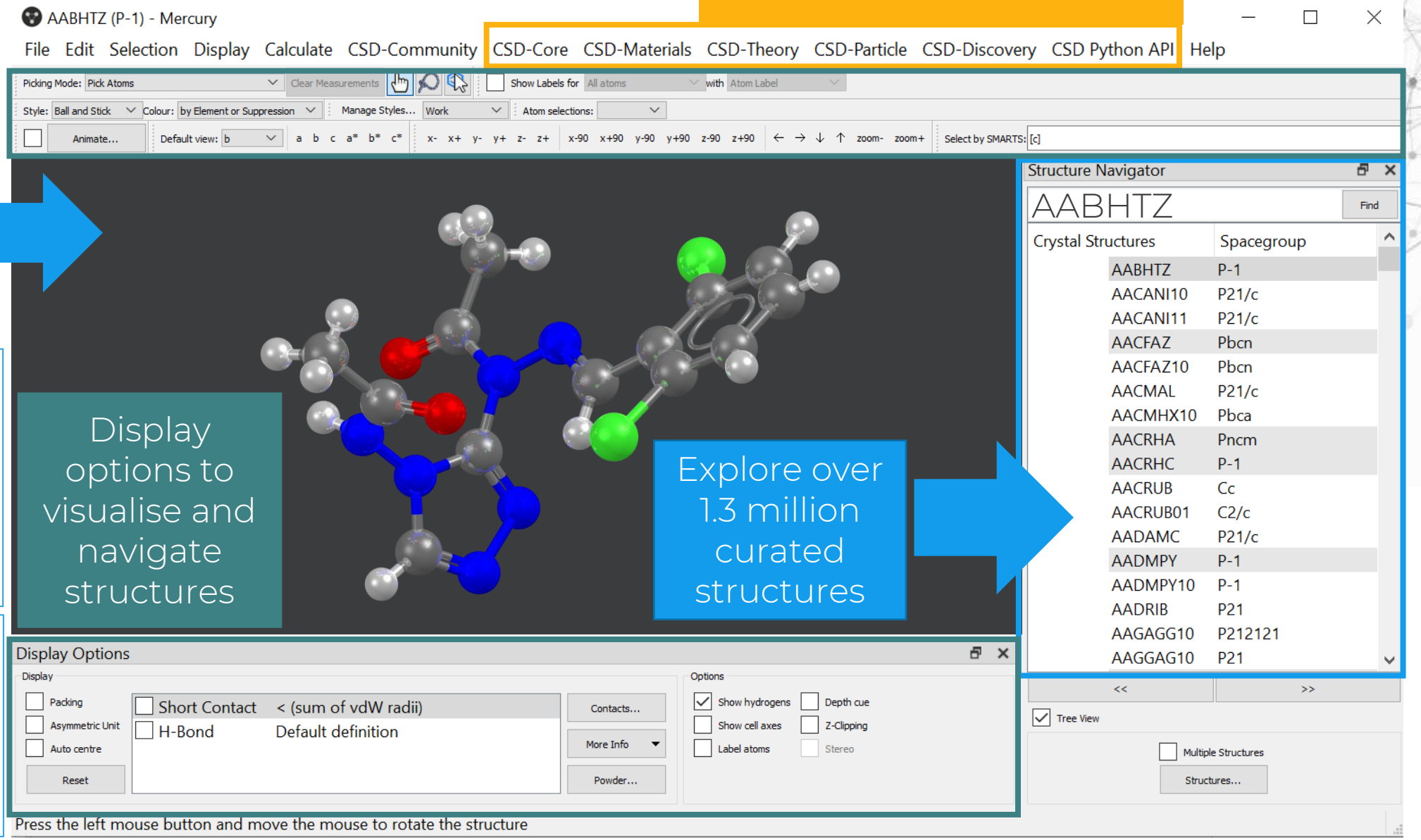
GitHub

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

CCDC

Mercury Overview

More advanced functionality to analyse and learn from structures

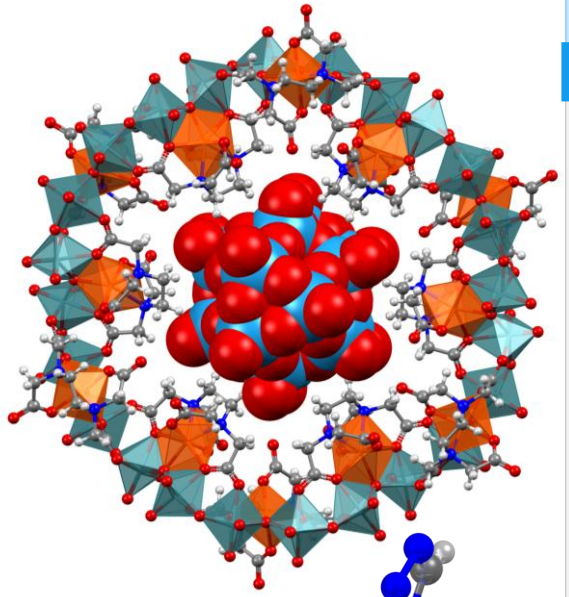


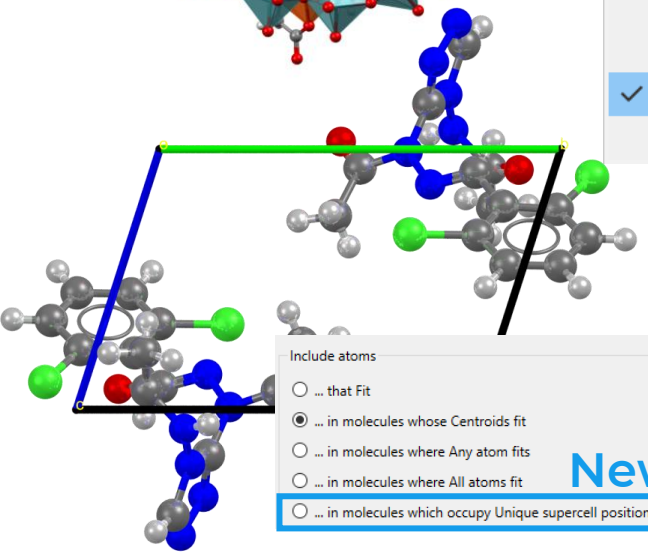
Mercury Visualisation 101

Learn more in this free online CSDU course

Self-guided exercises

Lots of display and analysis options!

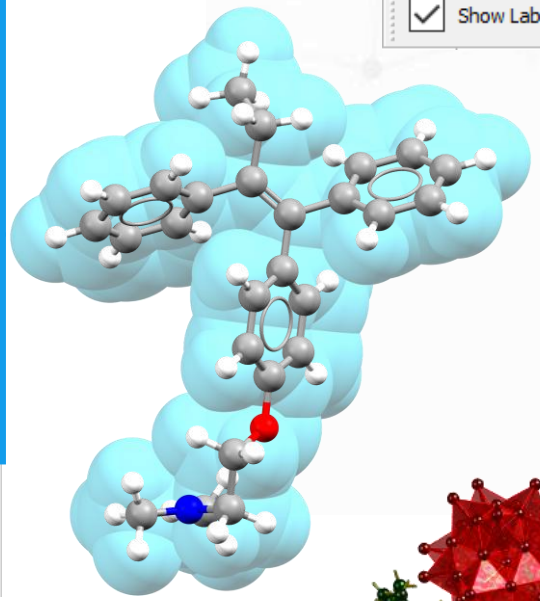




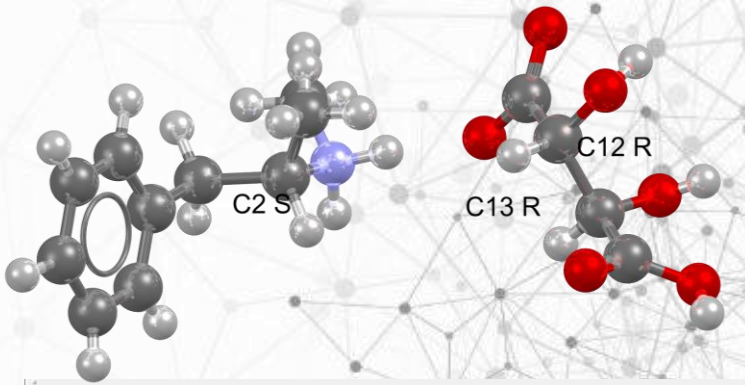
Display
- Styles
  - Wireframe
  - Stick
  - Ball and stick
  - Spacefill
  - Ellipsoid
  - Polyhedral
- Labels
- Colours
- Show/Hide
- More Information
- Symmetry Elements...
- Voids...
- Display Options...
- Manage Styles...
- View along
- Dial box...
- Spl
- Too

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

Stick settings...
Ball and Stick settings...
Spacefill settings...
Ellipsoid settings...
Polyhedral settings...
Contact settings...
Measurement settings...
ected atoms

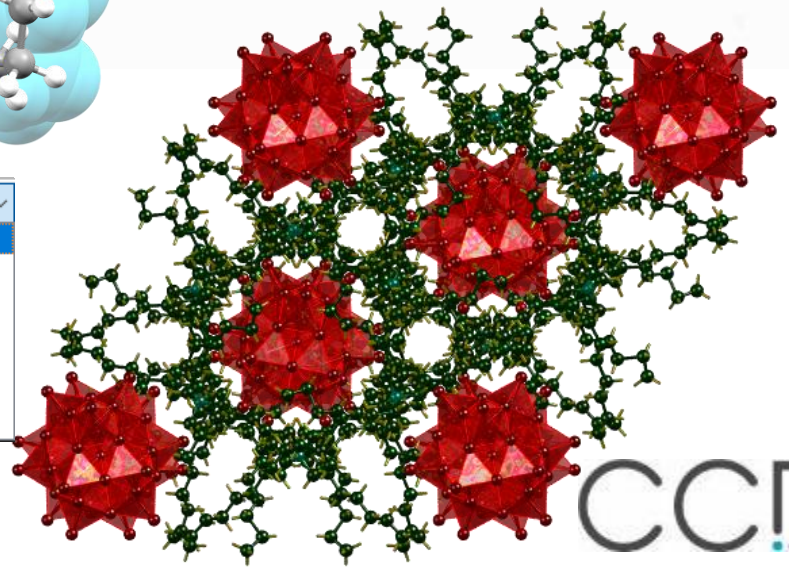


Colour: by Element or Suppression
- by Element
- by Symmetry equivalence
- by Atomic displacement
- by Symmetry operation
- by Gasteiger charge
- by Partial charge
- by Element or Suppression



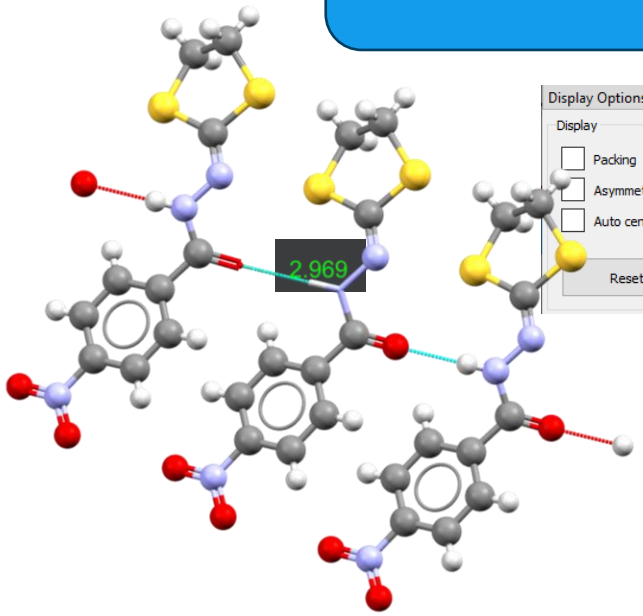
Show Labels for Stereocentres with Stereochemistry

