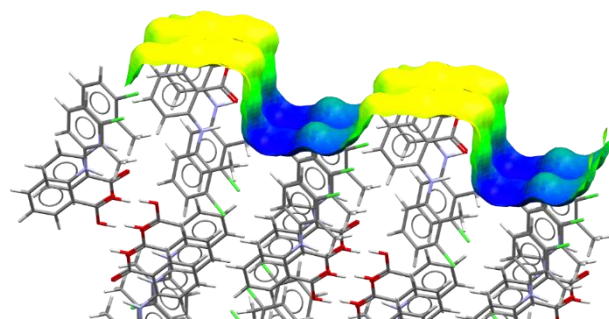


Surface Analysis with CSD-Particle Tools in Mercury

Developed using
2024.1 CSD Release



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advancing structural science

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Introduction

This workshop shows you how to use functionality from the CSD-Particle suite to visualize and analyse the mechanical and chemical properties of molecular crystals. It uses quick computational models and algorithms, alongside data from the Cambridge Structural Database (CSD), to provide both qualitative and quantitative analyses of particle shape as well as surface and bulk properties. Such features are found under the CSD-Particle menu in Mercury.

Before beginning this workshop, ensure that you have a registered copy of CSD-Materials or CSD-Enterprise installed on your computer. Please contact your site administrator or workshop host for further information.

Learning Outcomes

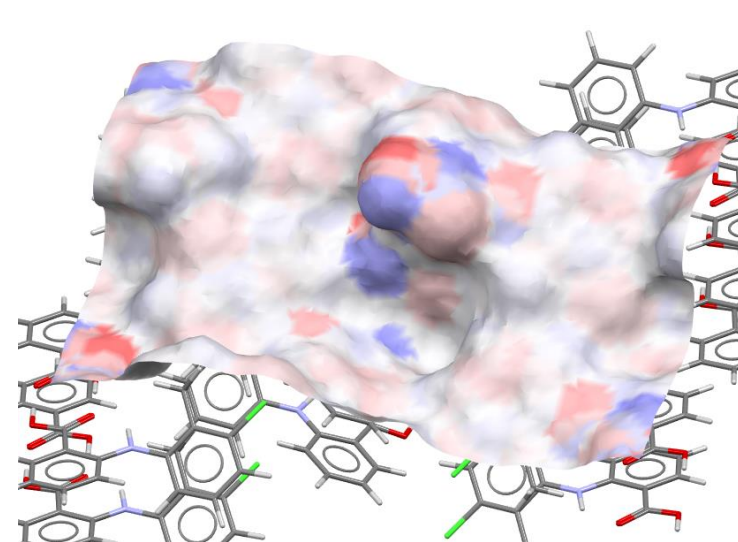
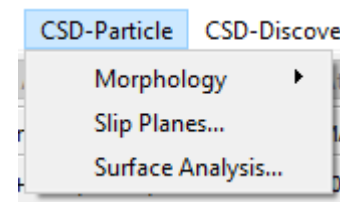
At the end of this workshop, you will be able to:

- Analyse particle surfaces.
- Calculate Full Interaction Maps on surfaces.
- Identify and analyse potential slip planes.

Note: The words in *Blue Italic* in the text are reported in the [Glossary](#) at the end of this handout. During the Virtual Workshop Try One part, work on one of the examples – you can pick the one on the components you are the most interested in. If you finish early, you may start a new example (if you have done example 1 or example 2, we suggest you then try example 3), or you can return to any of the examples at another time.

Pre-required Skills

The following exercises assume you have a working knowledge of the basics of visualizing structures with Mercury, namely, how to display and manipulate structures from a 3D coordinates file. Familiarity with Full Interaction Maps (FIMs) would also be helpful (See FIMs workshop [MER-002](#) and [CSDU module](#)). A basic review of the Mercury interface is provided at the end of this handout.

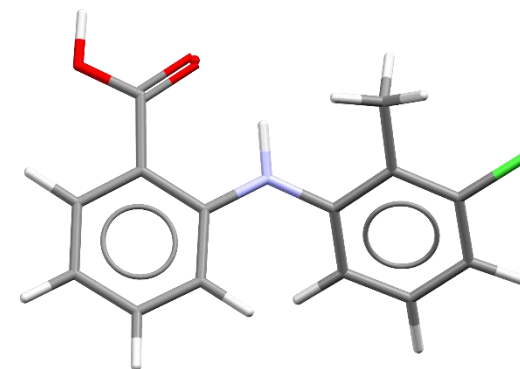


Materials


There are no additional materials required for this workshop.

Example 1. Surface Analysis

In this example, we will employ tools from the *Surface Analysis* feature in CSD-Particle to investigate two different surfaces of a 2-(3-chloro-2-methylanilino)benzoic acid crystal. The two surfaces under investigation are the (110) and the (020). By calculating these two surfaces and analysing their properties and the chemistry on each surface, we will learn more about their activities.



CSD Entry KAXXAI10 2-(3-chloro-2-methylanilino)benzoic acid

1. Open Mercury by double-clicking the Mercury icon  on the desktop.
2. In the **Structure Navigator** toolbar type the refcode KAXXAI10.

BFDH Morphology

3. We want to identify facets of interest in this morphology. We will first create the morphology using the [BFDH morphology](#) feature.
4. From the top-level menu select **CSD-Particle > Morphology > BFDH...** to generate the morphology. BFDH morphology uses the unit cell to create the morphology you see, therefore it does not account for the chemistry of the structure.
5. Rotate the structure to view the various facets that have been generated. For this exercise, we will explore two facets: (020) and (110). If you wish, explore options in the *Morphology* menu. Once you are ready to continue, close the *Morphology* menu and click the *Reset* button from the *Display Options* menu to return to the structure view.
6. The first surface that we will explore is the (110) facet.

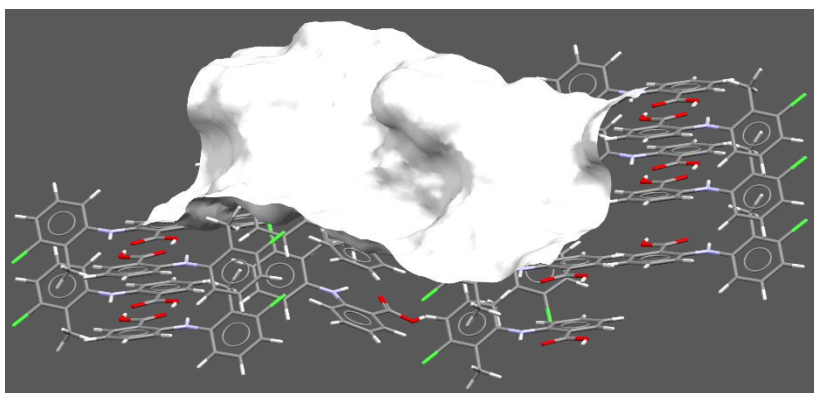
The screenshot illustrates the workflow in Mercury for generating a BFDH morphology and viewing specific facets. It includes the following elements:

- Step 1:** The Mercury icon on the desktop.
- Step 2:** The **Structure Navigator** window showing the search for refcode KAXXAI10. The results table is as follows:

Crystal Structures	Spacegroup
KAXXAI10	P21/n
KAXXAI11	P21/c
- Step 4:** The **CSD-Particle > Morphology > BFDH...** menu path.
- Step 5:** The **Display Options** window with the **Reset** button highlighted. The window contains checkboxes for Packing, Asymmetric Unit, Auto centre, Short Contact, and H-Bond, along with a text field for 'User defined'.
- Morphology View:** A 3D model of the crystal morphology with various facets labeled with Miller indices: (1-1-1), (1-10), (10-1), (11-1), (110), (101), (0-1-1), (0-20), (0-11), (01-1), (011), (-1-1-1), (-1-10), (-1-11), (-10-1), (-101), (-110), and (-111). The (020) facet is specifically highlighted with a red arrow.

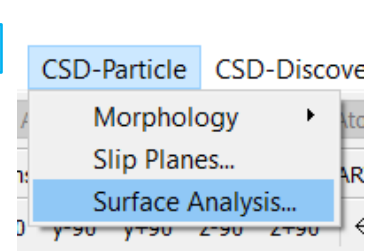
Surface Analysis

- From the top-level menu select **CSD-Particle > Surface Analysis...** to open the Surface Analysis dialog. Since we are interested in the (110) surface, we want to enter those values in the *Select surface orientation (hkl)* and *offset (o)* section. Change the value for *h* and *k* to 1, and leave *l* and *o* as 0, then click **Calculate Surface**.
- You will notice that a surface has been generated and the *Results* section of the *Surface Analysis* dialog has been populated. Let us go through the sections to understand what they mean.



- The *Results* section begins with the structure refcode and the surface generated as (orientation)[offset], here KAXXA110(110)[0.00]. The **Density Info (count/Å²)** portion tells us about the chemistry on the surface that is in contact with the topology (the white surface that has been generated). The density of hydrogen bond acceptors is higher than hydrogen bond donors on the surface. Observe that the density of *Unsatisfied H-Bond Donors* is lower than the density of hydrogen bond donors as they are a subset of this group. You can then rotate the surface to view the aromatic bonds in contact with the surface. The **Topology Info** section describes the physical roughness of the generated surface. The *Rugosity* is the ratio of the surface area to the projected area, and *RMSD* is the root mean squared deviation of the height from the mean plane. *Skewness* describes whether the surface is dominated by peaks (value higher than 0) or by valleys (lower than 0). Finally, *Kurtosis* describes the

7



9

Surface Analysis

Analyse

Select surface orientation (hkl) and offset (o)

h: 1 k: 1 l: 0 o: 0.00

☐ Preview Slab

☐ Show Advanced Options

Full Interaction Map

Calculate Surface

Results - KAXXA110 (110)[0.00]

Density Info (count/Å²)

H-Bond Acceptors:	0.051	Aromatic Bonds:	0.158
H-Bond Donors:	0.025	Unsatisfied H-Bond Donors:	0.006

Topology Info

Surface Area (Å ²):	449.533	Projected Area (Å ²):	315.890
Rugosity:	1.423	RMSD:	1.444
Skewness:	0.060	Kurtosis:	2.236

Display Options

Surface colouring: Single colour

Opacity: (%) 100

☐ Periodic View ☐ Hide Molecules

Atom Properties

☐ Charge ☐ H-Bond Acceptors

☐ Aromatic ☐ H-Bond Donors

☐ Unsatisfied H-Bond Donors

Reset Close

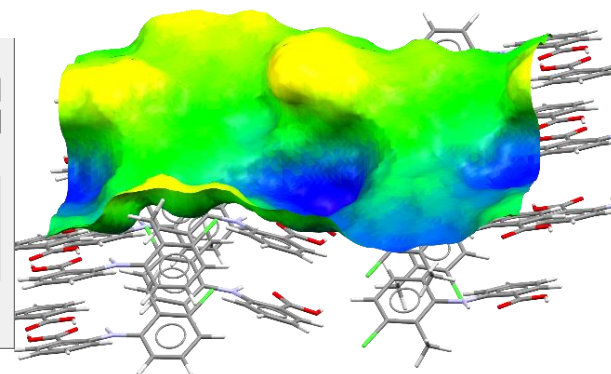
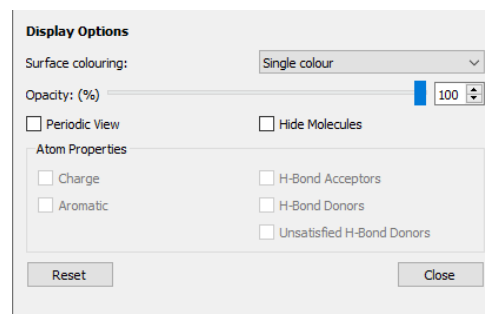
sharpness of the peak: values less than 3 signify a step-height change and values higher than 3 hint at a sharp peak.

