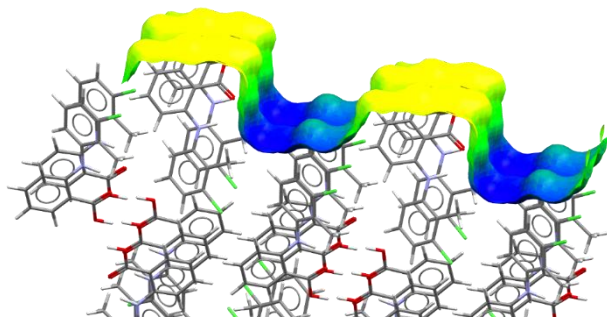


Surface Analysis with CSD-Particle U Try

Developed using
2022.3 CSD Release



CCDC
advancing structural science

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U Try – it's your turn!

In the second part of the *Surface Analysis with CSD-Particle* module, “U Try”, you will review the concepts and features presented in the first part, “U Watch”, and try them out yourself. If at any time you want to rewatch the videos, you can find them from the course webpage:

<https://www.ccdc.cam.ac.uk/community/training-and-learning/csdu-modules/particle-surface-analysis>

This tutorial will show you how to use CSD-Particle suite to visualize and analyse the mechanical and chemical properties of molecular crystals.

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

In this workshop you will learn how to:

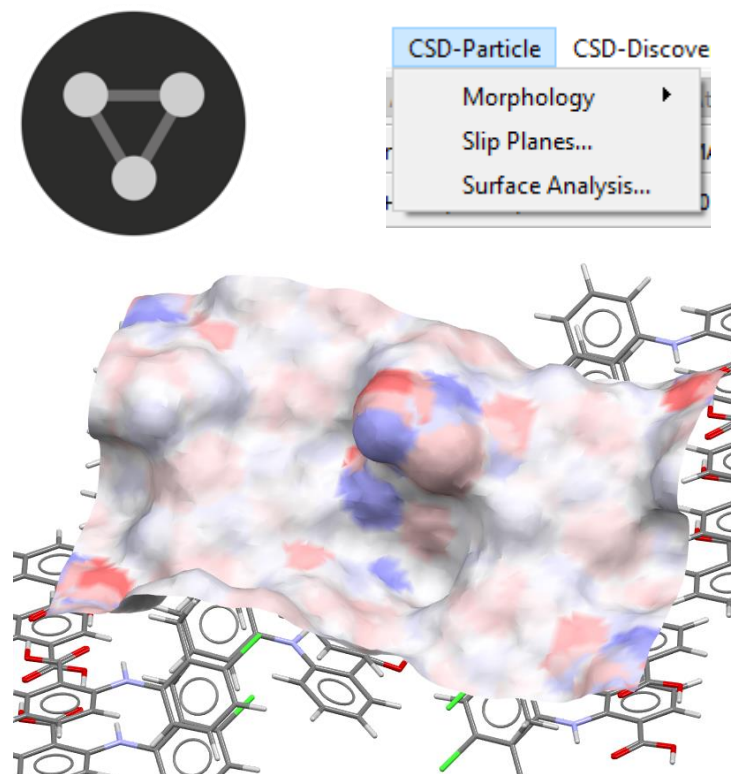
- Analyse particle surfaces.
- Calculate Full Interaction Maps on surfaces.

Note: The words in *Blue Italic* in the text are reported in the [Glossary](#) at the end of this handout. The exercise in this handout will take approximately **35-40 minutes** to be completed.

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 the relevant CSDU modules to get you started:

- <https://www.ccdc.cam.ac.uk/community/training-and-learning/csdu-modules/visualization-101/>
- <https://www.ccdc.cam.ac.uk/community/training-and-learning/csdu-modules/fims-101/>

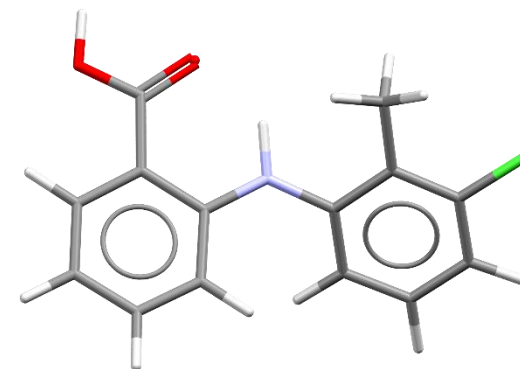


Materials


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.