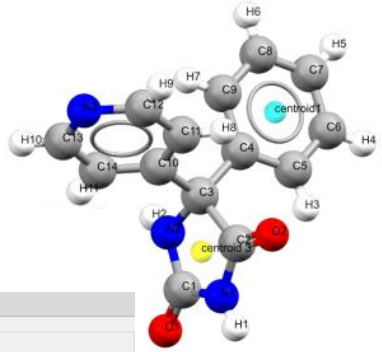
Watch the video on creating personalised styles

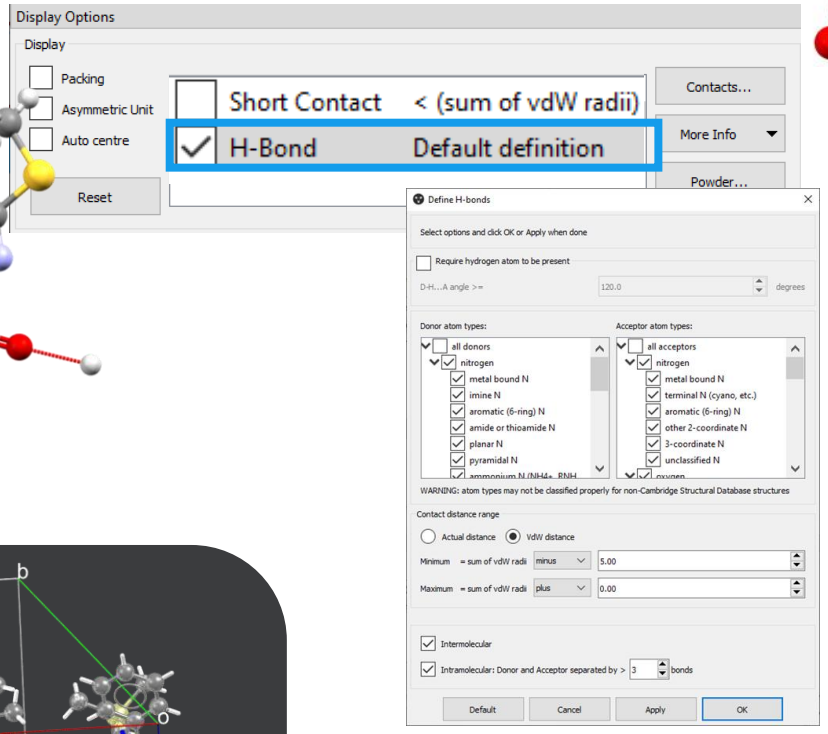


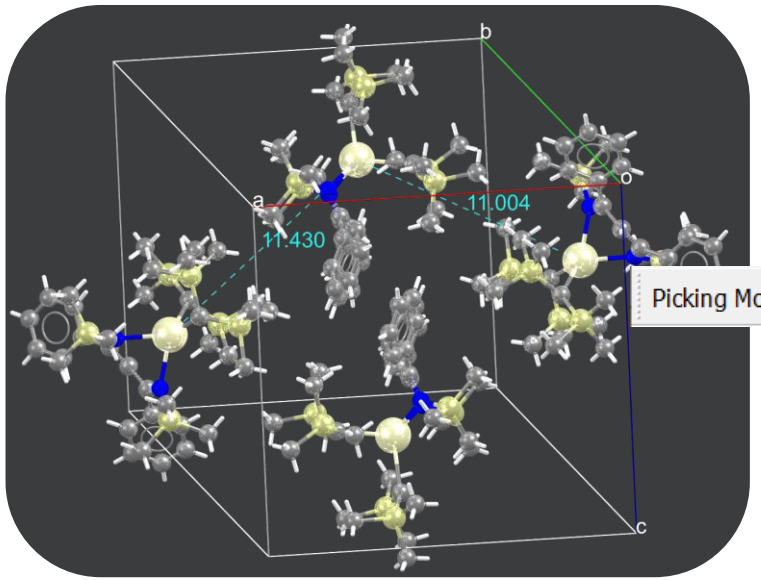
CCDC

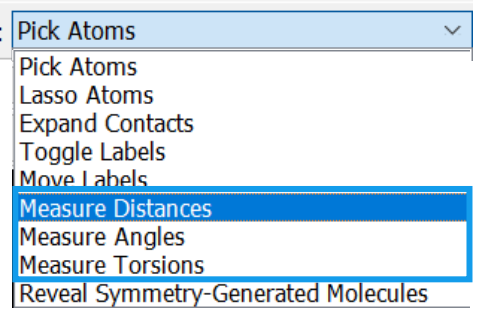
Lots of display and analysis options!