10. The *Display Options* section of the **Surface Analysis** dialog allows us to generate more dynamic views of the surface. We will adjust the values here to change the surface views.

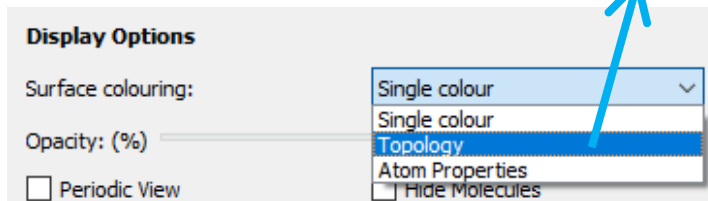
11. First, we will change the *Surface colouring* from *Single Colour* to *Topology* to get a better view of the height map of the surface. The areas closer to red are the peaks (note that in this case, we see a maximum of yellow), while the blue-purple areas are the valleys.

12. Next, select *Atom Properties* from the Surface Colouring menu. You will see that the surface is back to white and that it is now possible to tick the *Atom Properties* options below to visualize where specific chemistry is found on the surface. Explore the options to learn more about the surface. Tick H-Bond Acceptors (coloured red), H-Bond Donors (blue) and Aromatic (orange). We notice that what we observe on the surface is in line with the descriptors explored before. If some areas show both red and blue, the dominant colour will be hydrogen bond acceptors. To get a better view of which atoms are contributing to the maps, you can reduce the opacity.

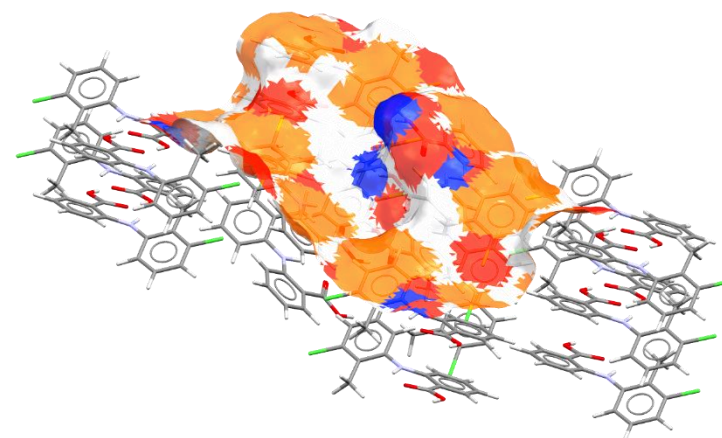
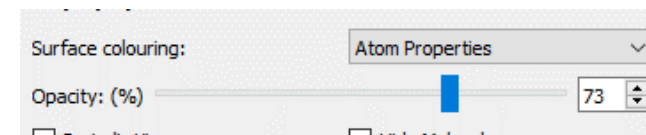
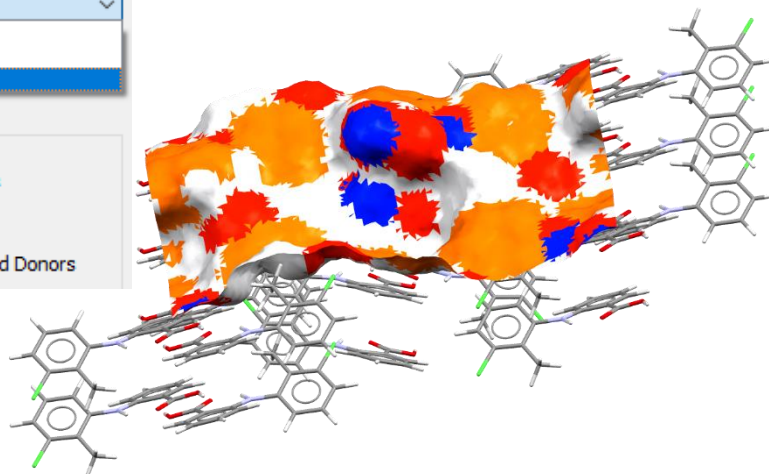
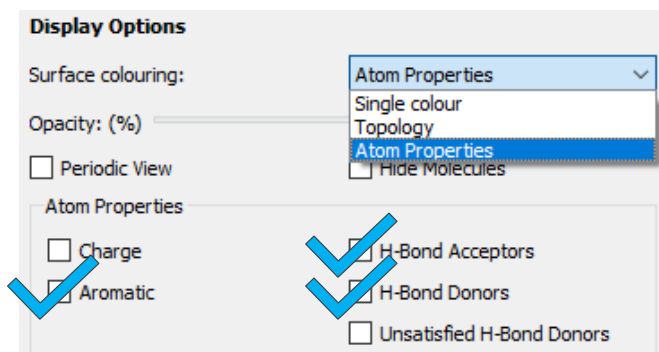
10



11

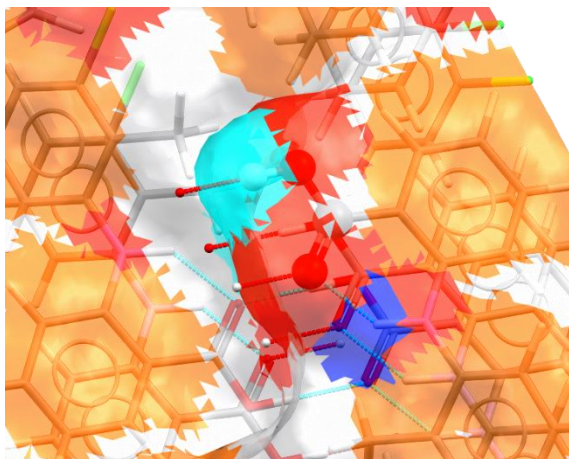


12



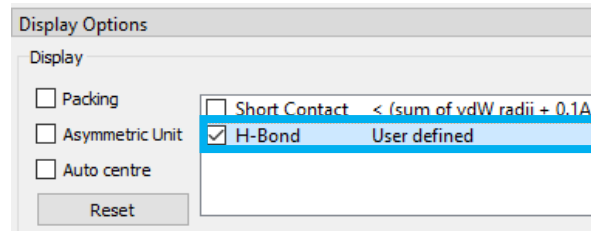
13. We will now visualize where hydrogen bond donors and acceptors are located by turning on H-Bonds in the *Display Options* box at the bottom of the Mercury interface.
14. The next atom property to investigate is the [Unsatisfied H-Bond Donors](#). Tick the corresponding box in the *Atoms Properties* section of the **Surface Analysis** dialog to colour the matching areas in teal (light blue shade).
15. Observe that not all the H-bond donors (blue) areas became teal, as some of the donors are satisfied. As an example, observe the hydrogen bond donors in the images on the side and on your structure: you will notice that (a) is protruding out of the surface and has a hydrogen to donate hence it is unsatisfied, while (b) is part of a dimer and the hydrogen donor is satisfied within the structure. This is important because it allows us to explore which hydrogens are available for donation, for incoming molecules for example, and which donors are not available as they are already involved in hydrogen bonds with the bulk of the surface.

15a

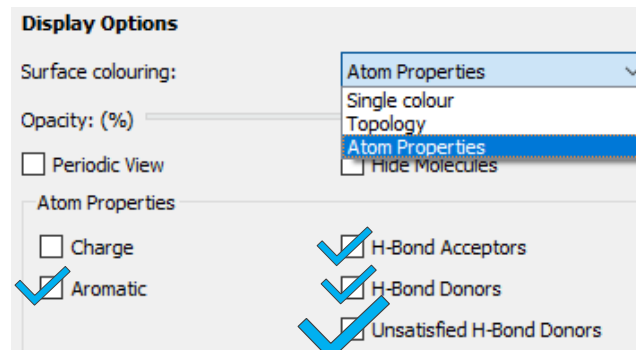


16. At the end of the analysis, turn off the hydrogen bonds by unticking the H-Bond box (opposite of **Step 13**).
17. The last atom property that we will see in this example is the charge. In the *Atoms Properties* section of the **Surface Analysis** dialog, untick all the properties that you currently have on and tick only *Charge*.

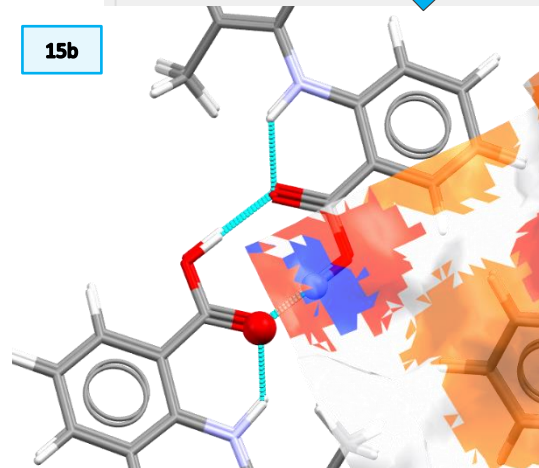
13



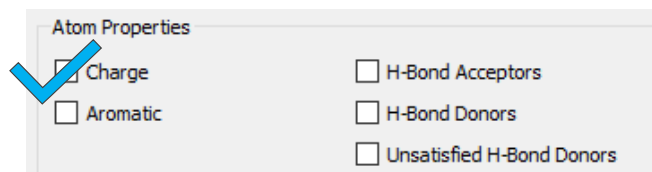
14



15b

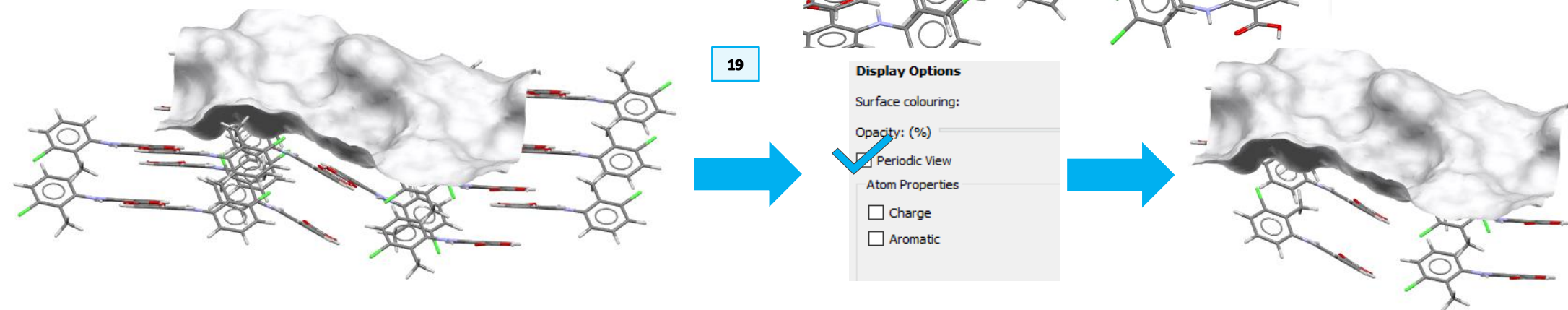


17



18. The surface is now coloured representing the [Gasteiger charges](#). You can observe areas of positive charge (blue) and negative charge (red). **Bonus tip:** if you have calculated your own charges, you can import them into a mol2 file by modifying the charges column and when you do the surface analysis, it will overlay the charges that you have given.

19. **Bonus tip:** If you tick the box next to *Periodic View* in the **Surface Analysis** dialog, you will only see the molecules that are within the bounding box of the surface. You may export this representation for further calculations, for example with Molecular Dynamics, Quantum Mechanics, or other computational techniques.