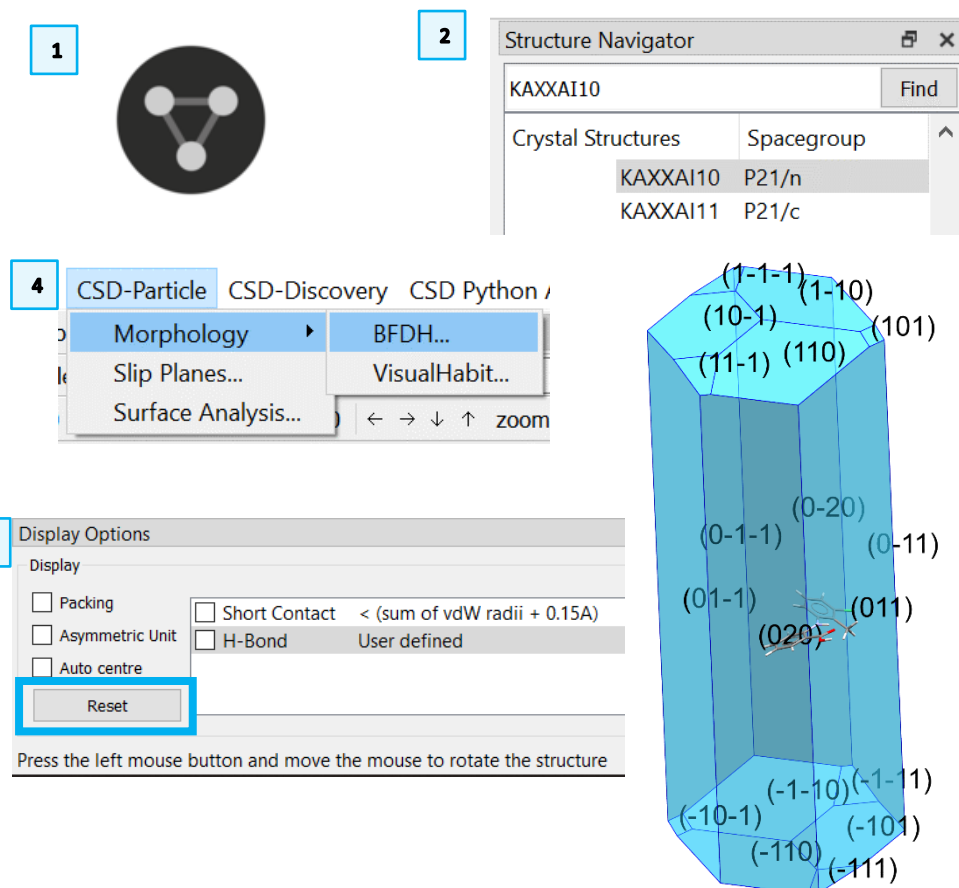


CSD Entry KAXXAI10 2-(3-chloro-2-methylanilino)benzoic acid

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.



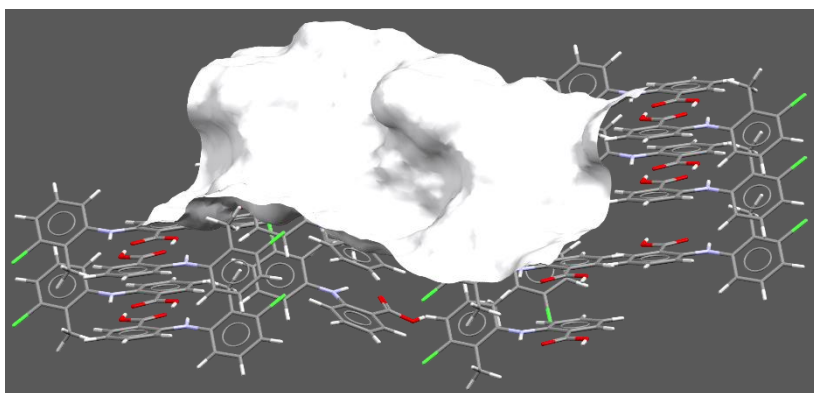
The screenshot illustrates the workflow in Mercury:

- Step 1:** The Mercury icon on the desktop.
- Step 2:** The **Structure Navigator** window showing the search for refcode KAXXAI10.
- Step 4:** The top-level menu path: **CSD-Particle > Morphology > BFDH...**
- Step 5:** The **Display Options** window with the **Reset** button highlighted.

On the right, a 3D model of the crystal morphology is shown, with various facets labeled with Miller indices: (1-1-1), (1-10), (10-1), (11-1), (110), (0-1-1), (0-20), (0-11), (01-1), (011), (-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 KAXXAI10 (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

CSD-Particle CSD-Discover

Morphology
Slip Planes...
Surface Analysis...

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

Density Info (count/Å²)

H-Bond Acceptors:	Aromatic Bonds:
H-Bond Donors:	Unsatisfied H-Bond Donors:

Topology Info

Surface Area (Å ²):	Projected Area (Å ²):
Rugosity:	RMSD:
Skewness:	Kurtosis:

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

Results - KAXXAI10 (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

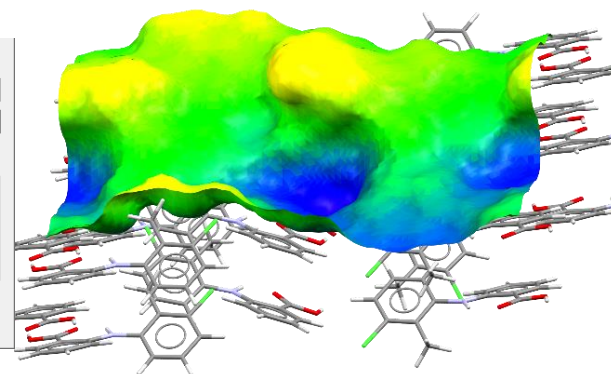
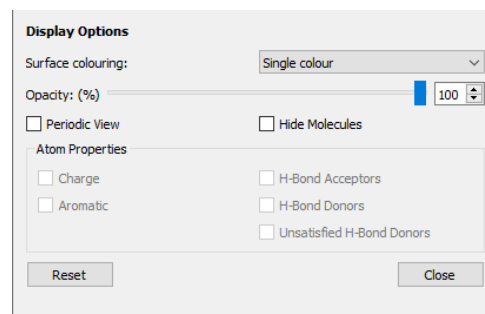
sharpness of the peak: values less than 3 signify a step-height change and values higher than 3 hint at a sharp peak.

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.

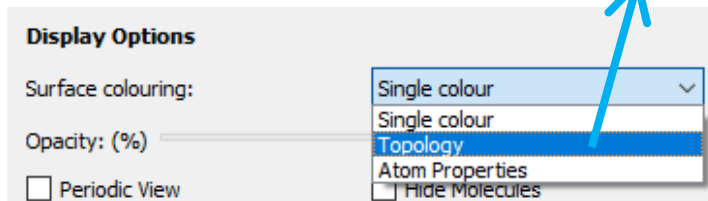
11. First, we will change the *Surface colouring* from *Single Colour* to *Topology* to get a better view of the height map of the surface. The areas closer to red are the peaks (note that in this case, we see a maximum of yellow), while the blue-purple areas are the valleys.