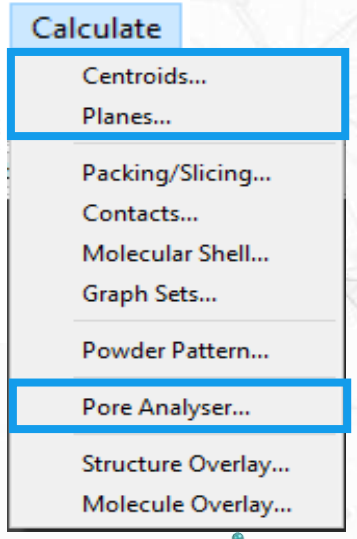


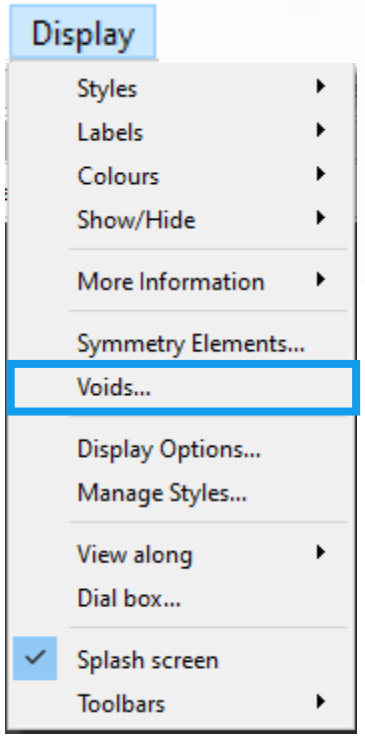


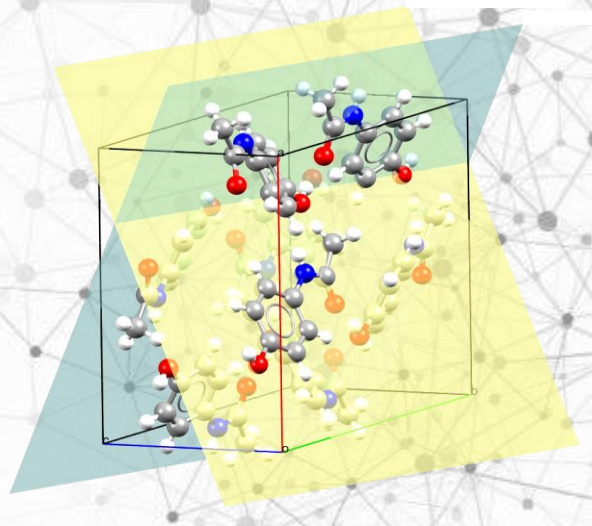


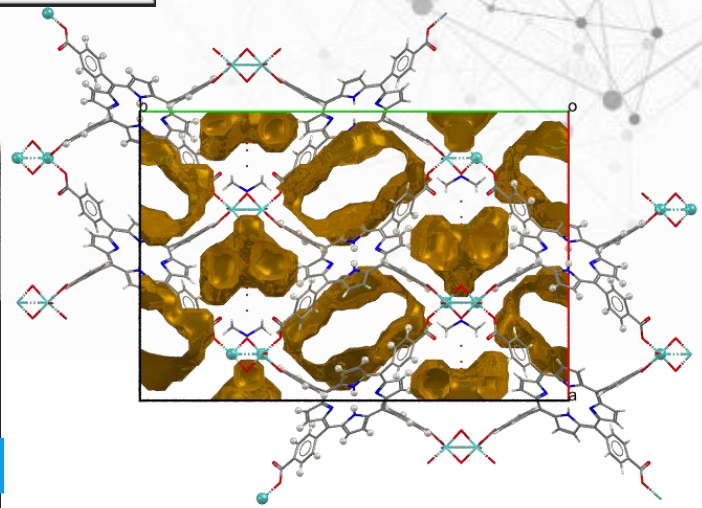








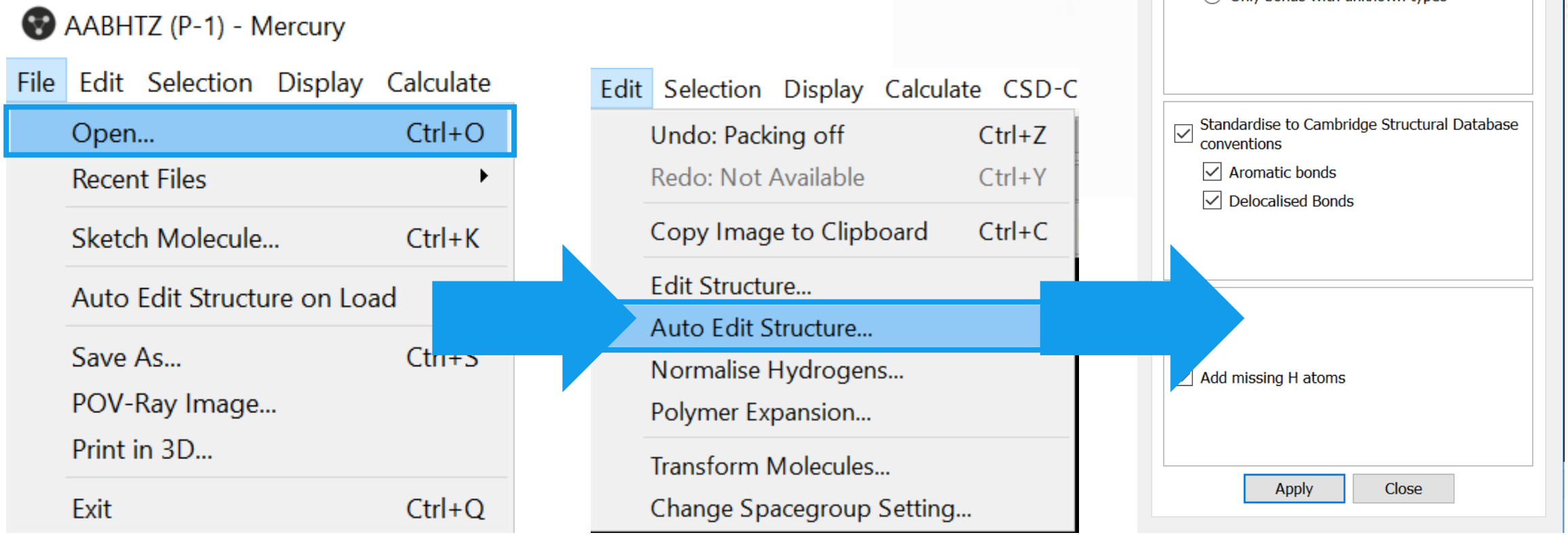




Watch the video on using voids and other functionality for porous materials

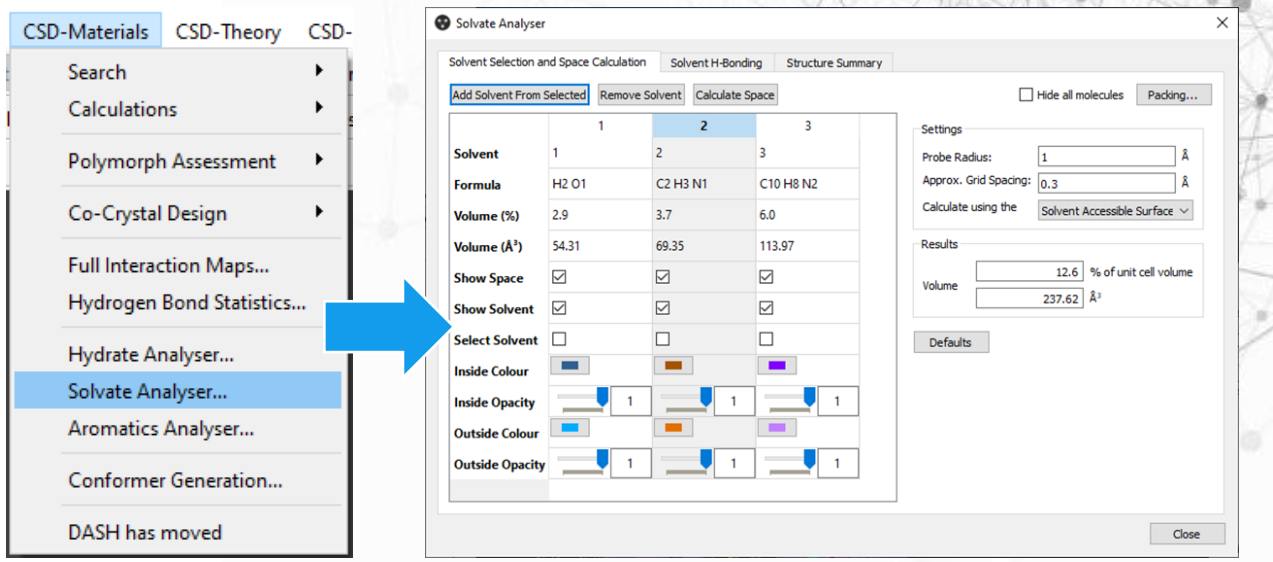
Using your own file or from the web

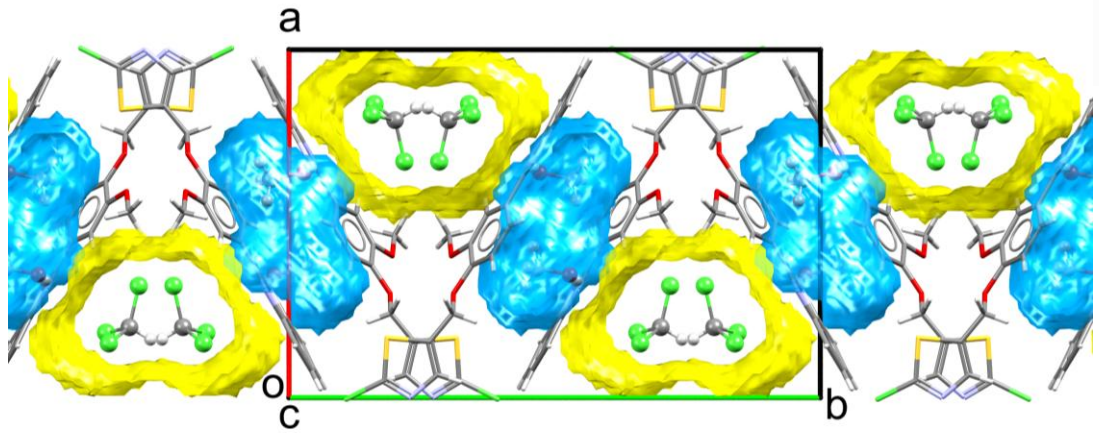
- File > Open – to open one of your own files for example a CIF
- Edit > Auto Edit Structure to assign bond types
- File > Auto Edit Structure on Load to automate



Solvate Analyser

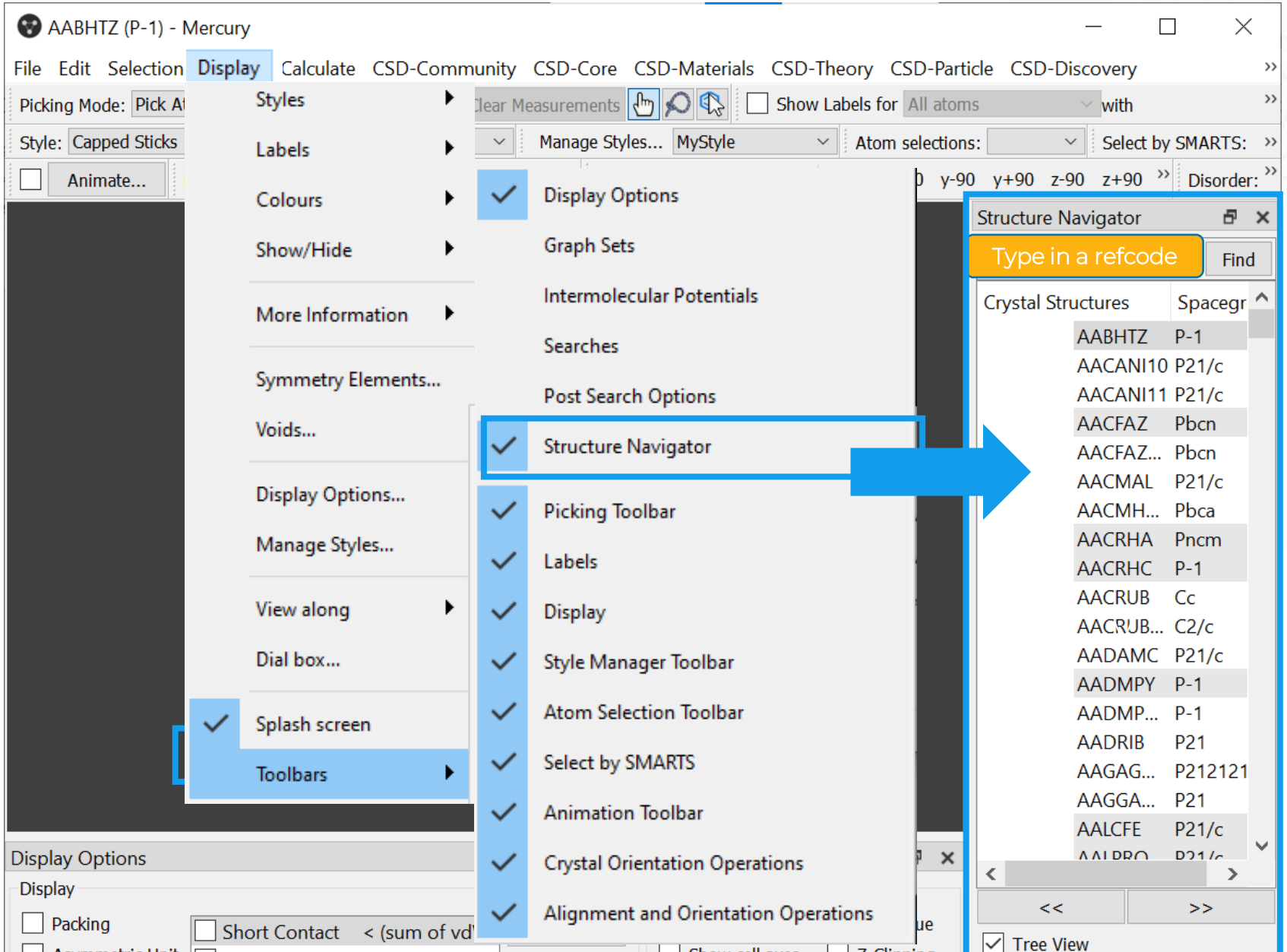
- **Calculation** and **display** of the space occupied by each of the different solvent molecules
- Easy selection of solvent molecule(s)
- **Assessment** of any hydrogen bonding motifs to/from the solvents
- Obtain reports
- Works **with disorder feature** producing different results based on the disorder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





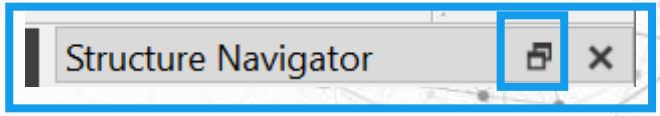
CCDC

Lost toolbars?



