



SURFKIT USER MANUAL

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Materials Integrated Computation and Intelligent Design

Catalogue

Overview	2
Install.....	2
Getting started	4
Help.....	4
Find conventional cell	4
Redefinition of crystal cell	5
Creation of crystal slab	6
Search twist angles with small strain	8
Merge slabs with twist angles	10
Search for adsorption site	12
Absorb molecule to site	13

Overview

Surfkit is a command-line program aim at for creating high Miller index crystal slab, twisted bilayer and heterostructured slab and manipulating molecular adsorption at surface models to adapt especially for first principles calculations. This program contains functions as follows:

Find conventional cell

Redefinition of crystal cell

Creation of crystal slab

Merge slabs with twist angles

Search twist angles with small strain

Search for adsorption site

Absorb molecule to site

The program supports VASP POSCAR format as input or output. Using Surfkit you can get an output POSCAR file of crystal slab, twisted bilayer and heterostructured slab with molecular adsorption at surface models.

Install

For compiled version for Windows, Mac and Linux system.

`$tar -zxvf Surfkit_*.tar.gz`

You can find Surfkit in bin folder as executable file. You can also find two folder exp for example, and doc for documents.

For source code version

```
$tar -zxvf Surfkit_src.tar.gz
```

```
cd src
```

```
make
```

You can then find Surfkit in bin folder as executable file. You can also find three folders: src for source code, exp for example, and doc for documents.

Getting started

Help

`./Surfkit -h`

Show commands in Surfkit.

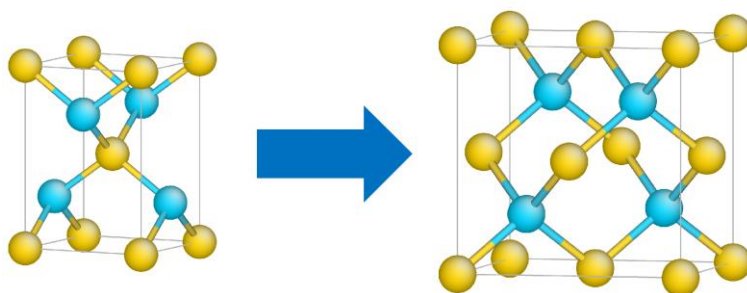
Find conventional cell

`Surfkit --conv [file1(In)] [file2(Out)]`

This command will convert any input cell into conventional cell. Running this step is highly recommend before redefinition. While [file1] means name of input POSCAR and the transformed cell is dumped to [file2].

For example: (run.sh in exp/BN folder)

`Surfkit --conv BN.POSCAR BN_conv.POSCAR`



This command will transform BN.POSCAR (left) to BN_conv.POSCAR (right).

Find 2D primitive cell

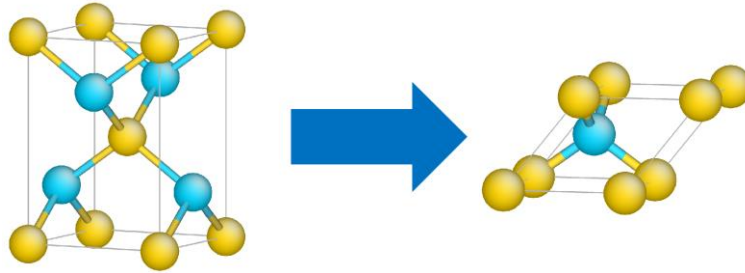
`Surfkit --prim2D [file1(In)] [file2(Out)]`

This command will convert any input cell into 2D primitive cell. Running this

step is highly recommend before redefinition. While [file1] means name of input POSCAR and the transformed cell is dumped to [file2].