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 visualise 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.

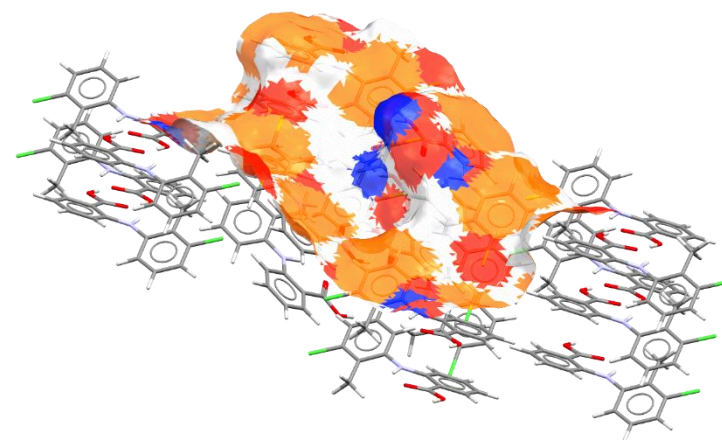
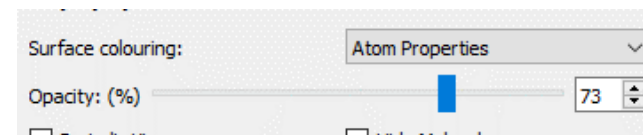
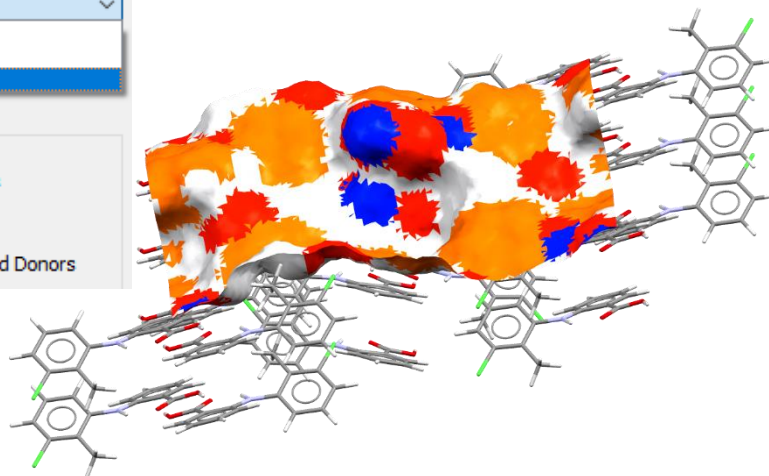
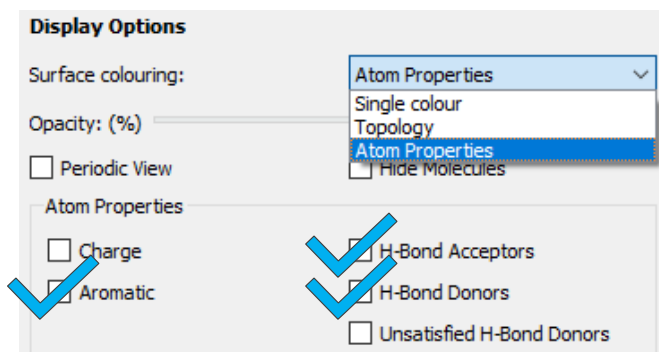
10



11



12

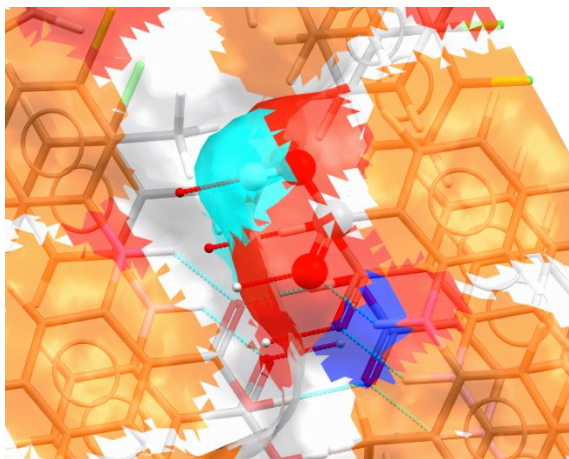


13. We will now visualise where hydrogen bond donors and acceptors are located by turning on H-Bonds in the *Display Options* box at the bottom of the Mercury interface.

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.

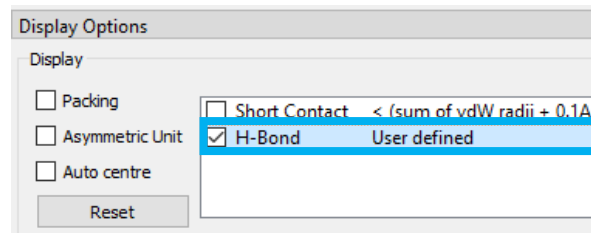
15a



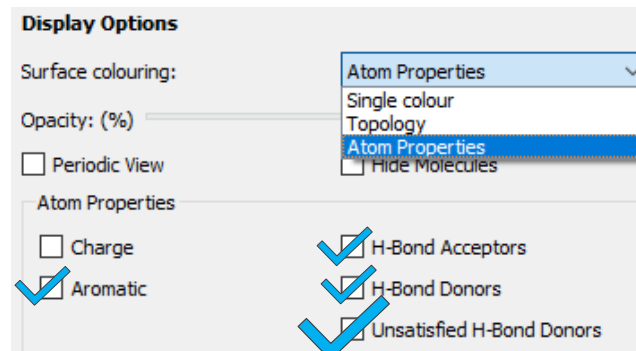
16. At the end of the analysis, turn off the hydrogen bonds by unticking the H-Bond box (opposite of **Step 13**).