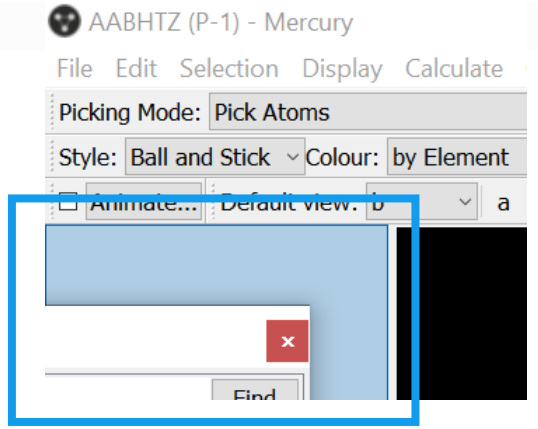
Extra Tip

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

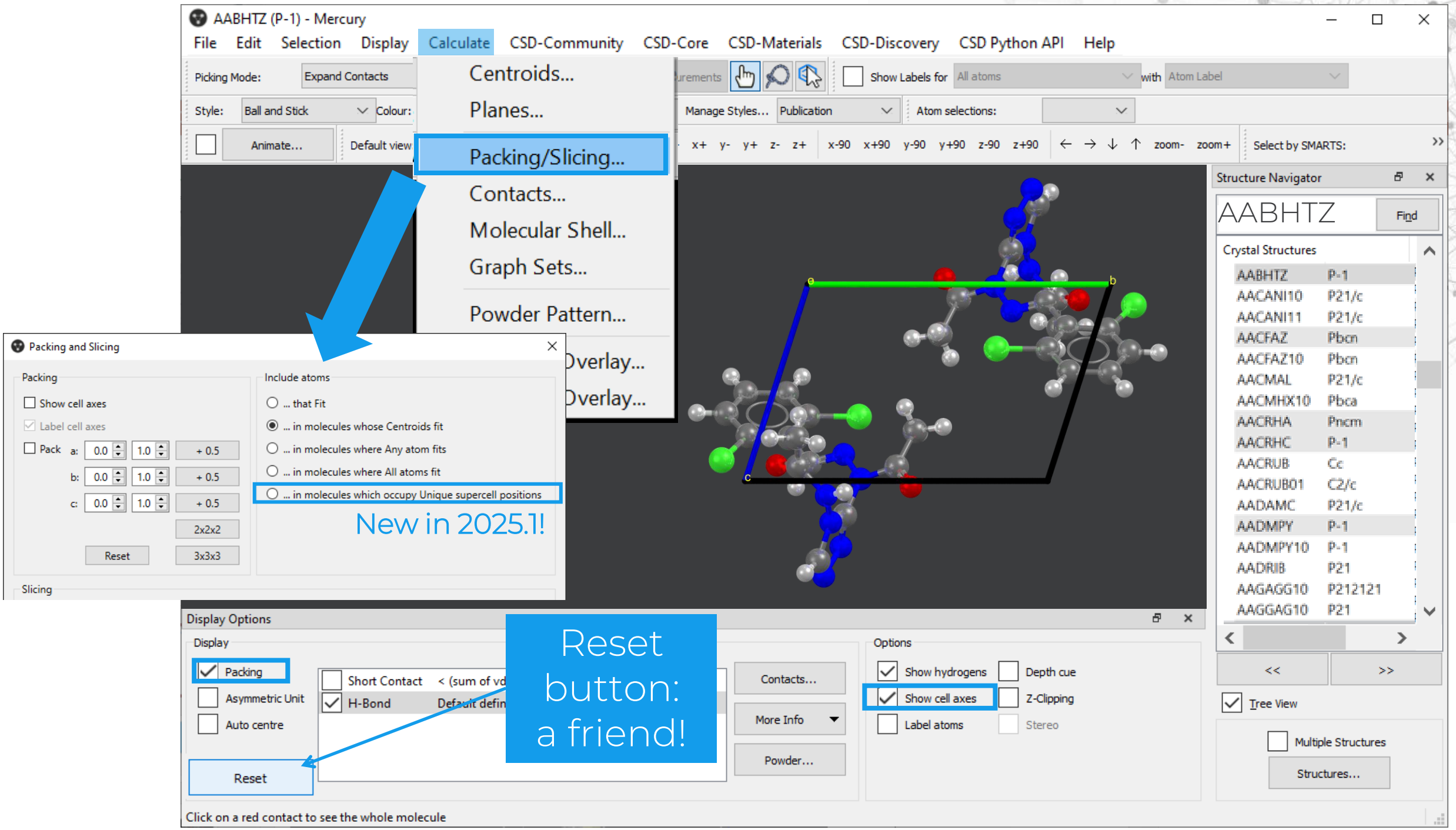


Extra Tip

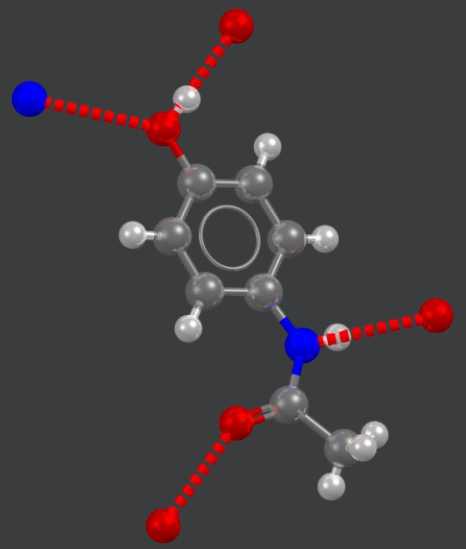
To pop the toolbar back in drag it to the area you want it.



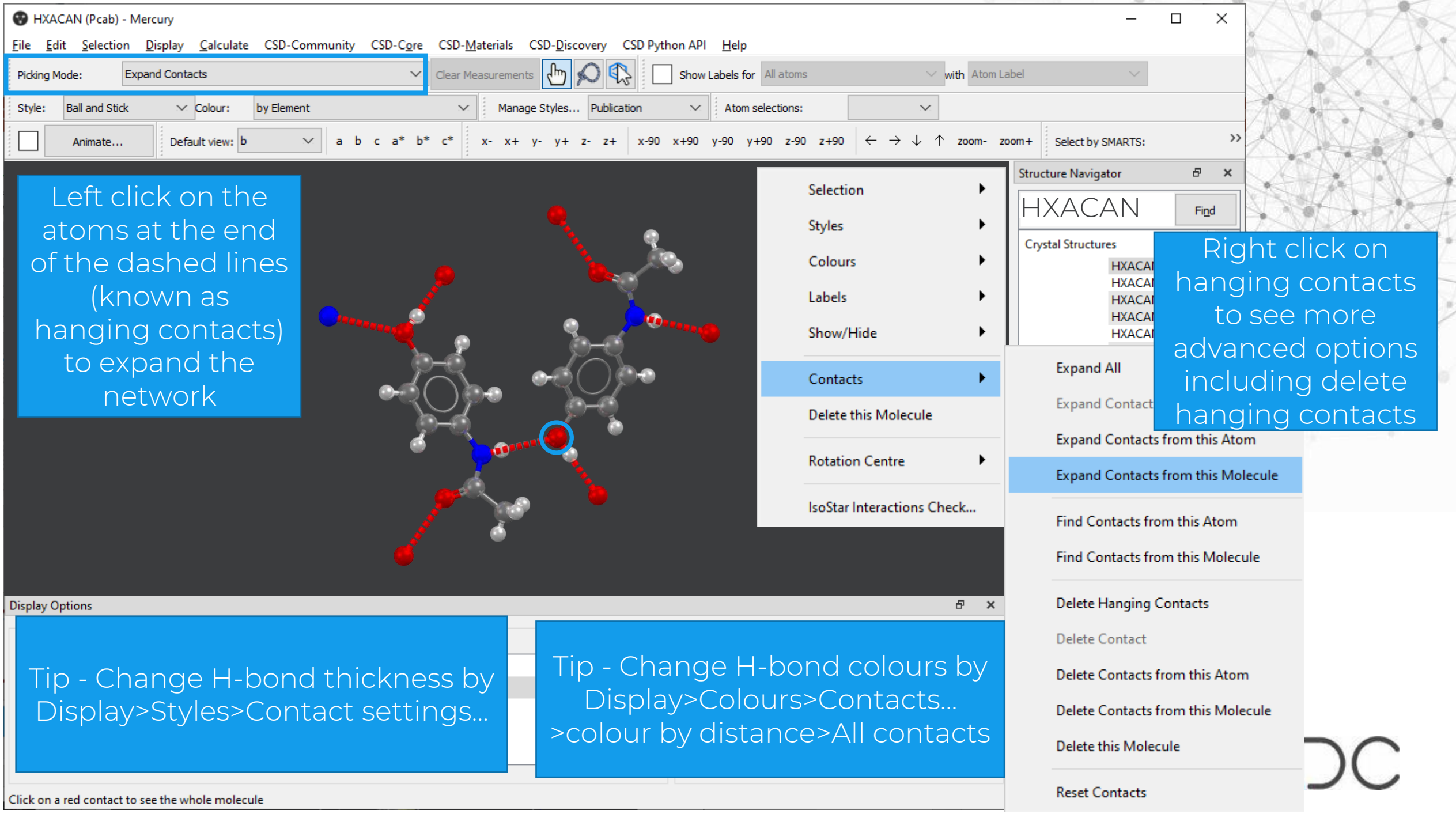
CCDC


AABHTZ (P-1) - Mercury
File Edit Selection Display Calculate CSD-Community CSD-Core CSD-Materials CSD-Discovery CSD Python API Help
Centroids...
Planes...
Packing/Slicing...
Contacts...
Molecular Shell...
Graph Sets...
Powder Pattern...
Packing and Slicing
Packing
Show cell axes
Label cell axes
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!
Reset
Slicing
Structure Navigator
AABHTZ
Find
Crystal Structures
Display Options
Display
Packing
Asymmetric Unit
Auto centre
Short Contact
H-Bond
Reset
Contacts...
More Info
Powder...
Options
Show hydrogens
Show cell axes
Label atoms
Depth cue
Z-Clipping
Stereo
Tree View
Multiple Structures
Structures...
Reset button: a friend!
Click on a red contact to see the whole molecule

Visualising hydrogen bonds



Click on “Default definition” to change the default H-bond definition


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 zoom- zoom+
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...
Structure Navigator
HXACAN
Find
Crystal Structures
Right click on hanging contacts to see more advanced options including delete hanging contacts
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

Agenda

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

- *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.