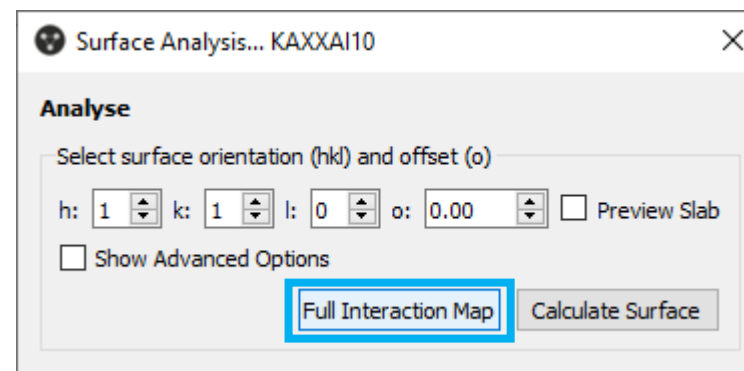


FIMs on Surface

20. For the next part, we will study the Full Interaction Maps (FIMs) on Surface. We will start with the same surface analysed in the previous part of this example.

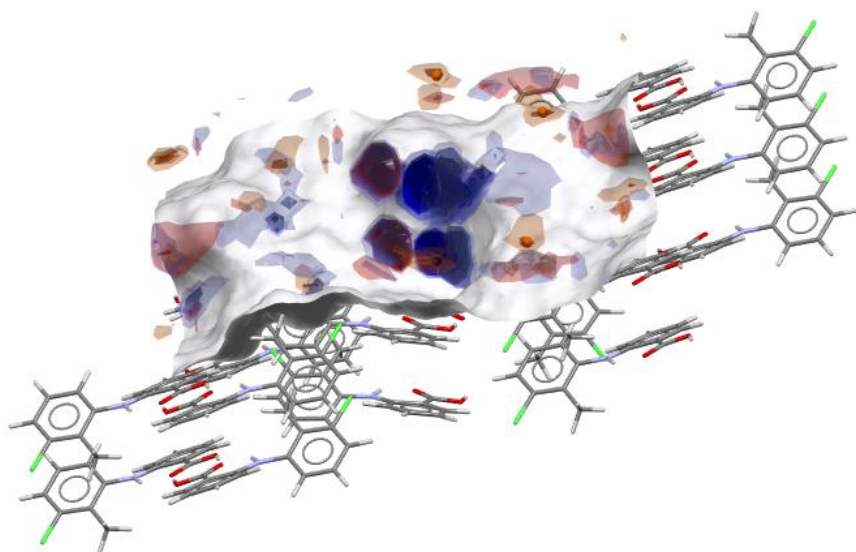
21. For this example, we will first untick all the options in the *Display Properties* section of the **Surface Analysis** dialog. Then, click the **Full Interaction Map** button at the top of the **Surface Analysis** dialog.

21



22. This will bring up the **Full Interaction Maps on Surface** window. For this example, we will keep the default settings and additionally, we will tick the *Generate hotspots in the map* box, and also select in the probes *Water Oxygen*. Then, click **Calculate Surface Maps**. A progress bar will appear.

23. FIMs have been generated on the surface and they show the likelihood of finding interactions of the selected probes on this surface. We can see maps and hotspots.



24. Let us investigate the maps. For ease of visualization, turn off the hotspots by going in the *Hotspots* tab and untick *All* above the *Visible* column.

25. Then, in the **Surface Analysis** dialog, tick again the atom properties *H-Bond Acceptors* and *H-Bond Donors*.

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 type="checkbox"/> Unsatisfied H-Bond Donors

22

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

- ☒ Uncharged NH Nitrogen
- ☐ Charged NH Nitrogen
- ☐ RNH3 Nitrogen
- ☐ Alcohol Oxygen
- ☒ Carbonyl Oxygen
- ☒ Water Oxygen
- ☐ Oxygen Atom
- ☐ Methyl Carbon
- ☒ Aromatic CH Carbon
- ☐ C-F Fluorine
- ☐ C-Cl Chlorine
- ☐ C-Br Bromine
- ☐ C-I Iodine

Colour

Defaults

Calculate Surface Maps Clear Maps & Hotspots Load Maps... Save Maps... Close

24

Full Interaction Maps on Surface

Options Maps Hotspots Log Files

Edit Hotspots

Probe	Display Min. Level	Level Range [min., max.]	Color	<input type="checkbox"/> All <input checked="" type="checkbox"/> Visible	Label	Use Opacity
1 Uncharged NH Nitrogen	5.00	[1.81, 35.45]	Blue	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
2 Carbonyl Oxygen	5.00	[1.21, 112.13]	Red	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
3 Water Oxygen	5.00	[1.03, 164.39]	Custom...	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
4 Aromatic CH Carbon	5.00	[1.02, 5.30]	Custom...	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>

Calculate Surface Maps Clear Maps & Hotspots Load Maps... Save Maps... Close

26. Observe that red areas on the surface (H-bond acceptors) match blue areas in the FIMs (NH Nitrogen, H-bond donors), while blue areas on the surface (H-bond donors) correspond to red areas in the FIMs (Carbonyl Oxygen, H-bond acceptors). **Hint:** Turn on and off parts of the plot for better visibility.

27. You can continue the analysis by turning on the *Unsatisfied H-Bond Donors* property for the surface. You will see that the unsatisfied hydrogen bond donors have a likely acceptor area on the maps, while satisfied donors do not as having already formed a H-bond in the surface would make the formation of any other hydrogen bond at an unlikely angle.

28. We can then explore FIMs numerically. Go to the *Maps* tab and observe the values in the *Level Range* column. These values express how likely over random it is to find such interaction.

Full Interaction Maps on Surface

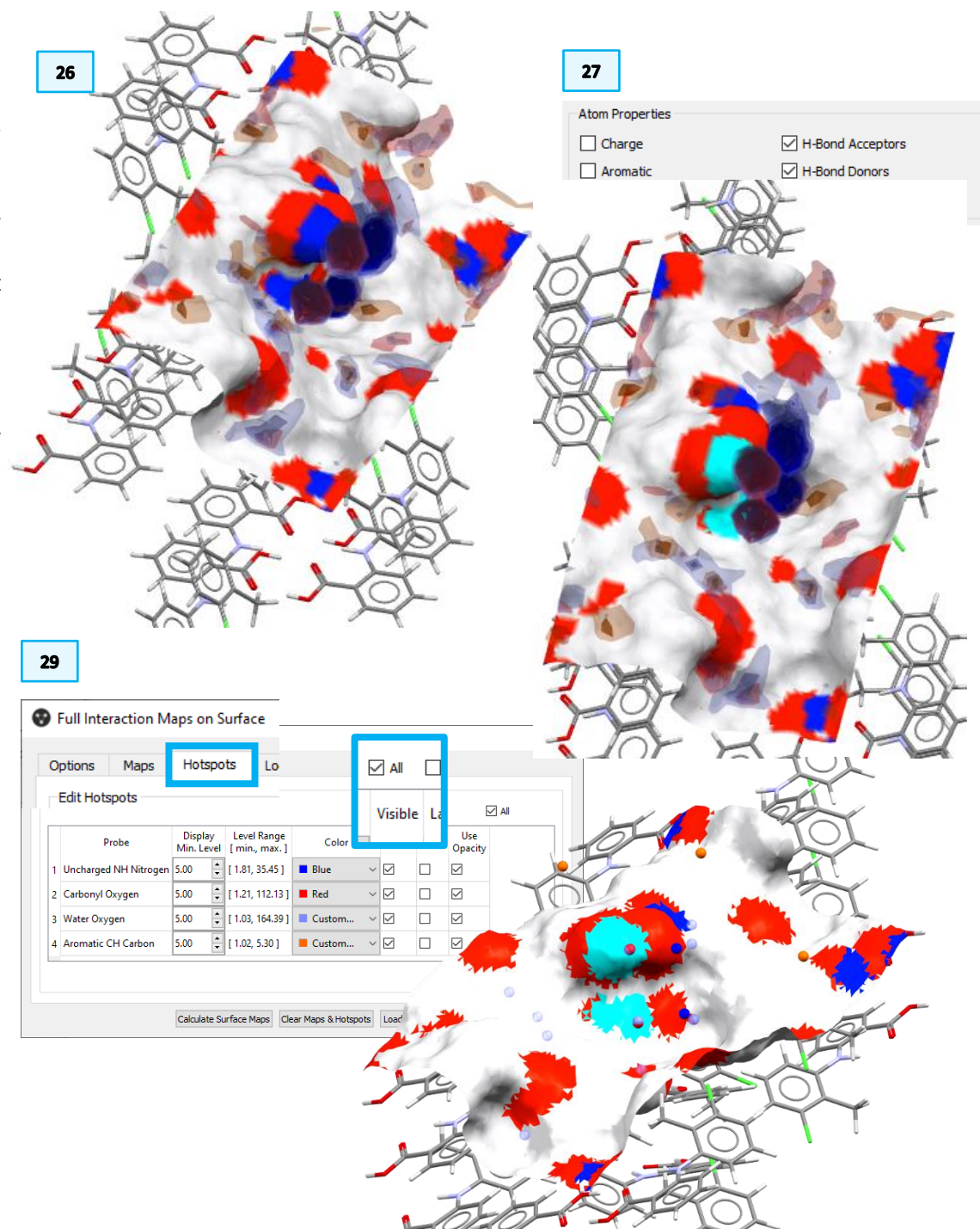
Options: **Maps** Hotspots Log Files

Edit Existing Contours

Probe	Level	Level Range [min., max.]	Color	Visible	Display Type	Opacity
1 Uncharged NH Nitrogen	2.00	[0.00, 35.45]	Blue	<input checked="" type="checkbox"/>	triangle	0.2
2 Uncharged NH Nitrogen	4.00	[0.00, 35.45]	Blue	<input checked="" type="checkbox"/>	triangle	0.5
3 Uncharged NH Nitrogen	6.00	[0.00, 35.45]	Blue	<input checked="" type="checkbox"/>	triangle	0.8
4 Carbonyl Oxygen	2.00	[0.00, 112.13]	Red	<input checked="" type="checkbox"/>	triangle	0.2
5 Carbonyl Oxygen	4.00	[0.00, 112.13]	Red	<input checked="" type="checkbox"/>	triangle	0.5
6 Carbonyl Oxygen	6.00	[0.00, 112.13]	Red	<input checked="" type="checkbox"/>	triangle	0.8
7 Water Oxygen	2.00	[0.00, 164.39]	Custom...	<input checked="" type="checkbox"/>	triangle	0.2
8 Water Oxygen	4.00	[0.00, 164.39]	Custom...	<input checked="" type="checkbox"/>	triangle	0.5
9 Water Oxygen	6.00	[0.00, 164.39]	Custom...	<input checked="" type="checkbox"/>	triangle	0.8
10 Aromatic CH Carbon	2.00	[0.00, 5.30]	Custom...	<input checked="" type="checkbox"/>	triangle	0.2

Calculate Surface Maps Clear Maps & Hotspots Load Maps... Save Maps... Close

29. We can now look in more detail at the [hotspots](#). For ease of visualization, turn off the maps by unticking *All* above the *Visible* column. Then, move to the *Hotspots* tab and tick *All* above the *Visible* column.



30. As hotspots represent the areas of the highest likelihood of interactions, observe where they are located on the surface and which atom properties they correspond to. [What do you observe?](#)

Comparison of different surfaces

31. Close the **Full Interaction Maps on Surface** window and click the **Reset** button in the *Display Options* menu at the bottom of the Mercury interface.