17. The last atom's 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*.

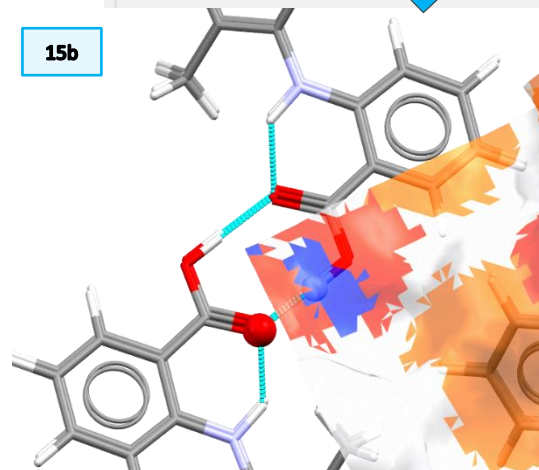
13



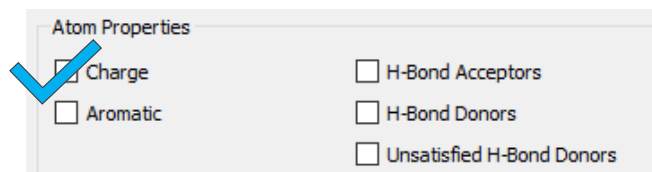
14



15b

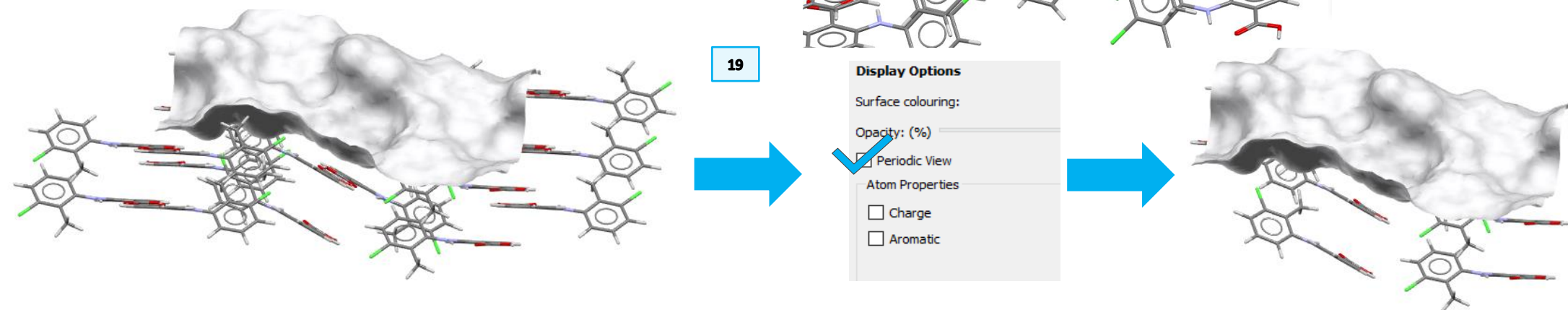


17



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.

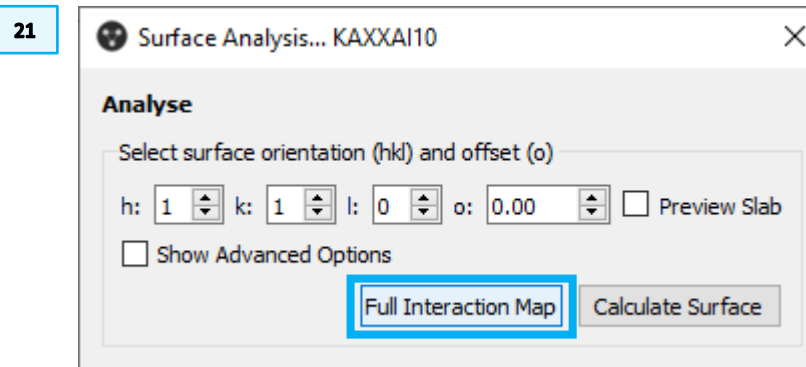
19. **Bonus tip:** If you tick the box next to *Periodic View* in the **Surface Analysis** dialog, you will only see the molecules that are within the bounding box of the surface. You may export this representation for further calculations, for example with Molecular Dynamics, Quantum Mechanics, or other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



FIMs on Surface

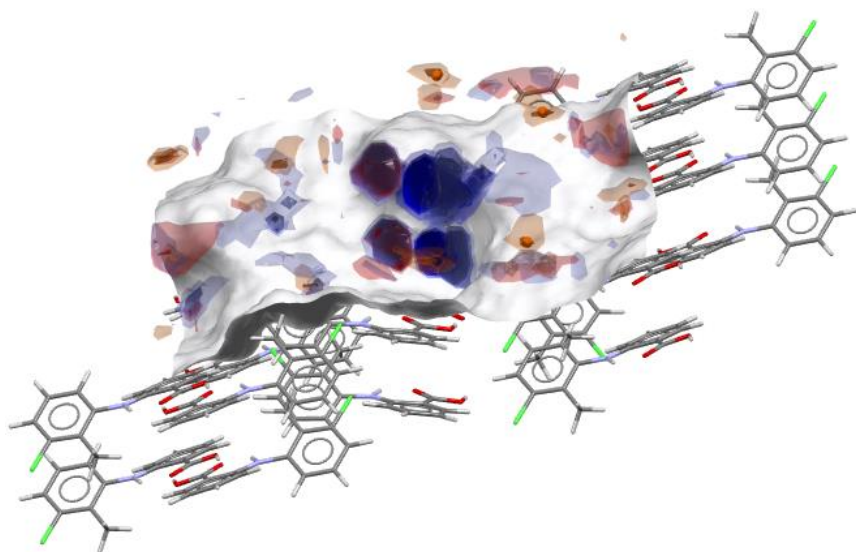
20. For the next part, we will study the Full Interaction Maps (FIMs) on Surface. We will start with the same surface analysed in the previous part of this example.