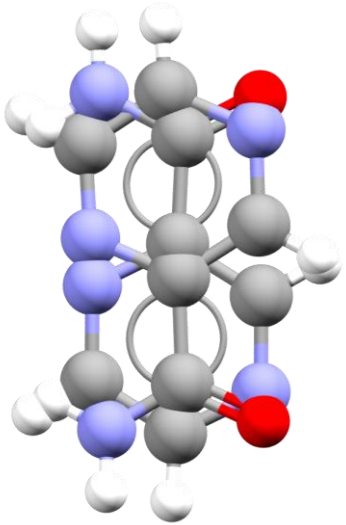
REC

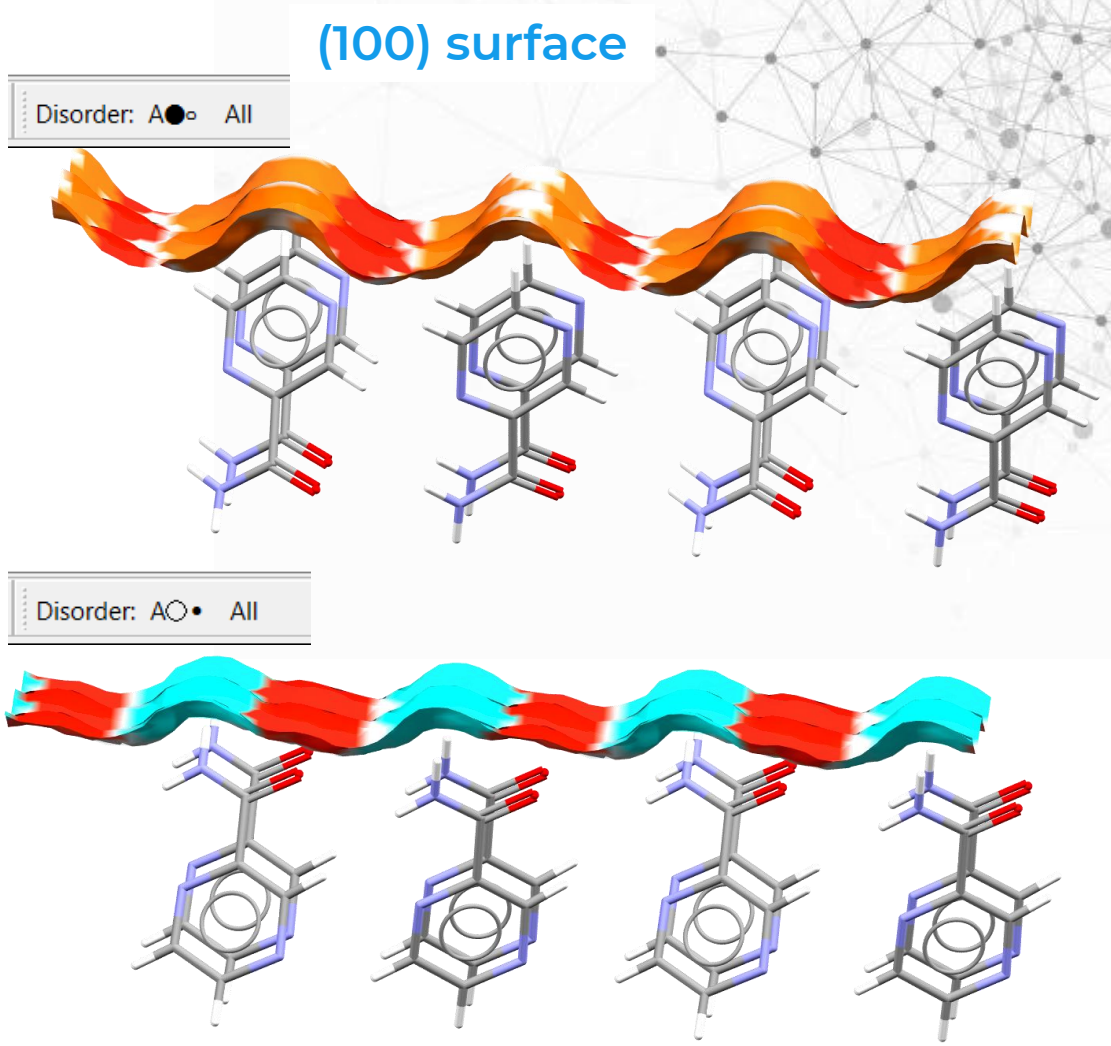
CCDC

Using Surface Analysis with disordered structures

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

CSD refcode:
PYRZIN19

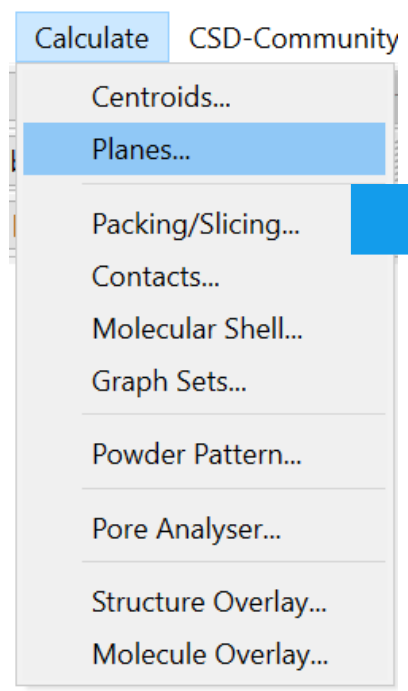


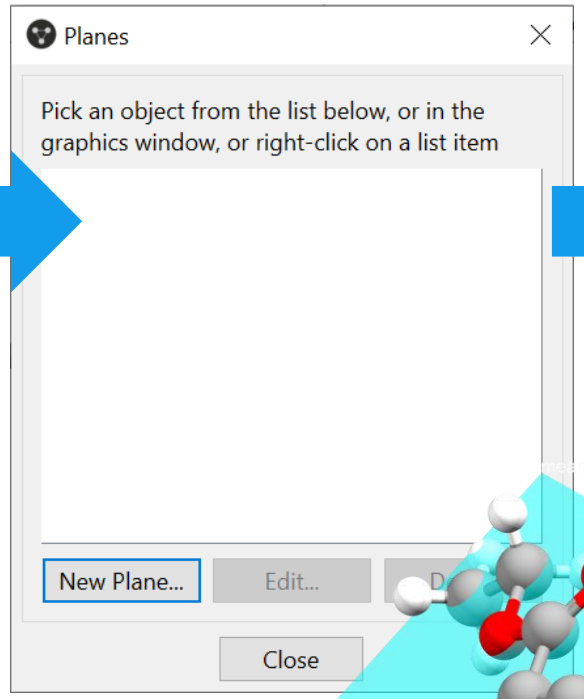


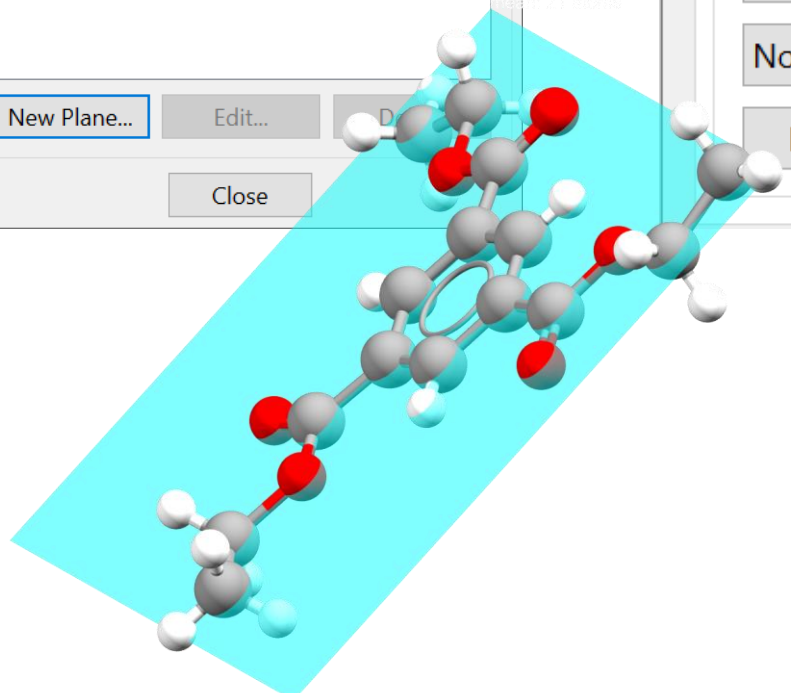
We learnt more about disorder in the previous Virtual Workshop!