32. Since we are now interested in the (020) facet, in the **Surface Analysis** dialog we want to enter those values in the *Select surface orientation (hkl) and offset (o)* section. Change the value for *h* and *l* to 0, for *k* to 2, and leave *o* as 0.

33. **Bonus tip:** before calculating the slab, it is possible to preview it by ticking the *Preview Slab* option. You can tick *Show Advanced Options* to explore different visualization options. For this exercise, change *U* and *V* to 2 to obtain a 2x2 surface. Observe the surface, then untick both *Preview Slab* and *Show Advanced Options*.

34. Now click **Calculate Surface** as in **Step 7**.

35. At the bottom of the **Surface Analysis** dialog select *Topology* from the Surface Colouring menu. We can observe how the surface is different from the previous one; this is reflected also in the topology values. Compare these with the results obtained in **Step 9** for surface (110). In particular, we observe a negative value of the *Skewness* and a lower *Kurtosis* value, meaning that we have a surface resembling more a step function rather than a round peak.

Results - KAXXAI10 (020)[0.00]			
Density Info (count/Å ²)			
H-Bond Acceptors:	0.055	Aromatic Bonds:	0.092
H-Bond Donors:	0.018	Unsatisfied H-Bond Donors:	0.018
Topology Info			
Surface Area (Å ²):	355.004	Projected Area (Å ²):	217.504
Rugosity:	1.632	RMSD:	1.883
Skewness:	-0.099	Kurtosis:	1.485

31 Display Options

Display

☐ Packing ☐ Short Contact

☐ Asymmetric Unit ☐ H-Bond

☐ Auto centre

Reset

32 Surface Analysis... KAXXAI10

Analyse

Select surface orientation (hkl) and offset (o)

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

☒ Show Advanced Options

Size of Surface: U: 1 V: 1

Default values for the following settings have been optimised for small molecule organic systems.

Size of Surface: U: 2 V: 2

Probe Radius: 1.2 Grid Spacing: 0.3

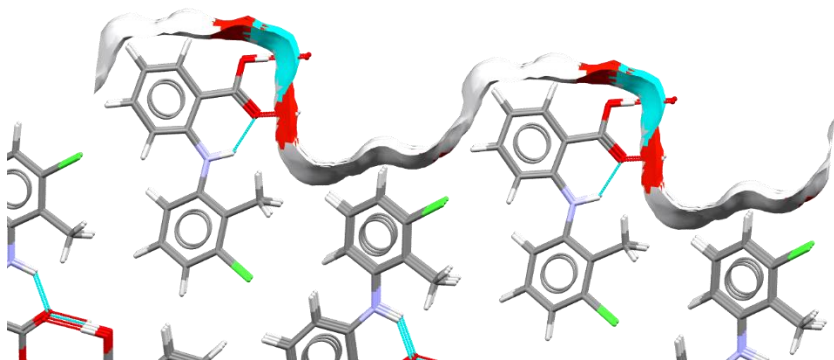
Thickness (W) Factor 1.60

Full Interaction Map **Calculate Surface**

35

36. Next, select *Atom Properties* from the Surface Colouring menu. Tick H-Bond Acceptors, H-Bond Donors, and Unsatisfied H-Bond Donors. Also, observe the *Density Info* values in the dialog (**Step 35**) and compare them with **Step 9** for surface (110). In particular, we observe that all the hydrogen bond donors are unsatisfied in this case; moreover, the unsatisfied H-bond donors count per Å² is higher than for the (110) surface, while the aromatic bonds density is lower.

37. Now turn on the hydrogen bonds as in **Step 13** to observe where potential hydrogen bonds could be formed on the surface.

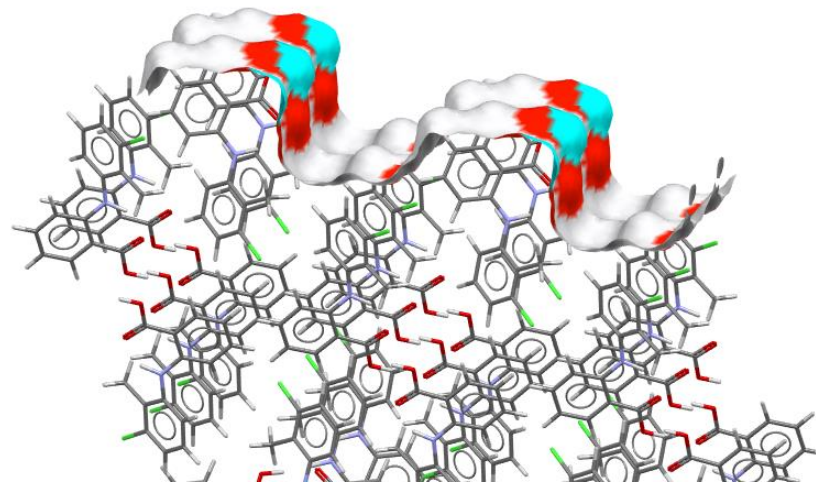


38. You may also observe the Gasteiger charges as in **Step 17** above.

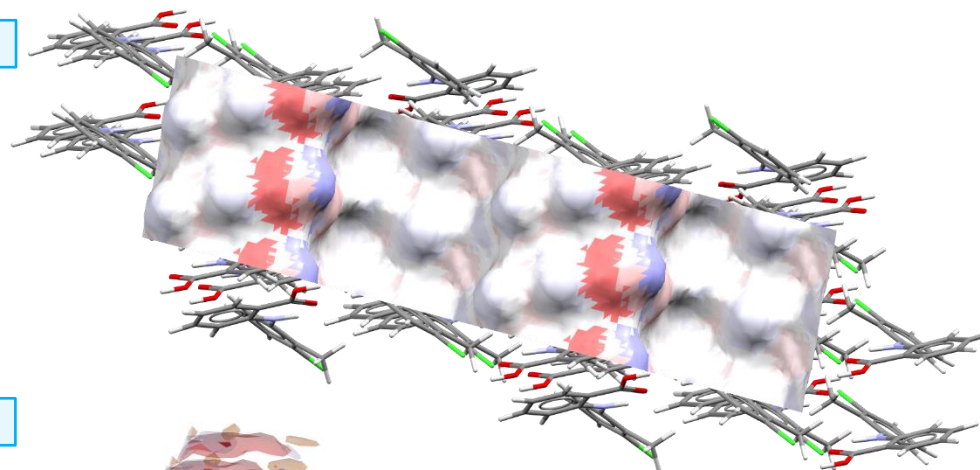
39. Next, we will generate FIMs on Surface, following **Steps 21 to 23** above.

40. Then, compare the values in the *Level Range* column of the table in the *Maps* tab with the ones obtained for surface (110) at **Step 28**. You will notice that in this case the values of the water oxygen and carbonyl oxygen are lower than in the previous case, suggesting a lower likelihood of interaction.

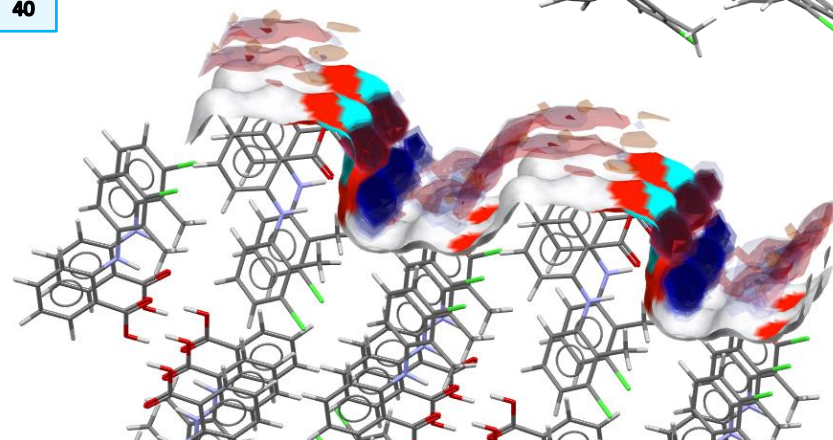
36



38

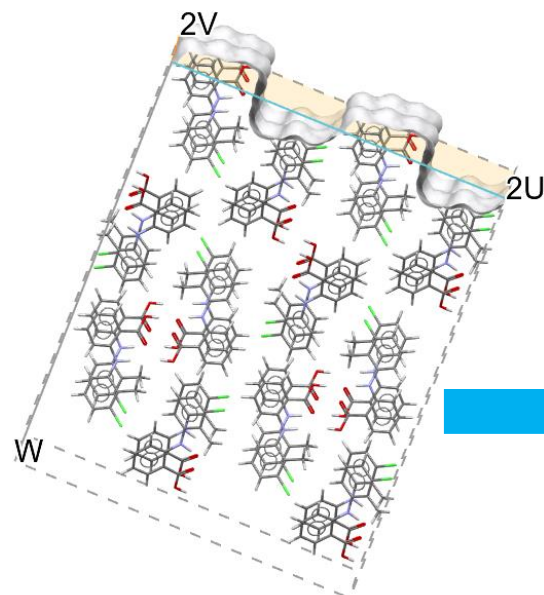


40



Exercise

41. Clear the maps and close the **Full Interaction Maps on Surface** window.
42. Bring up again the preview slab, as done in **Step 33**. This time, change the offset to observe how that impacts the surface terminations. We set the offset to 4 Å.



42

Surface Analysis... KAXXAI10

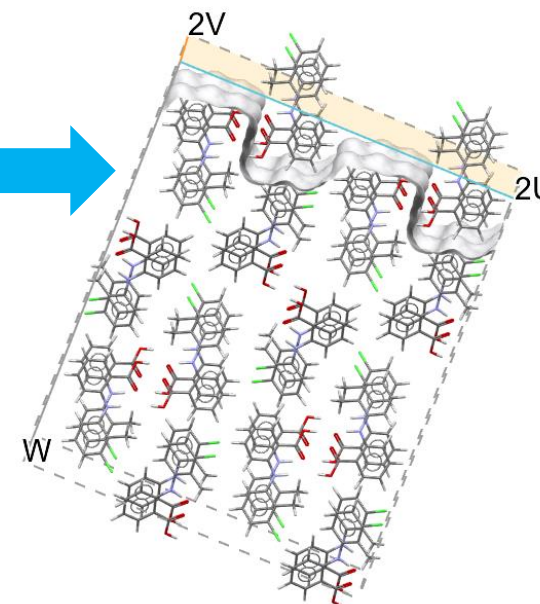
Analyse

Select surface orientation (hkl) and offset (o)

h: 0 k: 2 l: 0 o: 4.00

☒ Preview Slab

☒ Show Advanced Options



43. Click **Calculate Surface** to generate the surface and observe how its properties differ from the one without offset.

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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

☒ Uncharged NH Nitrogen

☐ Charged NH Nitrogen

☐ RNH3 Nitrogen

☐ Alcohol Oxygen

☒ Carbonyl Oxygen

☒ Water Oxygen

☐ Oxygen Atom

☐ Methyl Carbon

☒ Aromatic CH Carbon

☐ C-F Fluorine

☐ C-Cl Chlorine

☐ C-Br Bromine

☐ C-I Iodine

Colour

Defaults

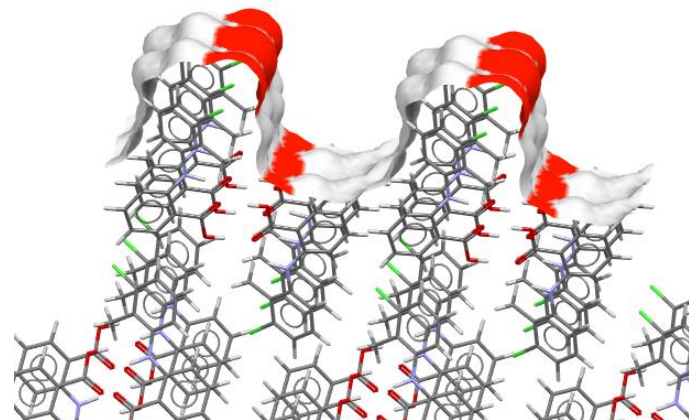
Calculate Surface Maps Clear Maps & Hotspots Load Maps... Save Maps... Close

44. Observe the chemistry and the properties: how does changing the terminations impact the properties of the surface? What does it mean?