For example: (run.sh in exp/BN folder)

Surfkit --prim2D BN.POSCAR BN_prim2D.POSCAR



This command will transform BN.POSCAR (left) to BN_prim2D.POSCAR (right)

Redefinition of crystal cell

Surfkit --proj -mat [file1(In)] [file2(Out)] a_h a_k a_l b_h b_k b_l c_h c_k c_l

This step will apply a transformation matrix to input cell. While [file1] means name of input POSCAR and the transformed cell is dumped to [file2]. Transform matrix is defined by:

$$\begin{pmatrix} \mathbf{a}' \\ \mathbf{b}' \\ \mathbf{c}' \end{pmatrix} = T \begin{pmatrix} \mathbf{a} \\ \mathbf{b} \\ \mathbf{c} \end{pmatrix} = \begin{pmatrix} a_h & a_k & a_l \\ b_h & b_k & b_l \\ c_h & c_k & c_l \end{pmatrix} \begin{pmatrix} \mathbf{a} \\ \mathbf{b} \\ \mathbf{c} \end{pmatrix}$$

Surfkit --proj -auto [file1(In)] [file2(Out)] c_h c_k c_l

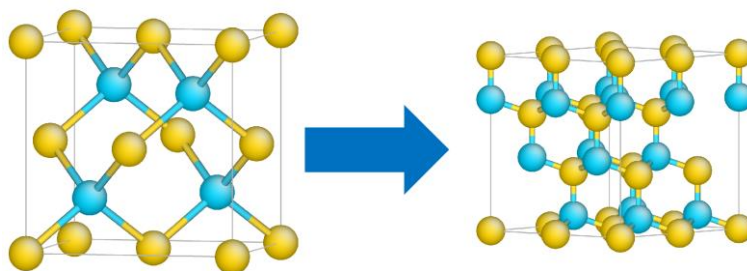
This step will auto generate a transformation matrix with given c_h c_k and c_l, and apply the transformation matrix to input cell. The automatically generated matrix will be printed to screen.

Surfkit --dup [file1(In)] [file2(Out)] a_h b_k c_l

This step will apply a diagonal matrix to input cell, while other element in matrix is set to zero.

For example: (run.sh in exp/BN folder)

Surfkit --proj -mat BN_conv.POSCAR BN_slab0.POSCAR 1 -1 0 1 0 -1 -1 -1



This command will transform BN_conv.POSCAR (left) to BN_slab0.POSCAR (right).

Cleavage of crystal slab

Surfkit --scan [file1(In)] [min height] [max height]

This command will dump all atomic layer and non-polar center in input POSCAR named [file1] between min height and max height unit Å.

Surfkit --shift [file1(In)] [file2(Out)] [shift height]

This command will convert input POSCAR named [file1] to output POSCAR named [file2] with shift demanded height unit Å.

Surfkit --cleav [file1(In)] [file2(Out)] [min height] [max height]

This command will convert input POSCAR named [file1] to crystal slab POSCAR named [file2] with min height and max height unit Å.

Surfkit --vacuum [file1(In)] [file2(Out)] [vacuum thickness]

This command will convert input POSCAR named [file1] to crystal slab POSCAR named [file2] with vacuum thickness L_v in unit Å.

New cell is defined as follows:

$$\mathbf{c}' = \frac{\mathbf{a} \times \mathbf{b}}{|\mathbf{a} \times \mathbf{b}|} \left[(c_{max} - c_{min}) \mathbf{c} \cdot \frac{\mathbf{a} \times \mathbf{b}}{|\mathbf{a} \times \mathbf{b}|} + L_v \right] \quad (4)$$