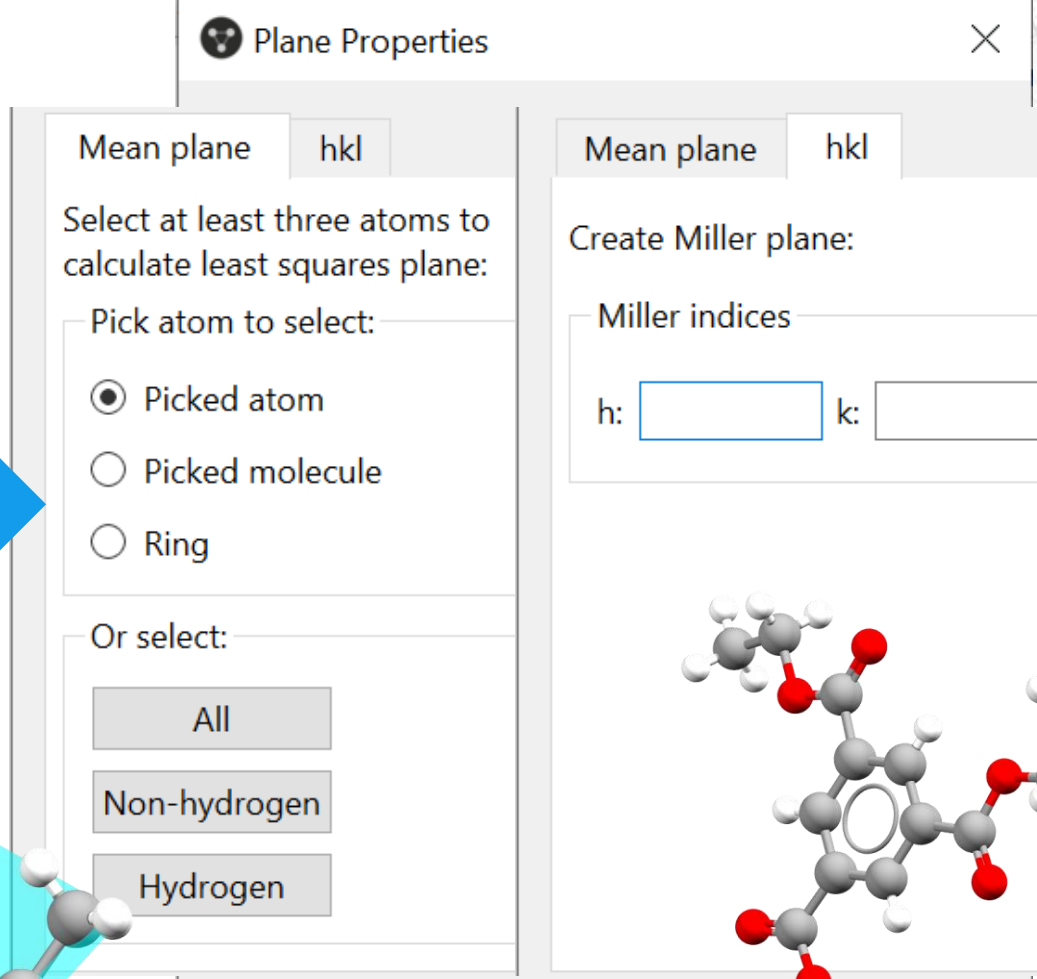
CCDC

Calculating planes

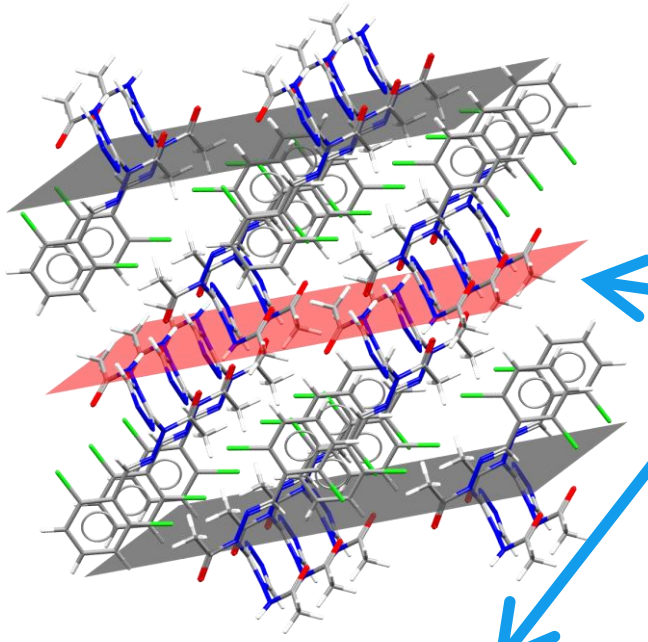


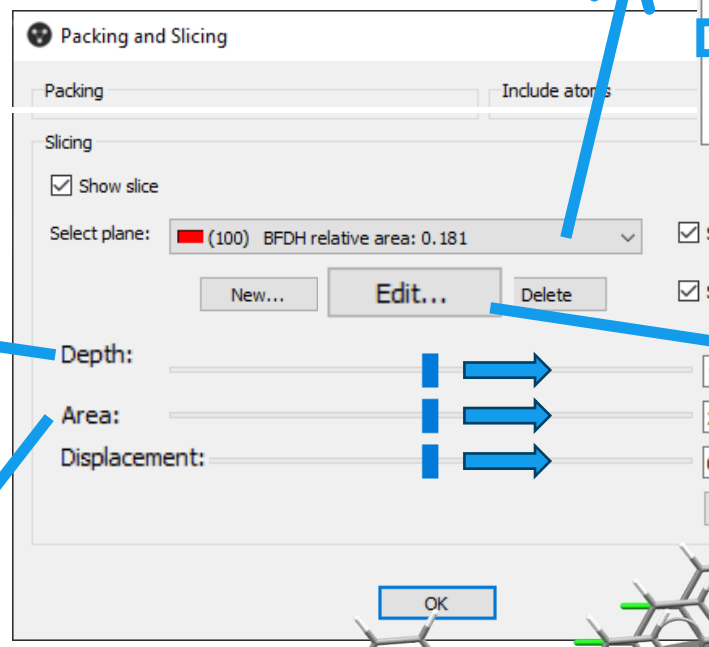


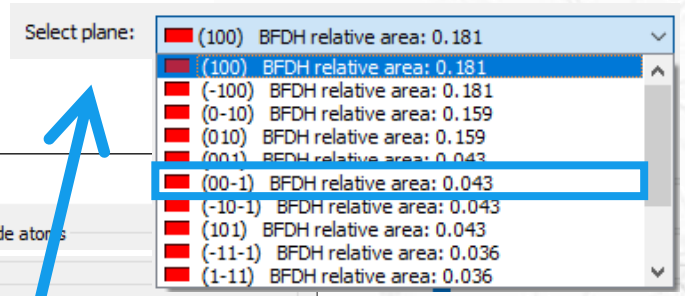


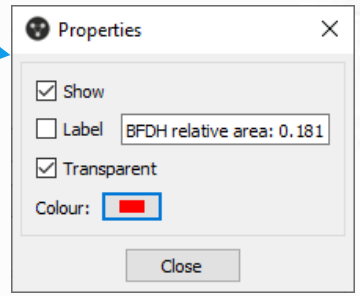


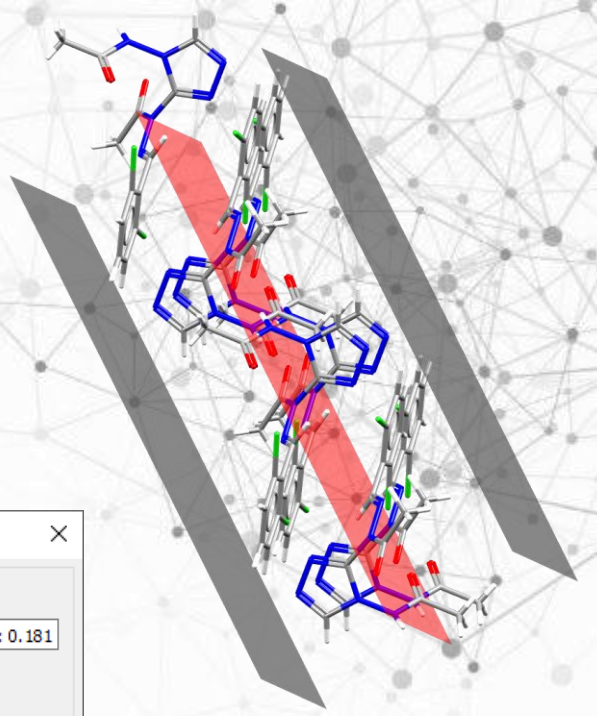
Slicing

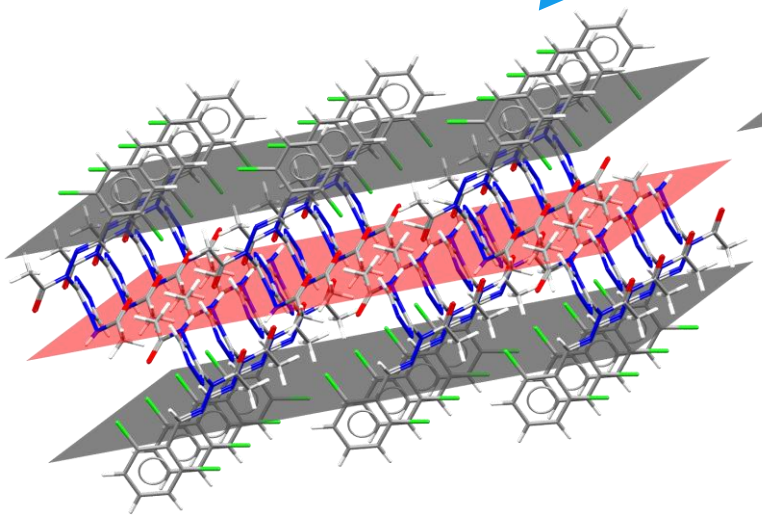


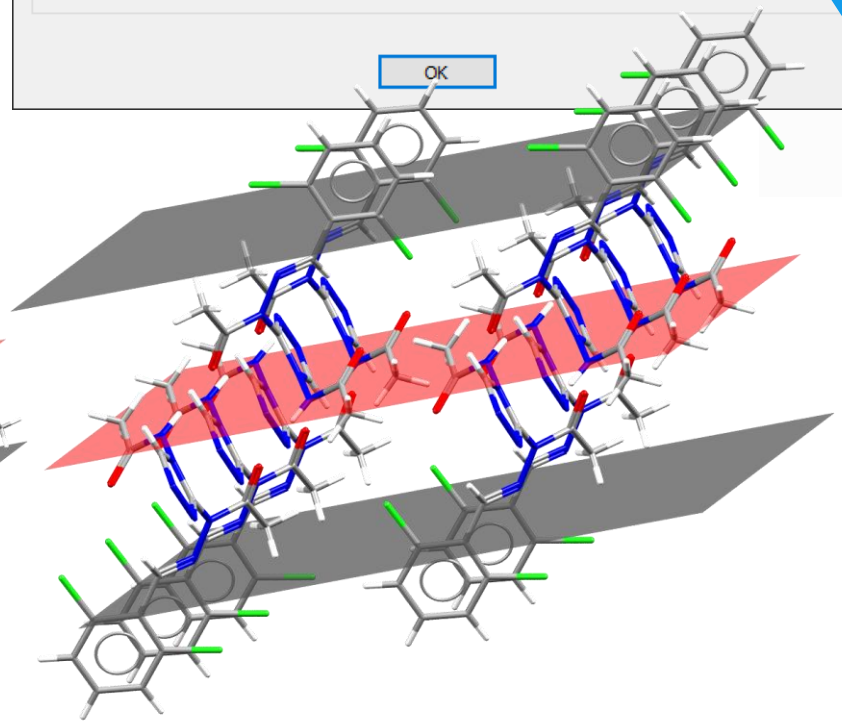


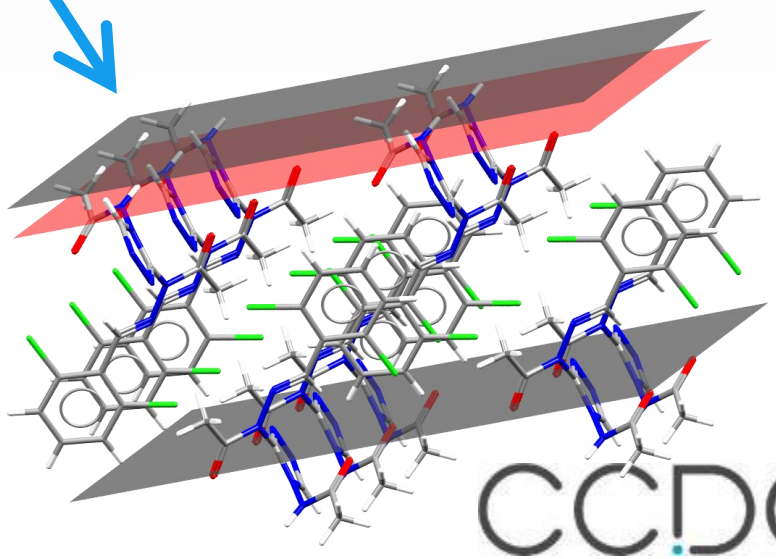












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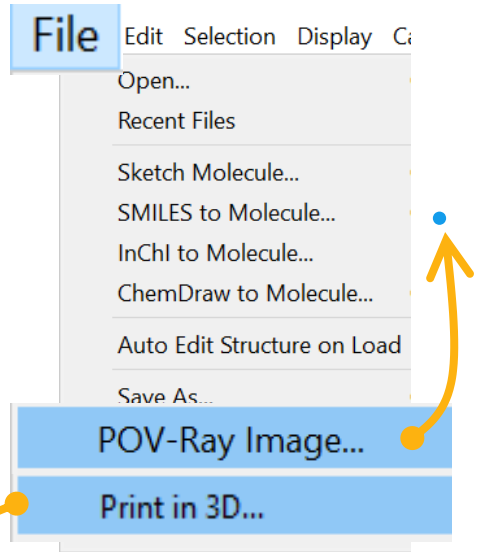
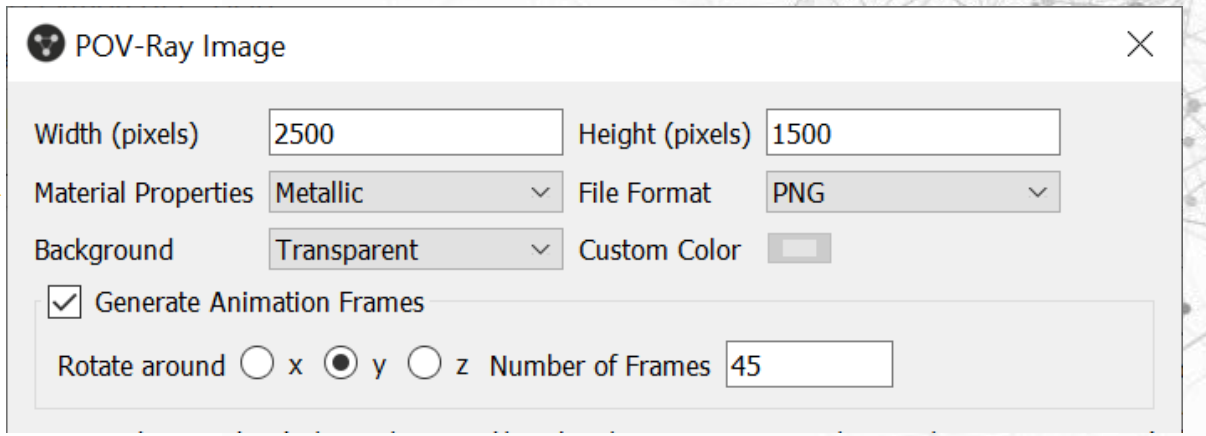
Features for effective visualization

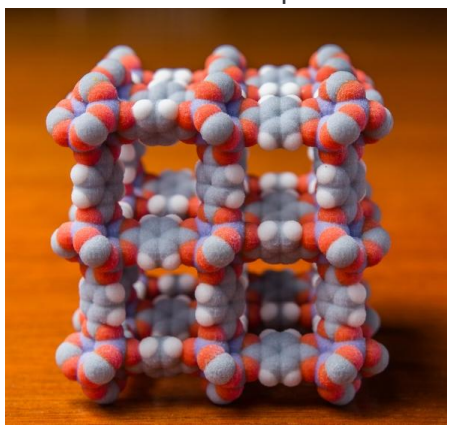


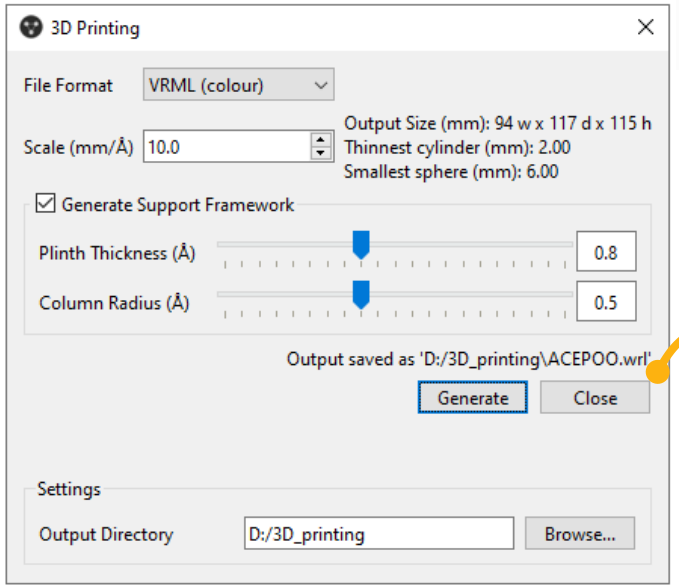
- Create high resolution images and frames for video or gifs