Results - KAXXA110 (020)[4.00]			
Density Info (count/Å ²)			
H-Bond Acceptors:	0.037	Aromatic Bonds:	0.129
H-Bond Donors:	0.018	Unsatisfied H-Bond Donors:	0.000
Topology Info			
Surface Area (Å ²):	420.815	Projected Area (Å ²):	217.504
Rugosity:	1.935	RMSD:	2.702
Skewness:	0.046	Kurtosis:	1.436

Conclusion

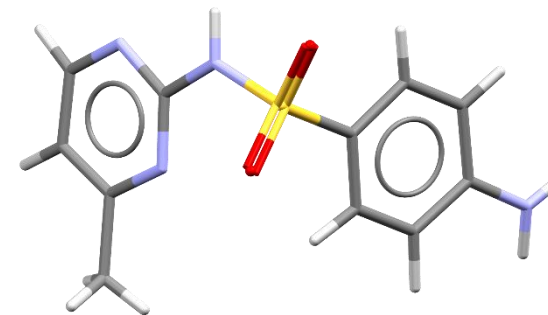
In this example, we saw in more detail how to use tools from *Surface Analysis* from CSD-Particle to analyse two *hkl* surfaces, namely the (110) and the (020), of a 2-(3-chloro-2-methylanilino)benzoic acid crystal. For each, we learnt how to investigate the chemistry and the topology of the surface and how to visualize such properties in the 3D visualizer in Mercury. We have also generated FIMs on each surface: FIMs allow us to quickly analyse where likely interactions are expected on the surface and which kind of chemistry we could expect. Changing the offset of the calculated surface also allows us to investigate how the activity of a surface would change.



Example 2. Slip Planes analysis to investigate elastic properties.

In this example, we will focus on two polymorphs of sulfamerazine to investigate their different tabletability and properties. Our focus will be on CSD Entries SLFNMA02 and SLFNMA01, displaying plastic and [elastic](#) behaviours respectively based on experimental data. We will use the [Slip Planes](#) tools to try and understand where the slip planes might indicate elastic or plastic behaviour.

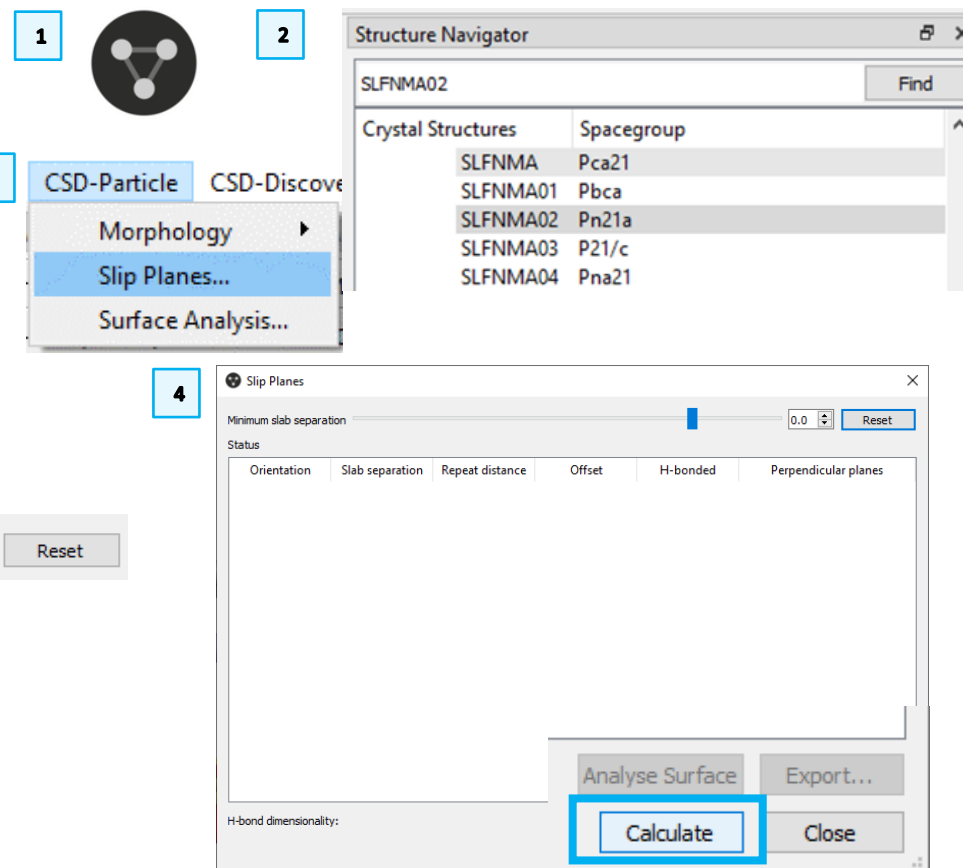
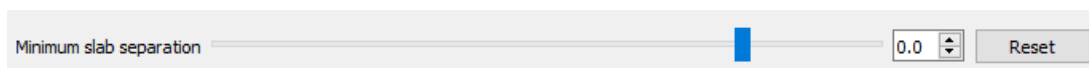
The Slip Planes tool shows potential slip planes based on the separation of the slabs.



A molecule of 2-p-Aminobenzene-sulfonamido-4-methylpyrimidine from CSD Entry SLFNMA02.

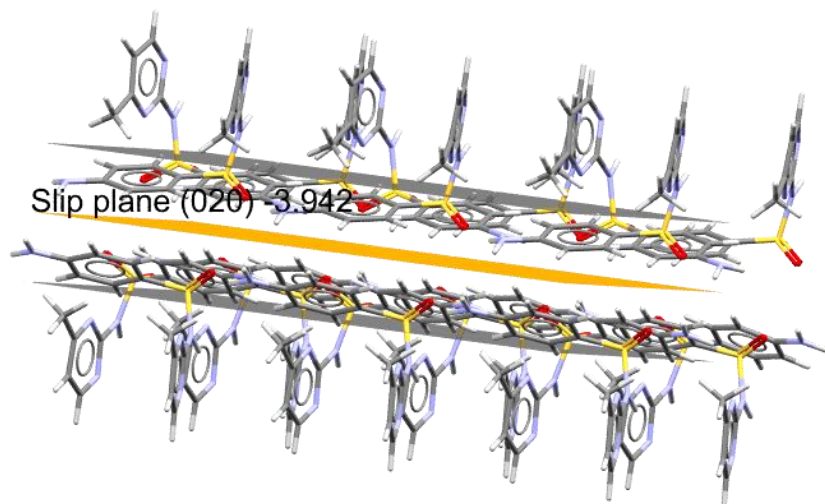
Calculation of potential slip planes

1. Open Mercury by double-clicking the Mercury icon on the desktop.
2. In the *Structure Navigator* on the right-hand side of the Mercury interface type the refcode SLFNMA02 to bring up the first [polymorph](#) of sulfamerazine that we are going to investigate, i.e. the [plastic](#) one.
3. From the top-level menu select **CSD-Particle** > **Slip Planes...** to launch the *Slip Planes* window.
4. Observe that the [minimum slab separation](#) is set to 0.0 Å. To start the calculation, click **Calculate** at the bottom of the *Slip Planes* window.

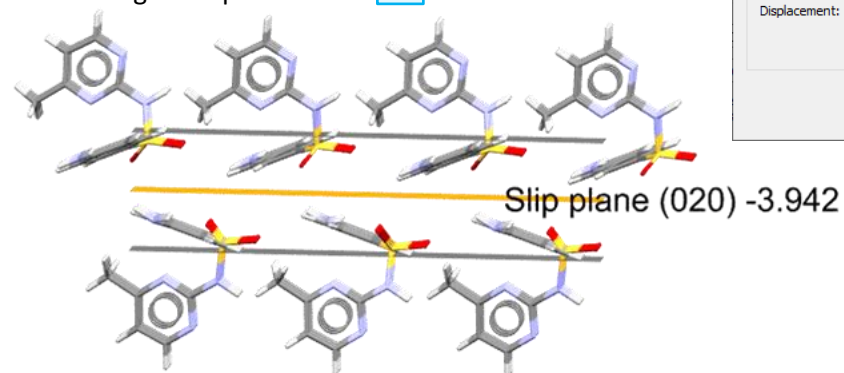


5. You will see that the table is now populated with an entry representing a potential slip plane with a slab separation of 1.561 Å. Observe the values in the table.

6. Click now on the entry in the table to visualize the planes in the Mercury visualizer. Note that this will also open the *Packing and Slicing* window.



7. You can rotate the structure to see the alignment of molecules around the slip plane. You can see that there is a significant separation between the two slabs with potential slips in directions parallel to the plane. This structure has a high likelihood of having a slip plane and it is indeed the one indicated as plastic in the literature. Structures with such features might be preferable when compression of the particle is involved.



5

	Orientation	Slab separation	Repeat distance	Offset	H-bonded	Perpendicular planes
1	(020)	1.561	10.977	-3.942	yes	

6

Slip Planes... SLFNMA02

Minimum slab separation: 0.0 [Reset]

Status: Calculation completed

	Orientation	Slab separation	Repeat distance	Offset	H-bonded	Perpendicular planes
1	(020)	1.561	10.977	-3.942	yes	

H-bond dimensionality: 3D network

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

Reset

2x2x2

3x3x3

Include atoms

☐ ... that Fit

☐ ... in molecules whose Centroids fit

☒ ... in molecules where Any atom fits

☐ ... in molecules where All atoms fit

Slicing

☒ Show slice

Select plane: Slip plane (020) -3.942 [Show plane]