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.



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

Probe	Colour
<input checked="" type="checkbox"/> Uncharged NH Nitrogen	Blue
<input type="checkbox"/> Charged NH Nitrogen	Light Blue
<input type="checkbox"/> RNH3 Nitrogen	Dark Blue
<input type="checkbox"/> Alcohol Oxygen	Red
<input checked="" type="checkbox"/> Carbonyl Oxygen	Red
<input checked="" type="checkbox"/> Water Oxygen	Blue
<input type="checkbox"/> Oxygen Atom	Red
<input type="checkbox"/> Methyl Carbon	Yellow
<input checked="" type="checkbox"/> Aromatic CH Carbon	Orange
<input type="checkbox"/> C-F Fluorine	Green
<input type="checkbox"/> C-Cl Chlorine	Green
<input type="checkbox"/> C-Br Bromine	Brown
<input type="checkbox"/> C-I Iodine	Purple

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"/> All <input checked="" type="checkbox"/> Visible	<input type="checkbox"/> All <input checked="" type="checkbox"/> Visible	<input checked="" type="checkbox"/>
2 Carbonyl Oxygen	5.00	[1.21, 112.13]	Red	<input type="checkbox"/> All <input checked="" type="checkbox"/> Visible	<input type="checkbox"/> All <input checked="" type="checkbox"/> Visible	<input checked="" type="checkbox"/>
3 Water Oxygen	5.00	[1.03, 164.39]	Custom...	<input type="checkbox"/> All <input checked="" type="checkbox"/> Visible	<input type="checkbox"/> All <input checked="" type="checkbox"/> Visible	<input checked="" type="checkbox"/>
4 Aromatic CH Carbon	5.00	[1.02, 5.30]	Custom...	<input type="checkbox"/> All <input checked="" type="checkbox"/> Visible	<input type="checkbox"/> All <input checked="" type="checkbox"/> Visible	<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).

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

28

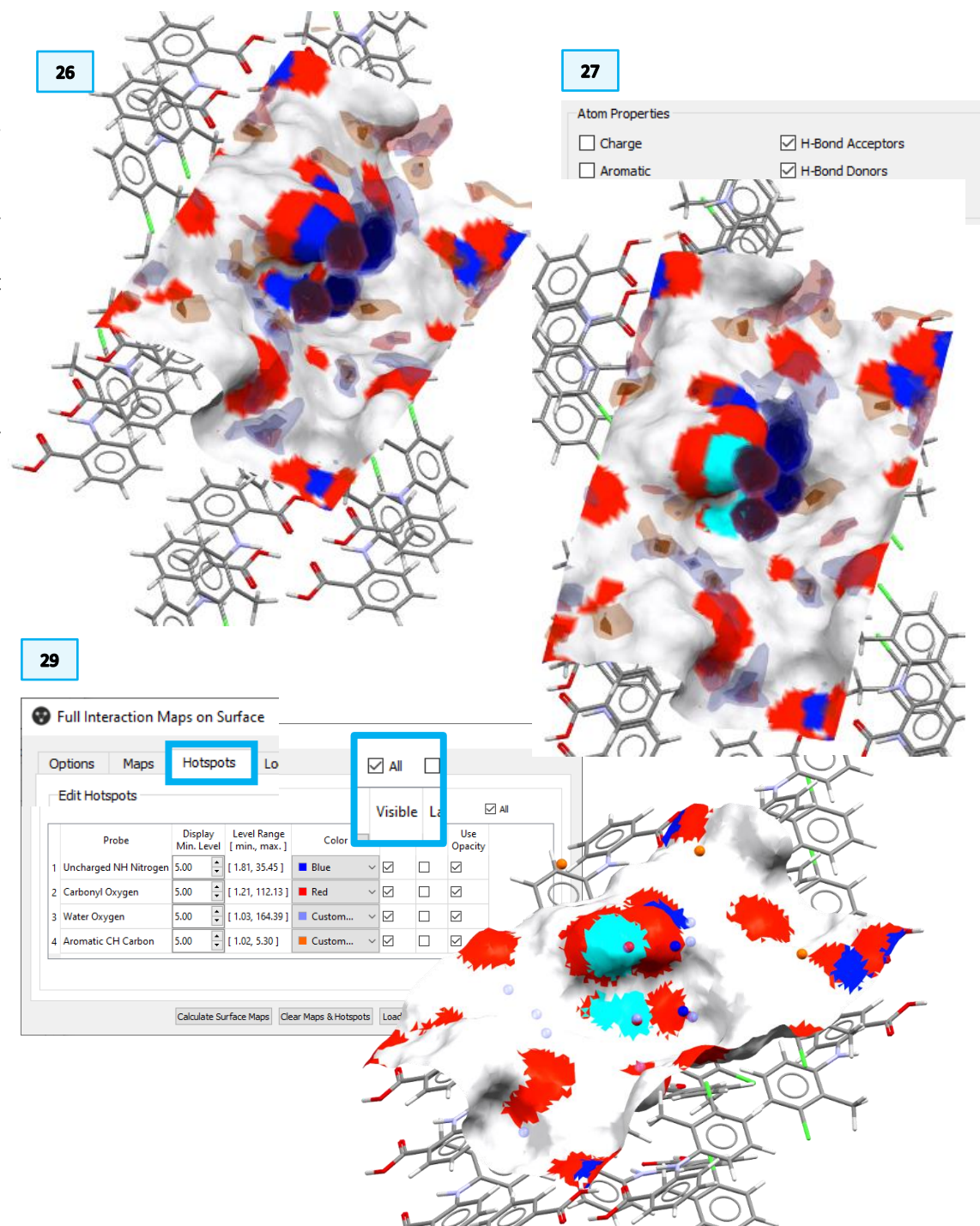
Probe	Level	Level Range [min., max.]	Color	Visible	Display Type	Opacity
1 Uncharged NH Nitrogen	2.00	[0.00, 35.45]	Blue	<input checked="" type="checkbox"/>	triangle	0.2
2 Uncharged NH Nitrogen	4.00	[0.00, 35.45]	Blue	<input checked="" type="checkbox"/>	triangle	0.5
3 Uncharged NH Nitrogen	6.00	[0.00, 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

29

☒ All

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 *k* to 0, for *l* 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 example by changing *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.