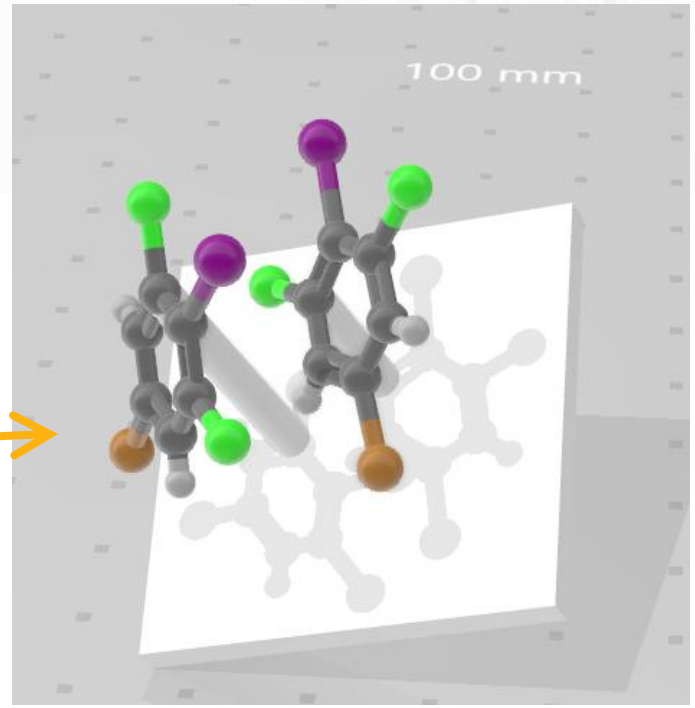


- Create files for 3D print

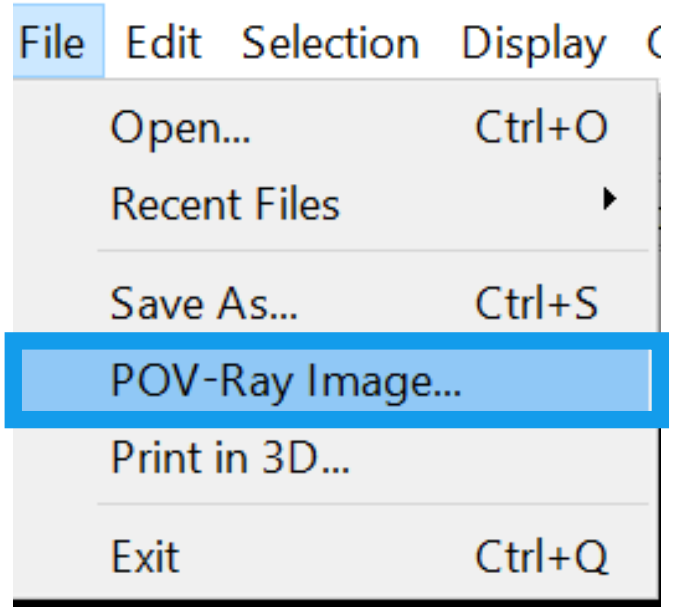
Example of 3D printed structure of CSD Refcode SAHYIK

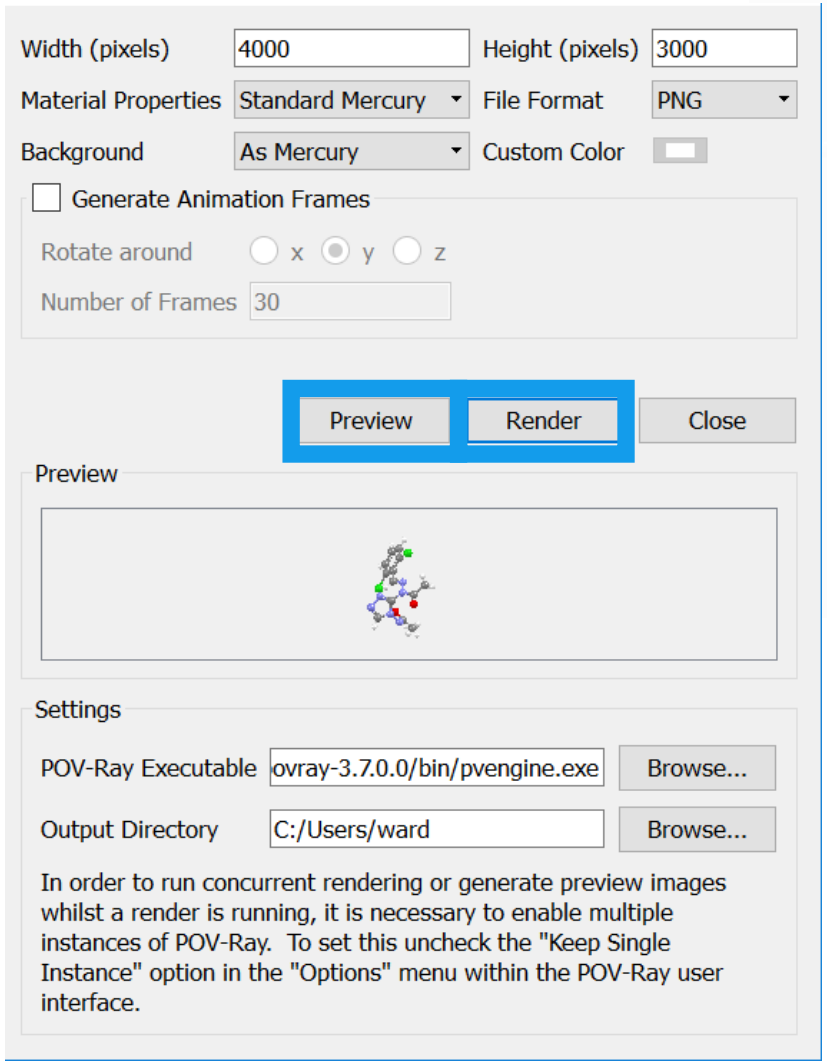






Generating high quality images





File > POV-Ray Image

Change Resolution

- Width = 4000
- Height = 3000

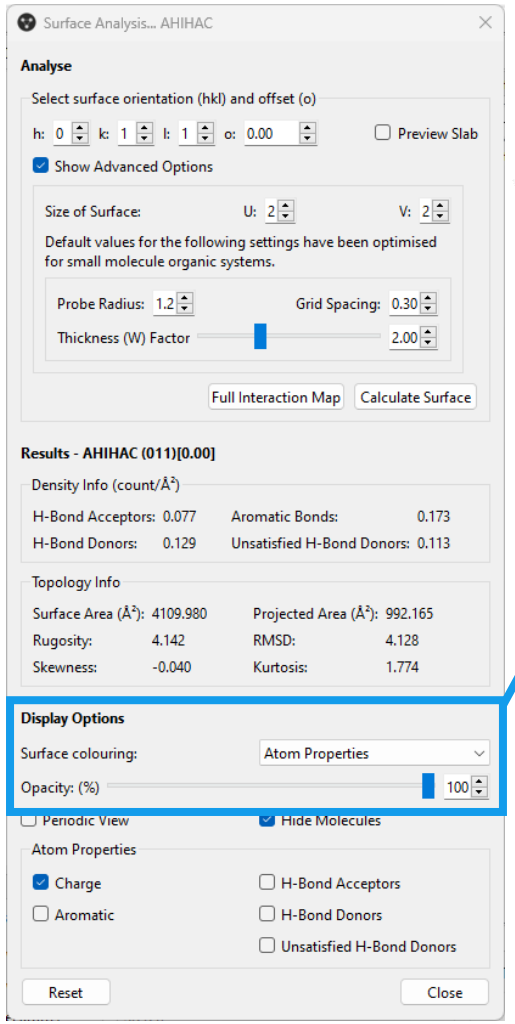
Change ‘Material Properties’ to ‘Metallic’

Set ‘Background’ to ‘Transparent’

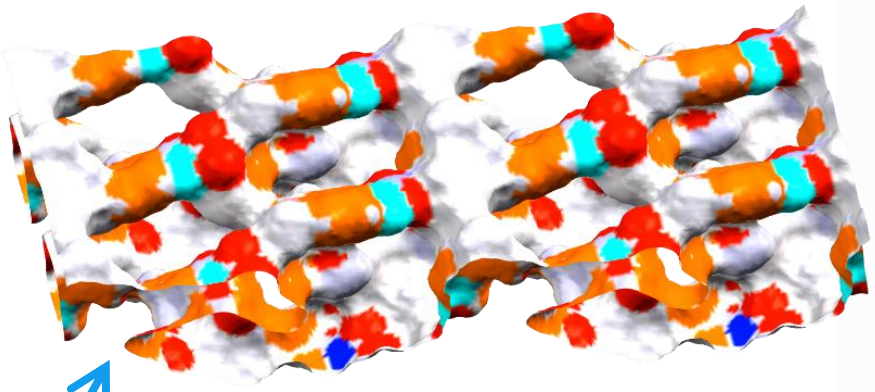
Press ‘Preview’