New... Edit... Delete

☒ Show bounds

Depth: 5.00

Area: 20.00

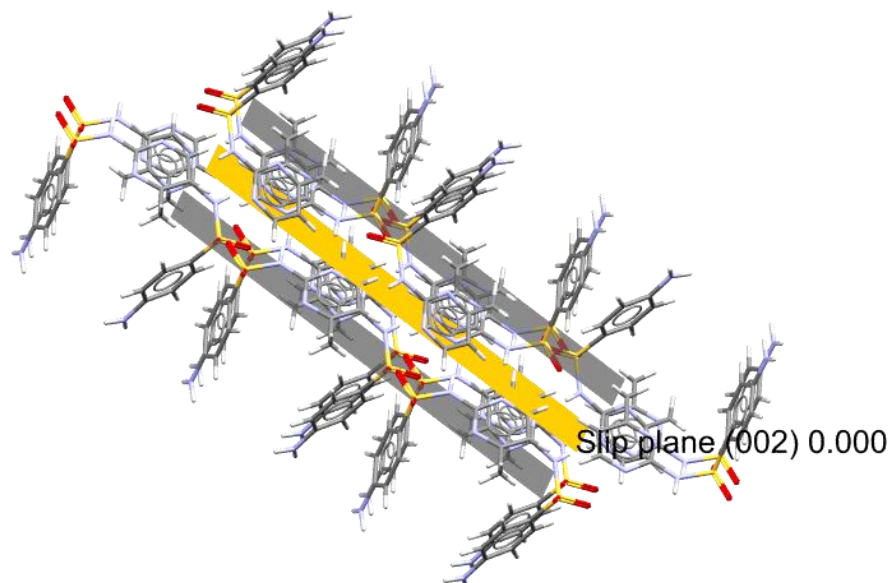
Displacement: 0.00

Reset

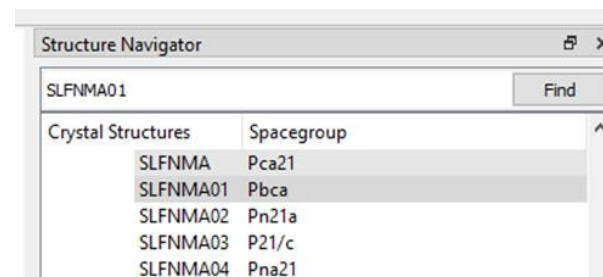
OK

7

8. We will now compare this structure with the [elastic](#) polymorph. Open another Mercury window by clicking on the icon again (on macOS, open a terminal window and run this command: `open -n -a "/path/to/CCDC/ccdc-software/mercury/mercury.app"`) and in the *Structure Navigator* on the right-hand side of the Mercury interface type the refcode SLFNMA01.
9. Re-open the slip planes menu; from the top-level menu select **CSD-Particle > Slip Planes...** as in **Step 3** above.
10. To start the calculation, click **Calculate** as in **Step 4** above. You will see that nothing has happened. The reason for this is that in this structure there are no potential slip planes with the minimum slab separation selected (0.0 Å).
11. Reduce the minimum slab separation by dragging the slider until the value is set to -1.6 Å. You will see in the dialog box that a new row has appeared with a slab separation value of -1.053 Å.
12. Observe the values in the table and then click on the row to visualize the plane in the structure. You will notice that for this polymorph the slabs are closer with more interlocked molecules compared to the structure analysed before. The potential slip plane appears more corrugated.



8



11

Minimum slab separation: -1.6 Å [Reset]

Slip Planes... SLFNMA01

Minimum slab separation: -1.6 Å [Reset]

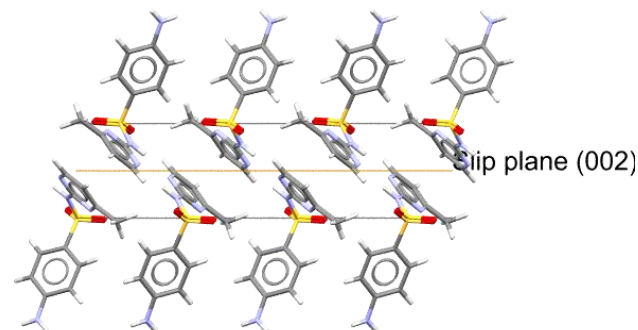
Status: Calculation completed

	Orientation	Slab separation	Repeat distance	Offset	H-bonded	Perpendicular planes
1	(002)	-1.053	11.442	0.000	yes	

H-bond dimensionality: 3D network

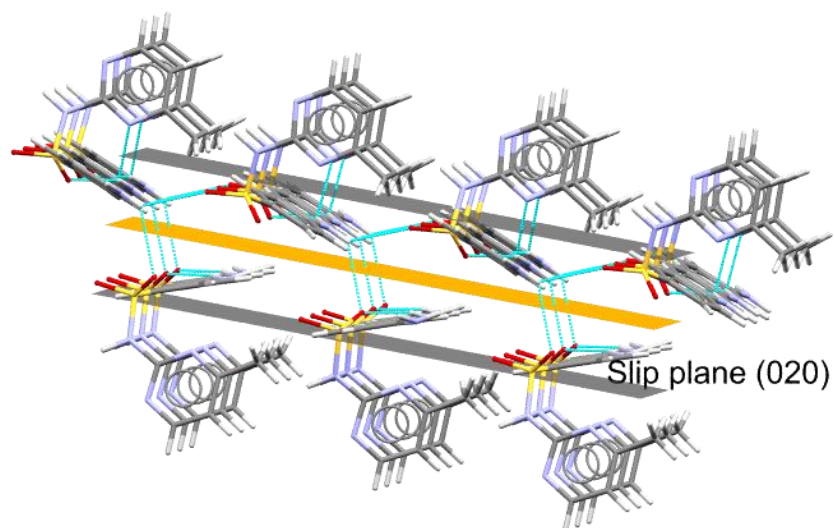
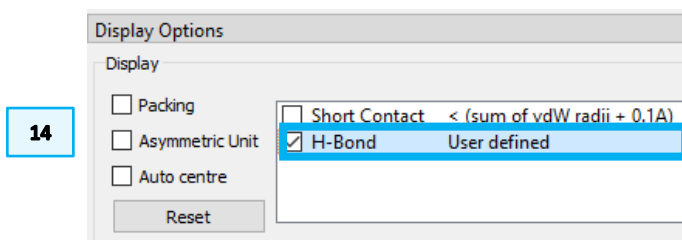
[Analyse Surface] [Export...] [Calculate] [Close]

12



Hydrogen bonds analysis

13. For both structures, we will explore the [hydrogen bonds](#) network. Hydrogen bonds are indeed really important for the stability of the structure. At the bottom of the Slip Planes window, you will see *H-bond dimensionality: 3D network*; and in the table, under *H-bonded* you can read “yes”, which means that there are hydrogen bonds across the defined slip plane.
14. Visualize hydrogen bonds by turning on H-Bonds in the *Display Options* box at the bottom of the Mercury interface.



Hydrogen bonds for the plastic deforming polymorph, CSD Entry SLFNMA02

13

Slip Planes... SLFNMA02

Minimum slab separation 0.0 Reset

Status: Calculation completed

	Orientation	Slab separation	Repeat distance	Offset	H-bonded	Perpendicular planes
1	(020)	1.561	10.977	-3.942	yes	

H-bond dimensionality: 3D network

Slip Planes... SLFNMA01

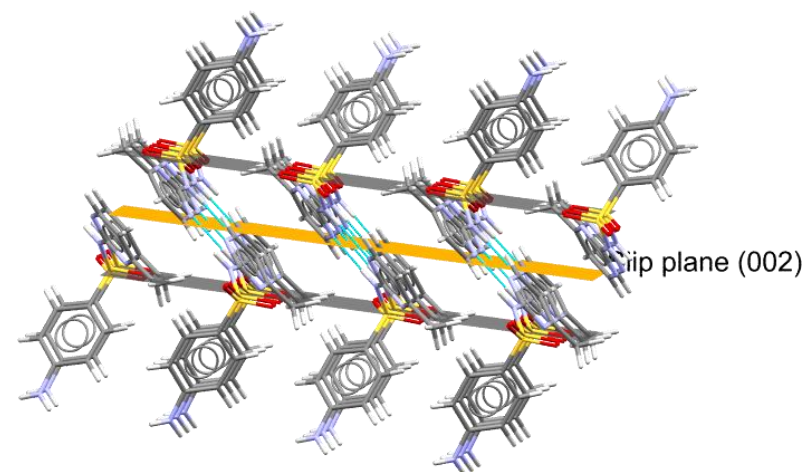
Minimum slab separation -1.6 Reset

Status: Calculation completed

	Orientation	Slab separation	Repeat distance	Offset	H-bonded	Perpendicular planes
1	(002)	-1.053	11.442	0.000	yes	

H-bond dimensionality: 3D network

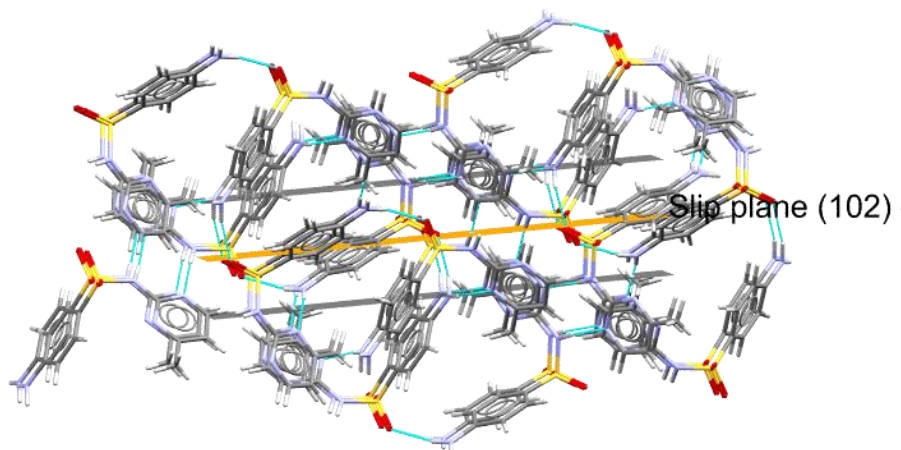
Analyse Surface Export... Calculate Close



Hydrogen bonds for the elastic deforming polymorph, CSD Entry SLFNMA01

Exploring more potential slip planes

15. Go back to the Mercury window with CSD Entry SLFNMA01.
16. To bring up more potential slip planes, drag the cursor at the top of the *Slip Planes* window to lower the minimum slab separation until a value of -4.0 Å. A total of 7 planes will populate the table.
17. If you explore the potential planes, by clicking on each entry, you will notice that plane (102) is very interlocked and connected so it seems very unlikely to be a slip plane. It is thus important to analyse in detail the potential planes.



18. You will also notice that the column with [perpendicular planes](#) is now populated and informs of which other potential slip planes are about perpendicular to the one in analysis. This might help assess where in an elastic system there might be a flexible crystal.

Conclusion

In this example, we explored an elastic and a plastic polymorph of sulfamerazine. Using the Slip Planes tool from CSD-Particle, we were able to investigate the location and properties of potential slip planes and consider how these could be related to the experimentally determined plastic or elastic properties.

16

Slip Planes... SLFNMA01

Minimum slab separation -4.0 Reset

Status: Calculation completed

	Orientation	Slab separation	Repeat distance	Offset	H-bonded	Perpendicular planes
1	(002)	-1.053	11.442	0.000	yes	(02-1), (10-2), (102)
2	(02-1)	-2.631	5.670	0.000	yes	(002), (10-2), (102)
3	(021)	-2.631	5.670	-2.835	yes	(002), (10-2), (102)
4	(020)	-2.973	5.852	0.000	yes	(002), (10-2), (102)
5	(020)	-3.909	5.852	-2.926	yes	(002), (10-2), (102)
6	(10-2)	-3.958	7.144	0.000	yes	(002), (02-1), (102)
7	(102)	-3.958	7.144	-3.572	yes	(002), (02-1), (10-2)

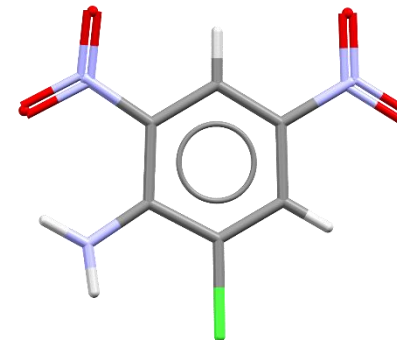
H-bond dimensionality: 3D network

Analyse Surface Export...

Calculate Close

Example 3. Slip planes analysis to investigate plastic properties of polymorphs.

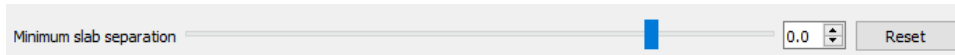
In the previous example, we looked at polymorphs that have different elastic properties: one plastic and the other elastic. In this example, we will look at polymorphs that exhibit similar plastic behaviours, however, one is more compressible than the other due to the type of planes observed.