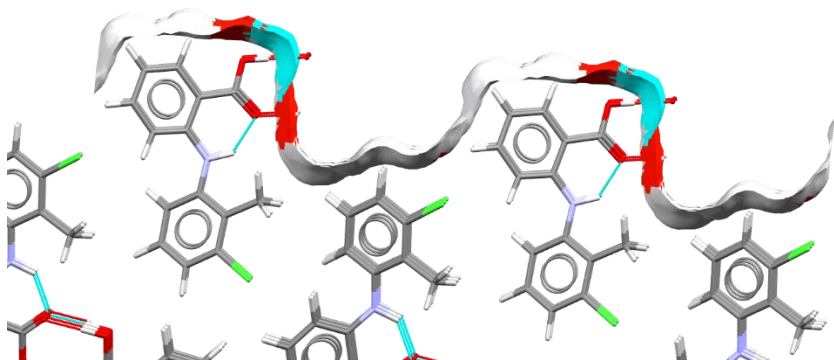
Probe Radius: 1.2 Grid Spacing: 0.3

Thickness (W) Factor 1.60

35 Full Interaction Map Calculate Surface

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.

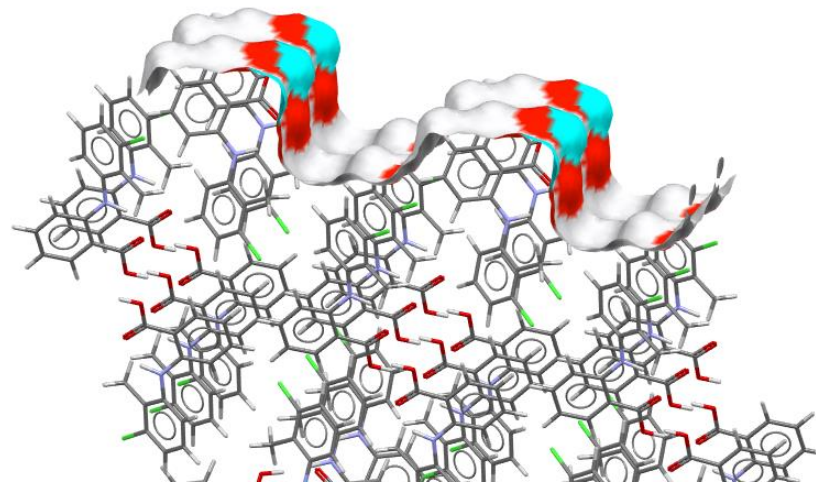


38. You may also observe the Gasteiger charges as in **Step 17** above.

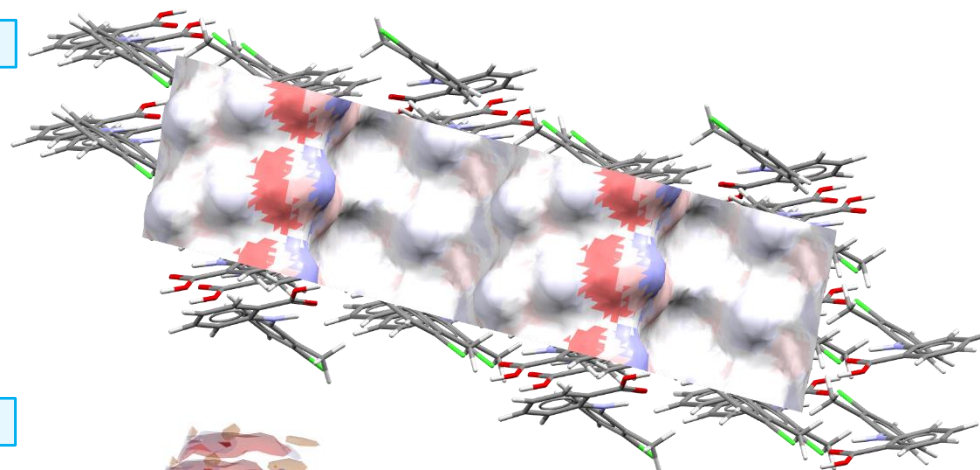
39. Next, we will generate FIMs on Surface, following **Steps 21 to 23** above.

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.