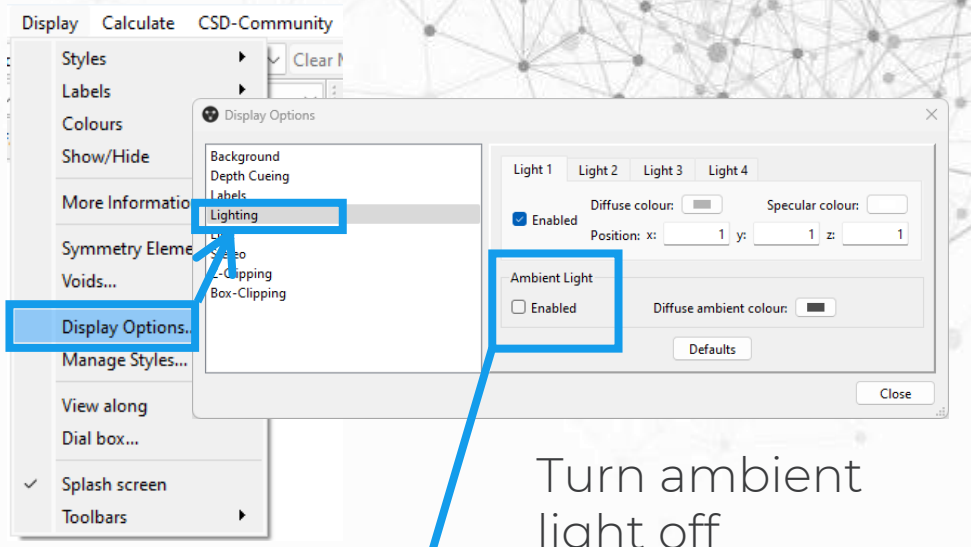
CCDC

Optimising display settings



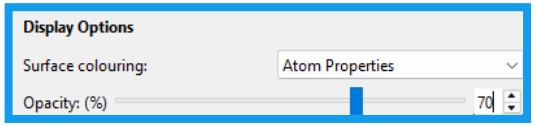
AHIHAC (011)[0.00] – default settings

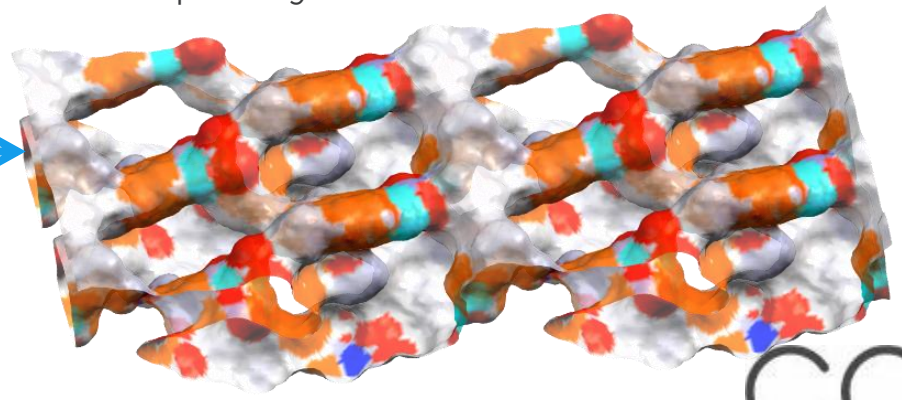




Turn ambient light off

Surface opacity at 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

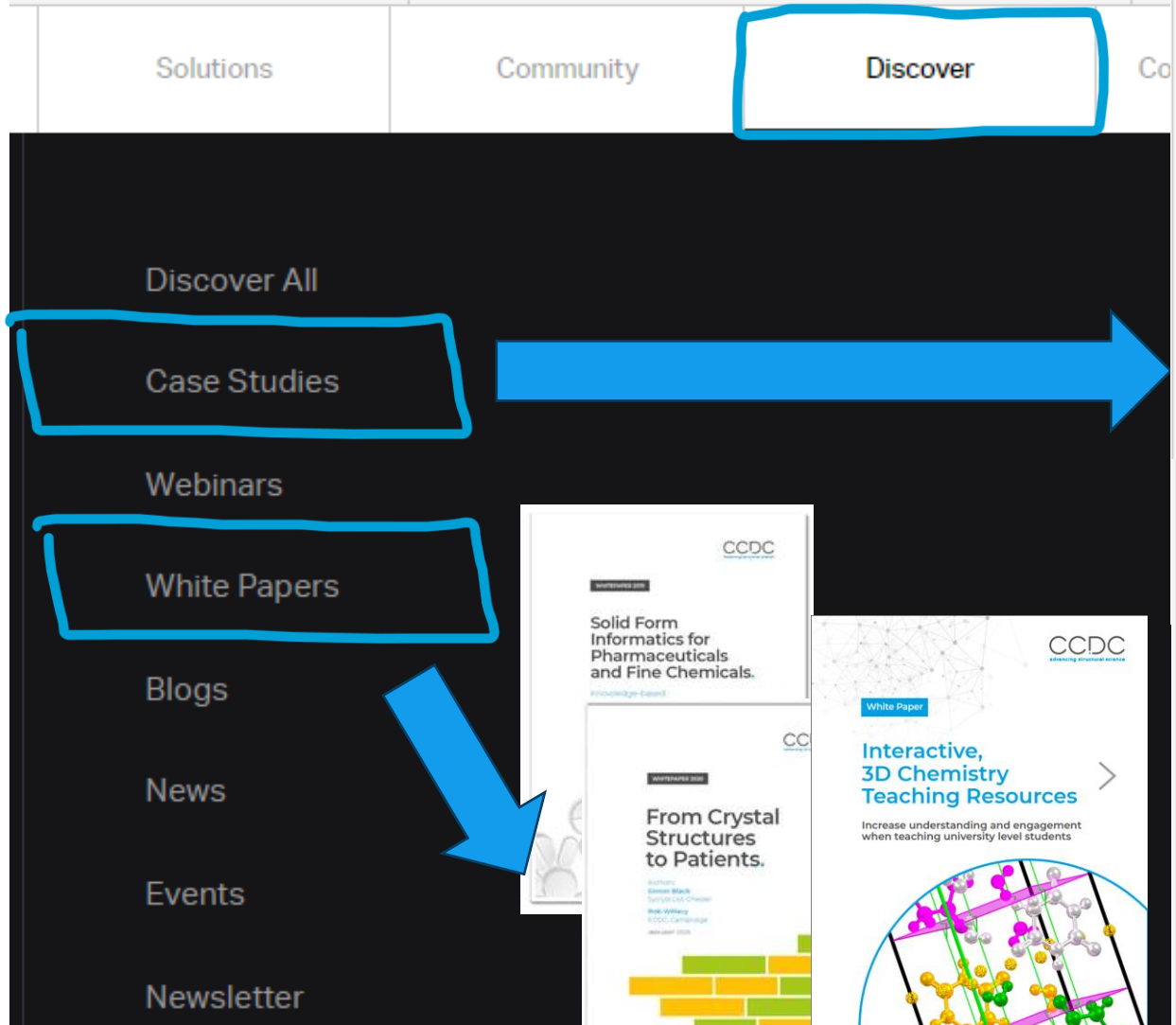
Legacy and Future Impact of the Cambridge Structural Database: A Tribute to Dr. Olga Kennard - special issue

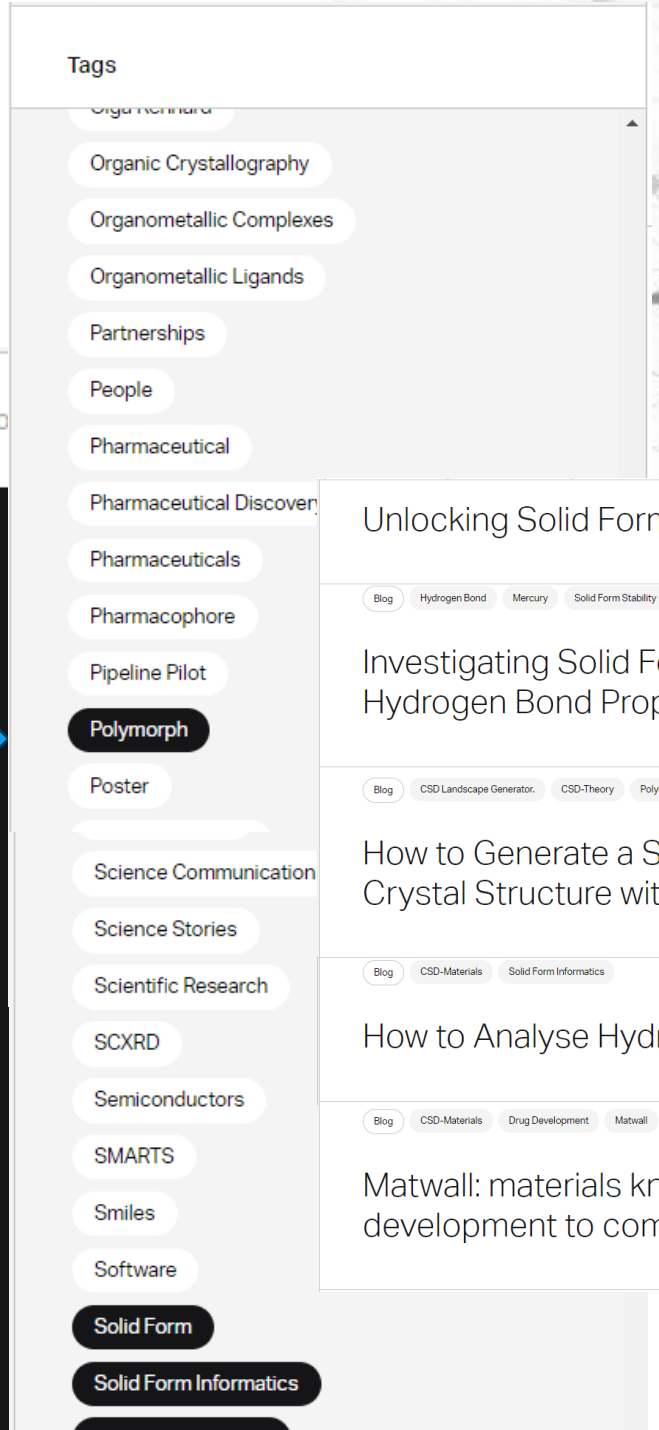
- 29 articles from industry and academia

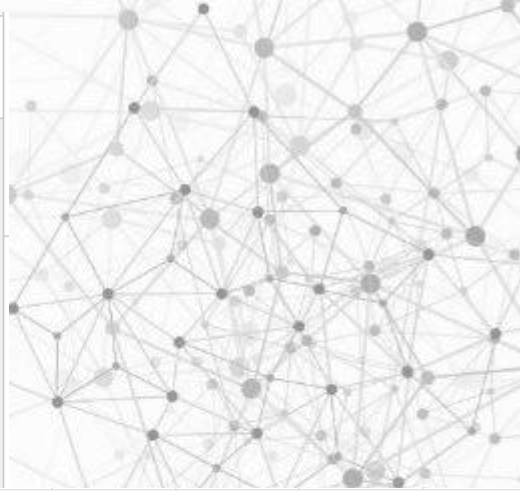
CRYSTAL GROWTH & DESIGN

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

More case studies







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 Hydr

Blog CSD-Materials Drug Development Matwall

Matwall: materials knc
development to comr

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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]
- **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

More reference papers for CSD-Particle

More reference papers for CSD Software

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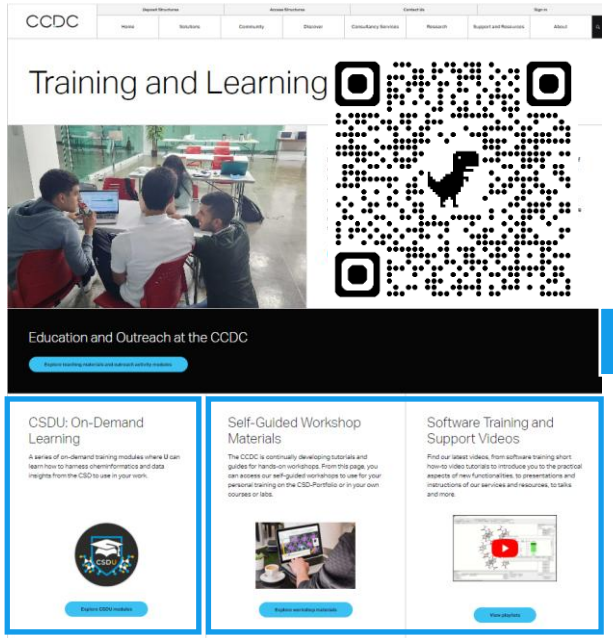
What we have learnt

- ✓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?

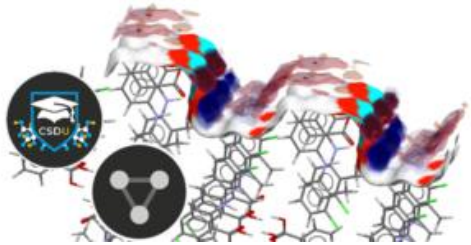
Training and learning



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

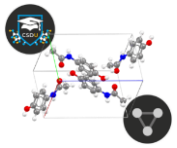
CSDU

Learn on demand with free online training courses

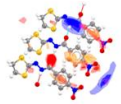


- Free
- Completion certificate upon passing a final test.
- In-depth review of today's topics and more software.

CSD Python API

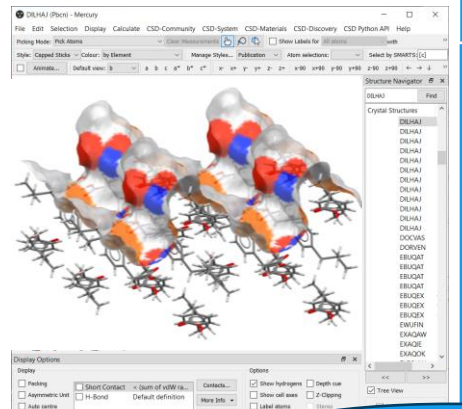


Basics of Mercury



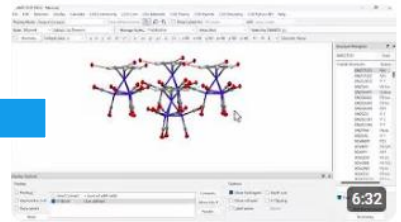
Full Interaction Maps

Self-guided workshops



Videos

YouTube channel



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

How to: Build and combine searches in ConQuest

And more!

https://www.ccdc.cam.ac.uk/community/training-and-learning/

Want to explore more?

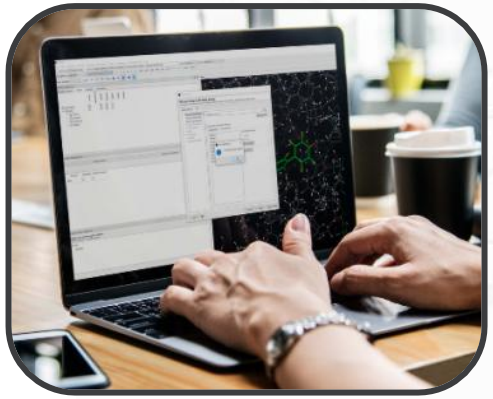
CCDC Virtual Workshops

- **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.



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Technical and scientific support

Getting set up
Technical support
Scientific questions

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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/*

Email
admin@ccdc.cam.ac.uk

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