6-Chloro-2,4-dinitroaniline molecule from CSD Entry UCECAG02.

Calculation of potential slip planes

1. Open Mercury by double-clicking the Mercury icon on the desktop.
2. In the *Structure Navigator* on the right-hand side of the Mercury interface type the refcode UCECAG02 to bring up the first polymorph that we are going to investigate.
3. From the top-level menu select **CSD-Particle > Slip Planes...** to launch the *Slip Planes* window.
4. Observe that the minimum slab separation is set to 0.0 Å. To start the calculation, click **Calculate** at the bottom of the *Slip Planes* window.



The image shows the Mercury software interface for performing a slip planes analysis. It includes the following components:

- Structure Navigator:** A window on the right showing a list of crystal structures. UCECAG02 is selected, showing a space group of P21.
- Top-level menu:** The 'CSD-Particle' menu is open, showing 'Slip Planes...' as an option.
- Slip Planes window:** A window titled 'Slip Planes' with a 'Minimum slab separation' slider set to 0.0 Å. The 'Calculate' button is highlighted.

5

5. You will see that the table is now populated with entries representing potential slip planes with the value of slab separations. You will also notice that the Perpendicular planes have also been populated. Perpendicular planes might help assess where in a system there might be a flexible crystal. Observe the values in the table.

	Orientation	Slab separation	Repeat distance	Offset	H-bonded	Perpendicular planes
1	(001)	2.190	13.275	0.000	no	(101), (01-1)
2	(101)	0.501	6.882	0.000	yes	(001), (01-1)
3	(01-1)	0.071	3.532	-2.116	yes	(001), (101)
4	(011)	0.071	3.532	-0.350	yes	(001), (101)

6

6. Click now on the first entry in the table to visualize the planes in the Mercury visualizer. Note that this will also open the *Packing and Slicing* window. You can move the Area slider to adjust the views in the main Mercury window.

Slip Planes... UCECAG02

Minimum slab separation: 0.0 (Reset)

Status: Calculation completed

	Orientation	Slab separation	Repeat distance	Offset	H-bonded	Perpendicular planes
1	(001)	2.190	13.275	0.000	no	(101), (01-1)
2	(101)	0.501	6.882	0.000	yes	(001), (01-1)
3	(01-1)	0.071	3.532	-2.116	yes	(001), (101)
4	(011)	0.071	3.532	-0.350	yes	(001), (101)

H-bond dimensionality: 2D sheet

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

Reset 2x2x2 3x3x3

Include atoms

☐ ... that Fit
☐ ... in molecules whose Centroids fit
☒ ... in molecules where Any atom fits
☐ ... in molecules where All atoms fit

Slicing

☒ Show slice

Select plane: Slip plane (001) 0.000

New... Edit... Delete

☒ Show plane
☒ Show bounds

Depth: 5.00
Area: 20.00
Displacement: 0.00

Reset

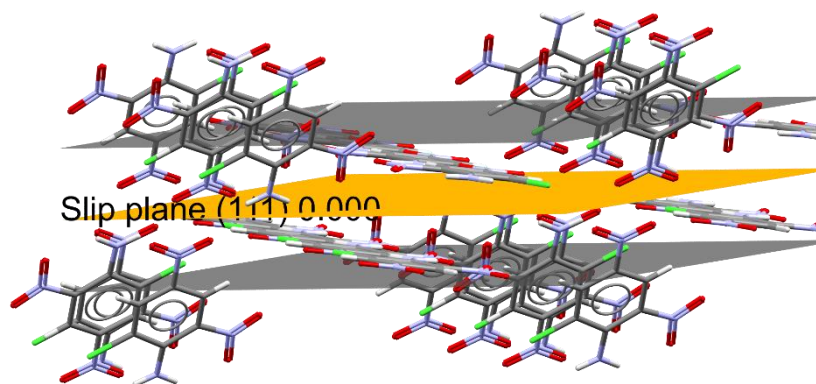
OK

Slip plane (001) 0.000

7. You can rotate the structure to see the alignment of molecules around the slip plane. You can see that there is a significant separation between the two slabs with potential slips in directions parallel and perpendicular to the plane. This structure has a high likelihood of having a slip plane. Structures with such features might be preferable when compression of the particle is involved. You can also view a different entry; select orientation (01-1) to view the planes.

Slip plane (01-1) -2.116

8. We will now compare this structure with the other polymorph. In the *Structure Navigator* on the right-hand side of the Mercury interface type the refcode UCECAG03.
9. If you have previously closed the *Slip Planes* window, re-open it from the top-level menu by selecting **CSD-Particle** > **Slip Planes...** as in **Step 3** above.
10. To start the calculation, click **Calculate** as in **Step 4** above. You will see the table populated with two entries. You will notice that there are no perpendicular planes observed in this structure.
11. Observe the values in the table and then click on each row to visualize the plane in the structure. You will notice that for this polymorph there are no perpendicular planes, only parallel ones. We can say that this polymorph is less likely to be flexible than the other.



8

Structure Navigator

UCECAG03 Find

Crystal Structures	Spacegroup
UCECAG01	P21/c
UCECAG02	P21
UCECAG03	P-1
UCECAH	P41
UCECAI	P-1
UCECAJ	P21/n

10

Slip Planes... UCECAG03

Minimum slab separation 0.0 Reset

Status Calculation completed

	Orientation	Slab separation	Repeat distance	Offset	H-bonded	Perpendicular planes
1	(111)	1.262	6.372	0.000	yes	
2	(110)	0.840	7.086	-3.543	yes	

H-bond dimensionality: 2D sheet

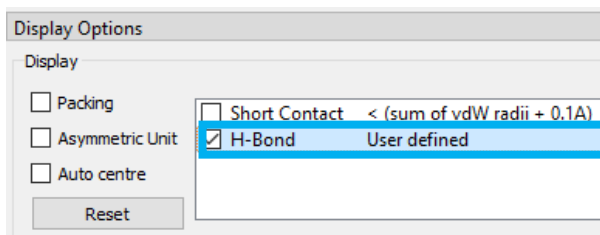
Analyse Surface Export... Calculate Close

11

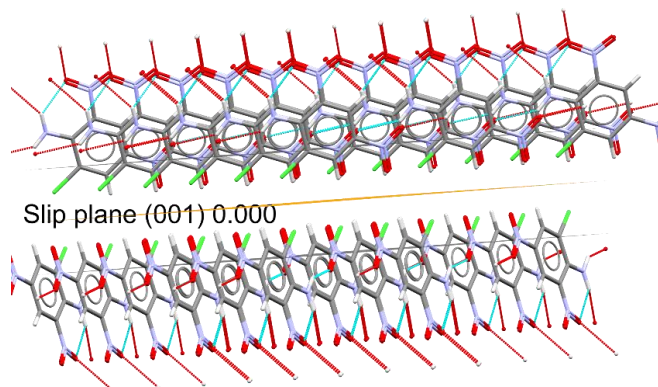
Hydrogen bonds analysis

12. For both structures, we will explore the hydrogen bonds network. Hydrogen bonds are indeed really important for the stability of the structure. At the bottom of the Slip Planes window, you will see *H-bond dimensionality: 2D sheet* for both structures. In the table for UCECAG02, under *H-bonded* you can read “no” for the first entry, which means that there are no hydrogen bonds across the plane. However, the other entries do exhibit hydrogen bonding for both structures

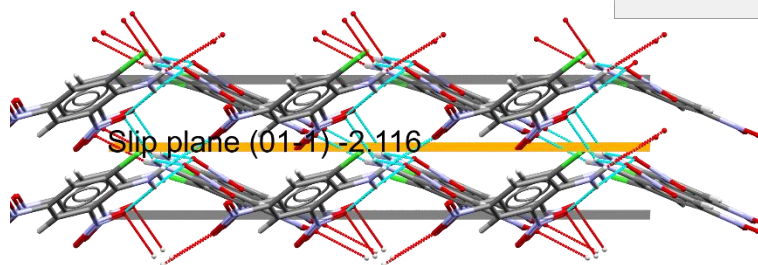
13. Visualize hydrogen bonds by turning on H-Bonds in the *Display Options* box at the bottom of the Mercury interface.



13

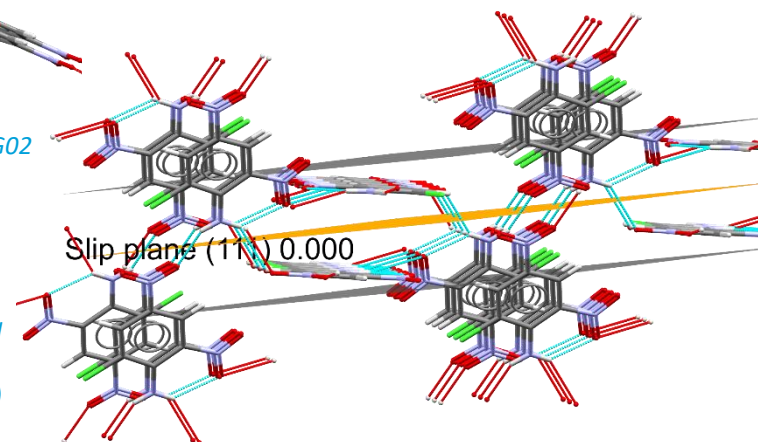


No hydrogen bonds for the first plane, the one with (001) orientation, in CSD Entry UCECAG02



Hydrogen bonds for the (01-1) orientation in CSD Entry UCECAG02

Hydrogen bonds for the second polymorph, CSD Entry UCECAG03, shown for the potential slip plane (111)



Slip Planes... UCECAG02

Minimum slab separation: 0.0 (Reset)

Status: Calculation completed

	Orientation	Slab separation	Repeat distance	Offset	H-bonded	Perpendicular planes
1	(001)	2.190	13.275	0.000	no	(01), (01-1)
2	(101)	0.501	6.882	0.000	yes	(001), (01-1)
3	(01-1)	0.071	3.532	-2.116	yes	(001), (101)
4	(011)	0.071	3.532	-0.350	yes	(001), (101)

H-bond dimensionality: 2D sheet

Slip Planes... UCECAG03

Minimum slab separation: 0.0 (Reset)

Status: Calculation completed

	Orientation	Slab separation	Repeat distance	Offset	H-bonded	Perpendicular planes
1	(111)	1.262	6.372	0.000	yes	
2	(110)	0.840	7.086	-3.543	yes	

H-bond dimensionality: 2D sheet

Analyse Surface Export... Calculate Close

Conclusion

In this example, we used the *Slip Planes* tool from CSD-Particle to investigate polymorphs with similar behaviours, where one is more compressible than the others. We studied the potential slip planes in both polymorphs to investigate such properties.

Summary

After this workshop you should now be able to:

- Calculate *hkl* surfaces and investigate their chemical and topological properties.
- Display different properties on the generated surface to visualize its potential activity and personalise the surface view to enhance clarity.
- Calculate Full Interaction Maps on such a surface to quickly identify likely interactions.
- Visualize hydrogen bonds in Mercury.
- Use the Slip Planes tool from CSD-Particle to explore the potential for slip planes, including, for example, to investigate elastic vs plastic behaviours.

Next Steps

If you have completed one of the three exercises proposed and still have time, you can start any of the other two exercises or try these components on one of your own structures. Or ask the tutors for more examples!

After this workshop, you can explore more exercises in the self-guided workshops available in the [CSD-Particle workshops area](#) on our website and the [Surface Analysis CSDU module](#). We suggest trying the Particle shape calculation with CSD-Particle workshop.