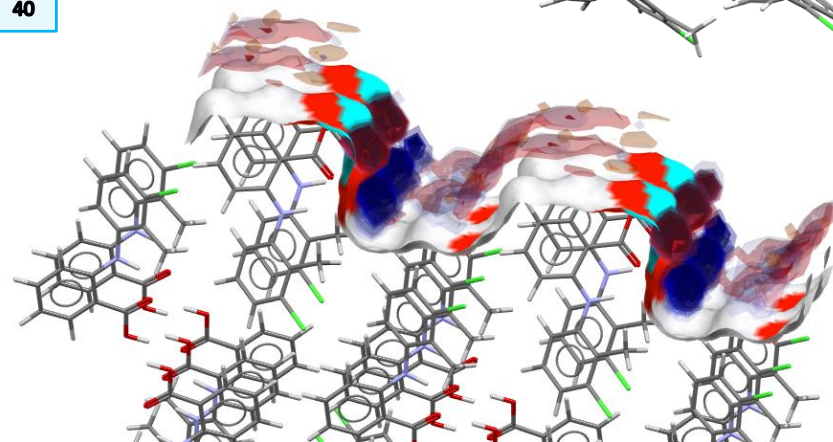
36



38

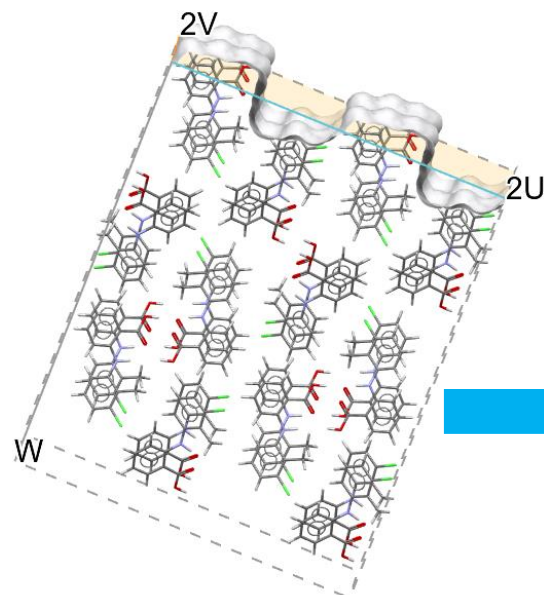


40

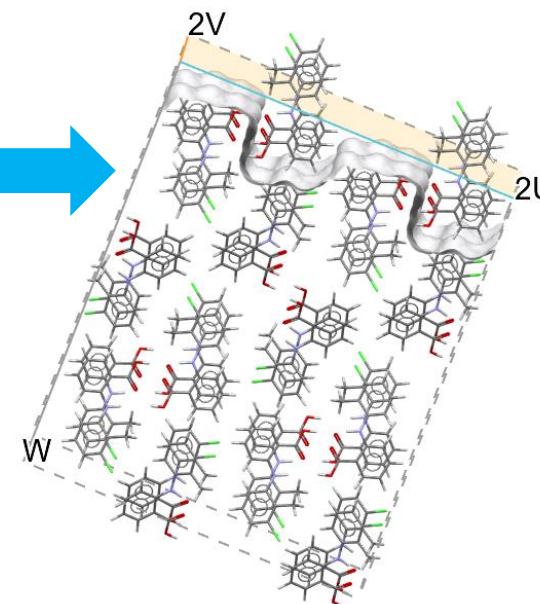
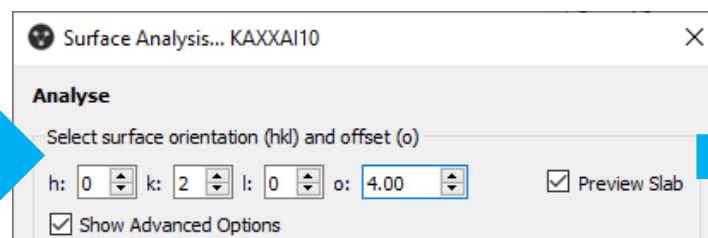


Exercise

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 impact the surface terminations. We set the offset to 4 Å.

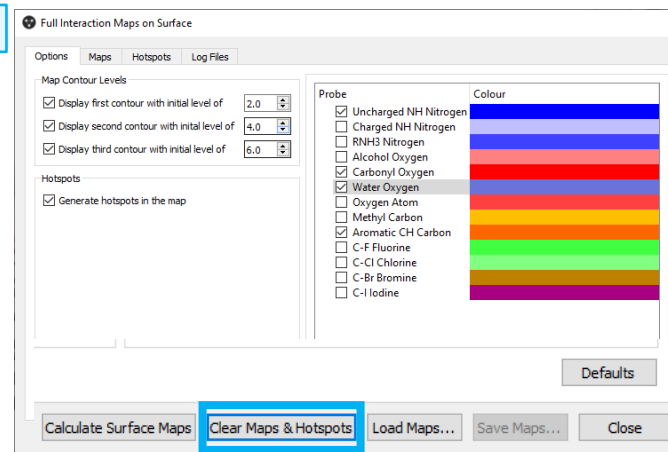


42



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

41

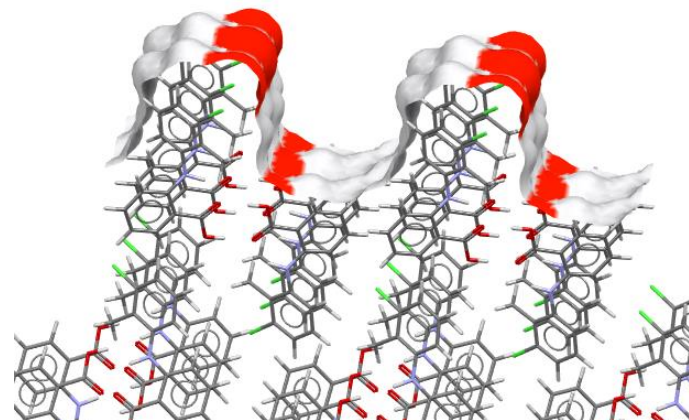


44. Observe the chemistry and the properties: how does changing the terminations impact the properties of the surface? What does it mean?

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 more in detail how to use tools from *Surface Analysis* from CSD-Particle to analyse two 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 visualise such properties in the 3D visualiser 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.