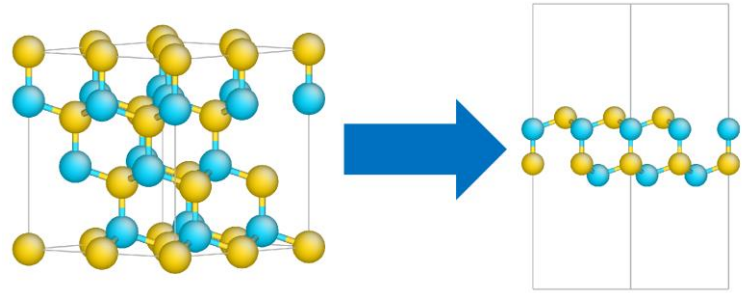
where L_v is the thickness of the vacuum layer to ensure that the lattice vector perpendicular to the crystal plane is sufficiently large to avoid interactions with its periodic image, $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ and $(\mathbf{a}', \mathbf{b}', \mathbf{c}')$ are the basis vectors of crystal cell before and after convention. To be noted that c_{max} and c_{min} is the minimum and maximum fractional coordinates of current slab cell in range of $\left(\frac{h_{min}|\mathbf{a} \times \mathbf{b}|}{|\mathbf{c} \cdot (\mathbf{a} \times \mathbf{b})|}, \frac{h_{max}|\mathbf{a} \times \mathbf{b}|}{|\mathbf{c} \cdot (\mathbf{a} \times \mathbf{b})|} \right)$, where h_{min} , h_{max} represent the minimum and maximum height of the cleavage plane respectively. Atoms with heights higher than h_{max} and lower than h_{min} will be removed. Subsequently, by adjusting the atomic coordinates along the c-axis, the atoms can be positioned at the midpoint between the minimum and maximum fractional coordinates. This ensures that the top and bottom vacuum thickness on each side of the slab is equal.

For example: (run.sh in exp/BN folder)

Surfkit --scan BN_slab0.POSCAR -5 5

Surfkit --thick BN_slab0.POSCAR BN_slab1.POSCAR -2 0

Surfkit --vacuum BN_slab1.POSCAR BN_slab2.POSCAR 10



These commands will transform BN_slab0.POSCAR (left) to BN_slab2.POSCAR (right).

Search twist angles with small strain

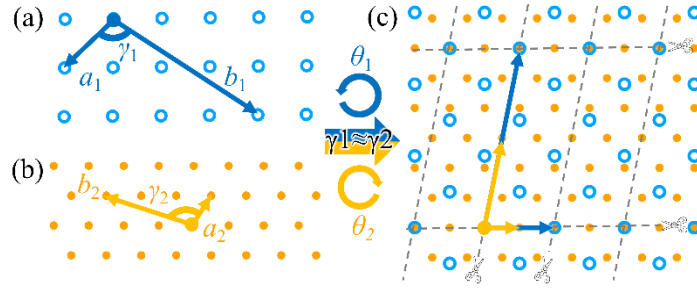
Surfkit --match [file1(Slab)] [file2(Slab)] {[limit] [parameter]}...

Surfkit --match [file1(Slab)] [file2(Slab)] maln [max vector length] miln [min vector length] mbox [max box length] mtwi [max twist angle] mvec [max axial mismatch] mang [max angle mismatch] magm [max rotate angle] migm [min rotate angle]

This command will search any possible twisted bilayer and heterostructure slab under limitation from POSCAR file named [file1] and [file2]. Limitation command can be added after file name or default value will be used. You can check this table for meaning of limitation:

Limit	Meaning	Symbol	Default
maln	Max length of vector, unit: Å	a_1, a_2, b_1, b_2	20
miln	Min length of vector, unit: Å	a_1, a_2, b_1, b_2	0
mbox	Max length of box, unit: Å	$n_a a_1, n_b b_1$	40

mtwi	Max twist angle, unit: degree	$ \theta_1 - \theta_2 $	20
magn	Max lattice angle, unit: degree	γ_1, γ_2	160
migm	Min lattice angle, unit: degree	γ_1, γ_2	20
mvec	Max axial mismatch	$\varepsilon_a, \varepsilon_b$	0.005
mang	Max angle mismatch, unit: degree	$ \gamma_1 - \gamma_2 $	1



Vector, twist angle, lattice angle and angle mismatch are defined by above figure.