Reading suggestions

You might find the following publications of interest:

- “Particle Informatics”: Advancing Our Understanding of Particle Properties through Digital Design, *Cryst. Growth Des.*, 2019, **19**, 9, 5258–5266 - <https://doi.org/10.1021/acs.cgd.9b00654>
- Elastically flexible molecular crystals, *Chem. Soc. Rev.*, 2021, **50**, 11725–11740 - <https://doi.org/10.1039/D1CS00469G>

Glossary

BFDH Morphology

Simulation of morphology using the Bravais Friedel Donnay Harker (BFDH) method. BFDH crystal morphology is an approximation based on crystallographic geometrical considerations. For a given structure, the BFDH algorithm will predict the habit or shape of a crystal using the corresponding unit cell and symmetry operator information.

Gasteiger Charges

Gasteiger charges refer to partial charges calculated with the Marsili-Gasteiger method.

In Mercury, for atoms in a molecule increasing red colour represents an increasing positive charge and increasing blue colour represents an increasing negative charge. For surfaces instead, colouring by Charge colours the surface with a continuous scale from negative (red) to positive (blue).

Hotspots

Hotspots represent the positions of the highest local density for each contour.

Hydrogen Bonds

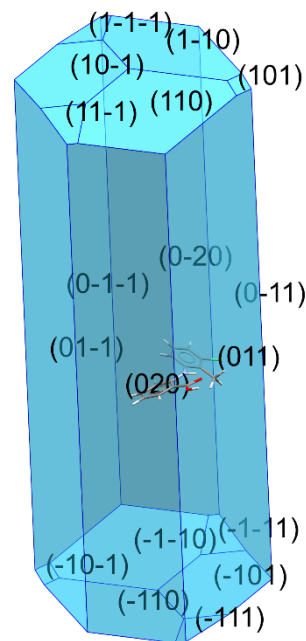
Hydrogen bonding occurs between donor-acceptor interactions involving hydrogen atoms. The H-bond interactions are classified as: strong (mostly covalent), moderate (mostly electrostatic) and weak (electrostatic). Their strength is observed to be between 12 and 30 kJ/mol.

Kurtosis

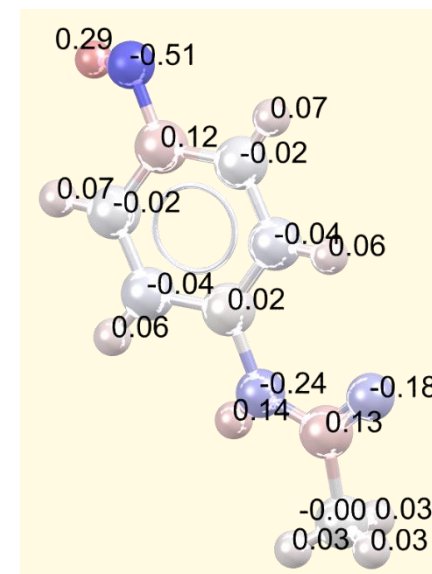
Kurtosis is a statistical characterisation of a dataset, such as surface topology, which measures the sharpness of height distribution and has a value of zero for a normal distribution. Positive values indicate a distribution with a sharp peak and long, "thick" tails. Negative values indicate a rounded peak with short, "thin" tails.

Minimum Slab Separation

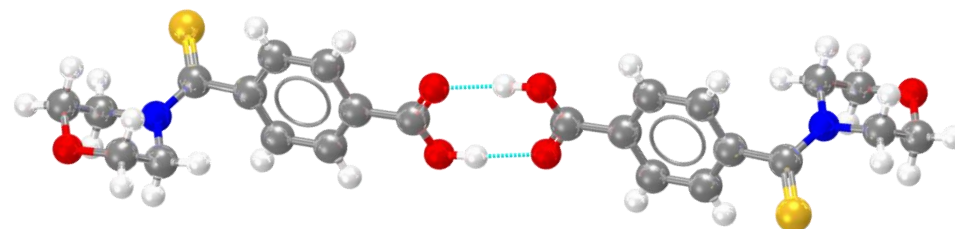
Potential slip planes will only be shown if the slab separation value is greater than the minimum slab separation which is 0 Å. The slab distance is the shortest distance between slabs of molecules on either side of this slip plane (Å).



Example of BFDH Morphology
for CSD Entry KAXXA10.



Molecule of paracetamol (CSD Entry HXACAN)
with atoms coloured by Gasteiger charge,
also expressed in the label.



In light blue, example of hydrogen bonds
for refcode MULWIC.

Offset

This is the value in Å of the distance to the calculated surface from the parallel Miller plane.

Perpendicular Planes

The *Perpendicular Planes* column in the Slip Planes table contains a list of any potential slip planes >45° from the given plane.

Polymorph

Polymorphism is the occurrence of two or more crystalline forms of the same substance. Where available, polymorph information can be displayed for Cambridge Structural Database (CSD) structures. Structures known to be polymorphic contain comments which include the word polymorph (when reported by the author), e.g., non-triboluminescent polymorph. There is also a CSD subset of polymorphic structures.

Rugosity

Rugosity is used to describe the roughness of the surfaces and is calculated as the surface area divided by the projected area.

Skewness

Statistical characterisation of a dataset, such as surface topology. Skewness measures the lack of symmetry, so in the case of surface topology, equal peaks and valleys would have a skewness of 0. If the surface was mostly valleys, then the skewness would be a negative value close to -1 and if the value is higher than 0, then the surface was mostly dominated by peaks.

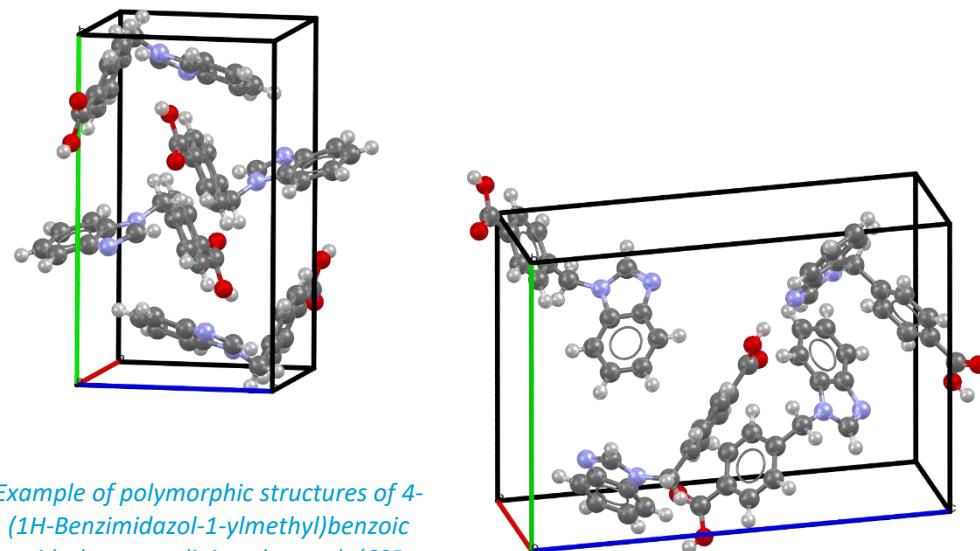
Slip Planes

Slip planes represent planes in a crystal structure along which a slip can take place.

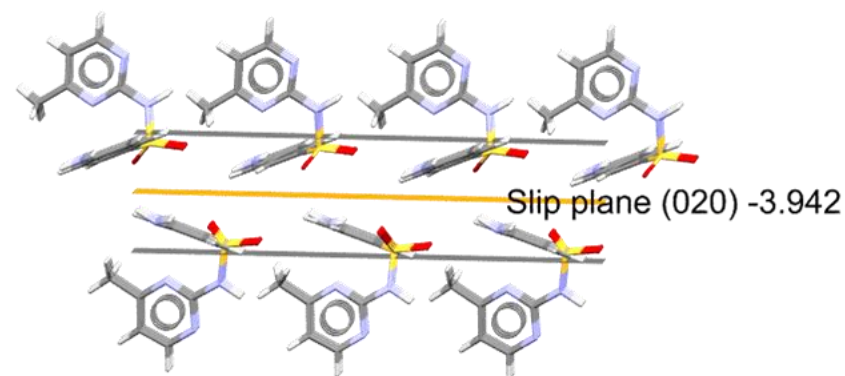
Please note that in CSD-Particle, the Slip Planes functionality identifies potential slip planes in a crystal structure.

Root Mean Square Deviation (RMSD)

The root mean square deviation (RMSD) is a commonly used measure of the difference between two sets of values (usually comparing observed data to



Example of polymorphic structures of 4-(1H-Benzimidazol-1-ylmethyl)benzoic acid: the monoclinic polymorph (CSD Entry ABADIS) at the top, and the orthorhombic polymorph (CSD Entry ABADIS01) on the right.



Example of potential slip plane in CSD Entry SLFNMA02.

estimated data). The RMSD is defined as the square root of the mean squared error. In Mercury this is used to measure the geometric difference between packing features or packing patterns in crystal structures.

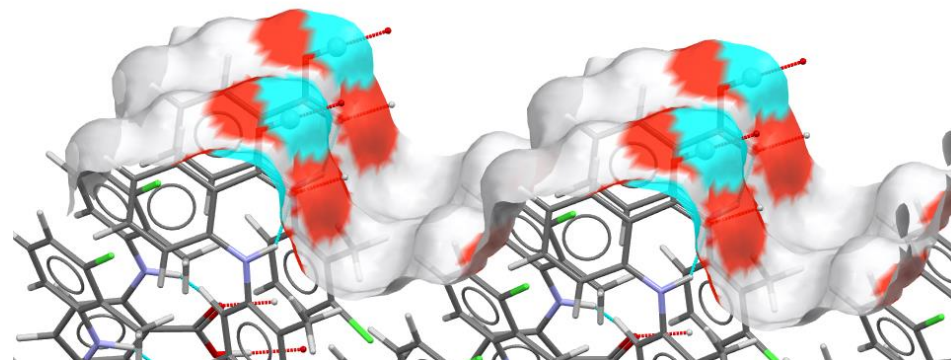
Unsatisfied Hydrogen Bonds

Unsatisfied hydrogen bond donors are defined as those whose hydrogen atom is surface-terminating and not being used in an existing hydrogen bond. They are reported as unsatisfied hydrogen bond donor density (count/Å²).

Elastic vs Plastic

An elastic material is a material that after compression can return to its initial shape and size once no more force is applied to it.

On the other hand, a plastic material would retain the deformation after the force has been removed.



Example of unsatisfied H-bond donors on the (020) surface of CSD Entry KAXXAI10.

Basics of Mercury Visualization






Mercury is the CCDC's visualization software to view 3D structures of small molecules, generate images, and animations of molecules.

In the following we will see some of the basics of navigation and visualization in Mercury that you will find helpful to support your analysis.

In the **Mercury interface** we find:

- **At the top:** list of menus from which we can access visualization and analysis options, and other CSD components such as CSD-Materials.
- **On the right-hand side:** the **Structure Navigator**, with the database loaded (depending on your licence). The Structure Navigator allows you to select a refcode to visualize in the main Mercury window.
- **Beneath the main display window:** **Display options toolbar**. You can quickly view a packing diagram, display Hydrogen bonding and detailed information about the molecule using the More Info option.

Using the **mouse to enhance visualization:**

-  Left mouse button and move – rotate molecules.
-  Middle Mouse wheel – move molecules up and down.
-  Right mouse button and move up and down – zoom in and out of molecules.
-  Shift + Left mouse button and move - rotate in the plane molecules.
-  Ctrl + Left mouse button and move - translate molecules.

Right click:

- Near a molecule and
- Away from a molecule