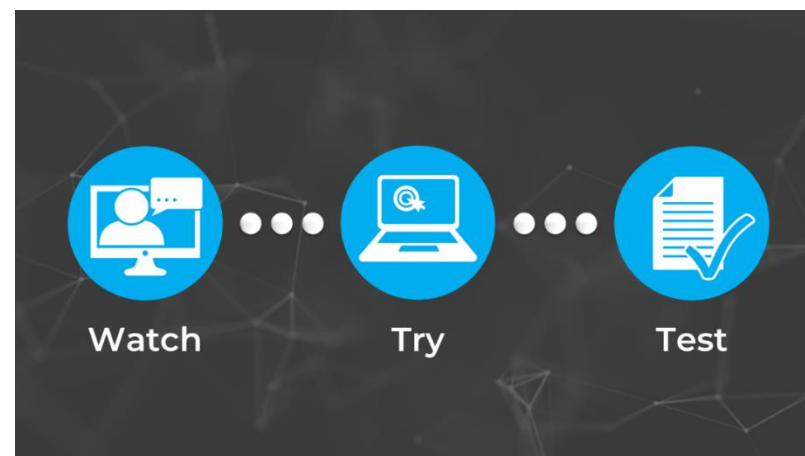
Summary

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 surface to quickly identify likely interactions.
- Visualise hydrogen bonds in Mercury.

Next Steps

Now that you have completed the Try part of this CSDU module, you can head to the final part: the quiz! Go back to the module webpage (<https://www.ccdc.cam.ac.uk/community/training-and-learning/csdu-modules/particle-surface-analysis>) and follow the instructions to complete the final test and earn a completion certificate.



Glossary

BFDH Morphology

Simulation of morphology using the Bravais Friedal 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

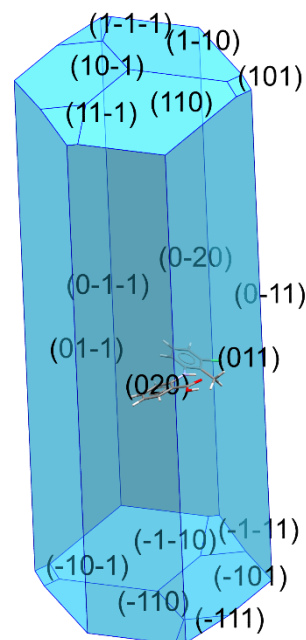
Hydrogen bonding occurs between donor-acceptor interactions precisely involving hydrogen atoms. The H-bonds interactions are classified as: strong (mostly covalent), moderate (mostly electrostatic) and weak (electrostatic). Their strength is observed to be between 12 and 30 kJ/mol.

Kurtosis

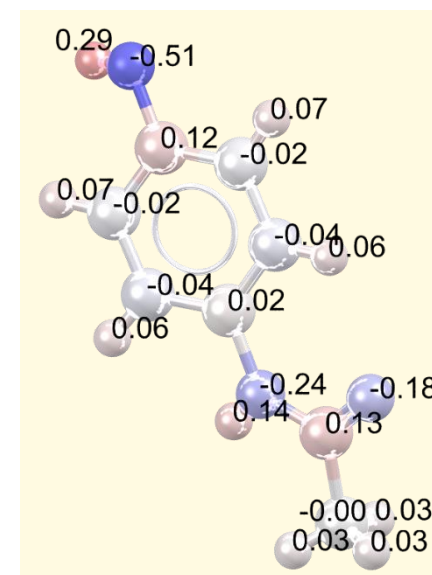
Kurtosis is a statistical characterisation of a dataset, such as surface topology, which measures the sharpness of height distribution and has a value of zero for a normal distribution. Positive values indicate a distribution with a sharp peak and long, "thick" tails. Negative values indicate a rounded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

Offset

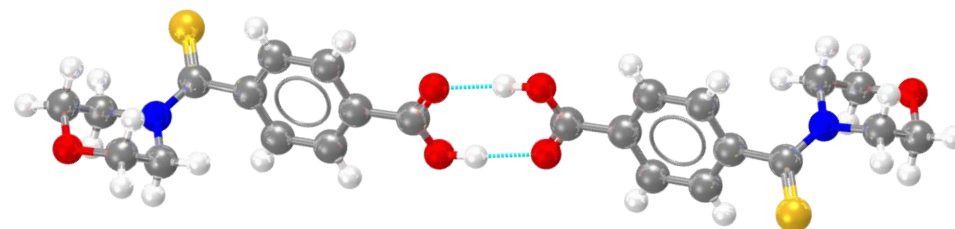
This is the value in Å of the distance to the calculated surface from the parallel Miller plane.



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.

Rugosity

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

Skewness

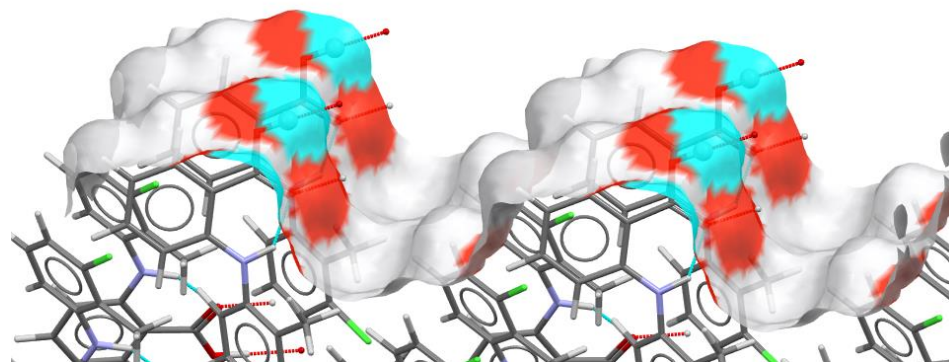
Statistical characterisation of a dataset, such as surface topology. Skewness measures the lack of symmetry, so in the case of surface topology, equal peaks and valleys would have a skewness of 0. If the surface was mostly valleys, then the skewness would be a negative value close to -1 and if the value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

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 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).



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