axial mismatch is defined as follows

$$\varepsilon_a = \min \left(\frac{a_1 \cdot n_a - a_2 \lfloor a_1 \cdot n_a / a_2 \rfloor}{a_1 \cdot n_a + a_2 \lfloor a_1 \cdot n_a / a_2 \rfloor}, \frac{a_2 \lceil a_1 \cdot n_a / a_2 \rceil - a_1 \cdot n_a}{a_1 \cdot n_a + a_2 \lceil a_1 \cdot n_a / a_2 \rceil} \right)$$

$$\varepsilon_b = \min \left(\frac{b_1 \cdot n_b - b_2 \lfloor b_1 \cdot n_b / b_2 \rfloor}{b_1 \cdot n_b + b_2 \lfloor b_1 \cdot n_b / b_2 \rfloor}, \frac{b_2 \lceil b_1 \cdot n_b / b_2 \rceil - b_1 \cdot n_b}{b_1 \cdot n_b + b_2 \lceil b_1 \cdot n_b / b_2 \rceil} \right)$$

where ε_a and ε_b is the axial strain along a and b, n_a and n_b are the scaling numbers of a_1 and b_1 , the algorithm will traverse all integer value until axial strain reaches minimum or until $a_1 \cdot n_a$ reach the upper limitation of box length. $\lfloor \cdot \rfloor$ means round to integer, $\lceil \cdot \rceil$ means ceiling to integer, min means the minimum value between two strains. If the minimum strain were calculated by round value $\lfloor a_1 \cdot n_a / a_2 \rfloor$ or $\lfloor b_1 \cdot n_b / b_2 \rfloor$ are scaling numbers of a_2 and b_2 , otherwise $\lceil a_1 \cdot n_a / a_2 \rceil$ or $\lceil b_1 \cdot n_b / b_2 \rceil$ are scaling number.

Using this command, you will get a CSV format file named “**mismatch.csv**” which can be viewed by excel or sorted by panda lib of python. However, editing data is not allowed because it will change result in the following step. “**mismatch.csv**” contains column as follows:

Column name	Meaning	Symbol
Twist Angle	Twist angle between file1 and file2	$ \theta_1 - \theta_2 $
Rotate Angle1	Rotate angle of file1	θ_1
Rotate Angle2	Rotate angle of file2	θ_2
Sigma1	Coincidence site lattice parameter reference to file 1	Σ
Sigma2	Coincidence site lattice parameter reference to file 2	Σ
a Axial Mismatch	Axial mismatch along a axis	ε_a
b Axial Mismatch	Axial mismatch along b axis	ε_b
Angle Mismatch	Angle Mismatch	$ \gamma_1 - \gamma_2 $
1M11 1M12 1M21 1M22	Deformation matrix of file 1	a_h, a_k, b_h, b_k
2M11 2M12 2M21 2M22	Deformation matrix of file 2	a_h, a_k, b_h, b_k

Merge slabs with twist angles

Surfkit --twist [file1(Slab)] [file2(Slab)] [file3(Output)] [twist angle]

This command will build selected twisted bilayer and heterostructure slab according to “**mismatch.csv**” under current folder, so make sure you are using same

[file1] [file2] when generating “**mismatch.csv**”. The twist angle which is most close to input parameter will be selected for generating POSCAR file named [file3].

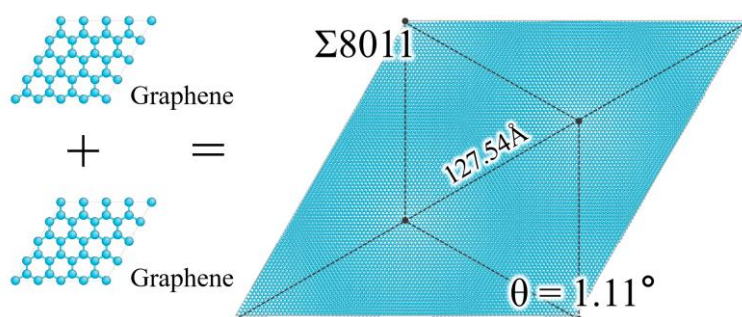
For example: (run.sh in exp/Graphene folder)

Surfkit --match GRAPHENE.POSCAR GRAPHENE.POSCAR maln 230 miln

220 mbox 230 mtwi 6 mvec 0.00001 magm 122 migm 118 mang 0.01

Surfkit --twist GRAPHENE.POSCAR GRAPHENE.POSCAR S8011.POSCAR

1.1



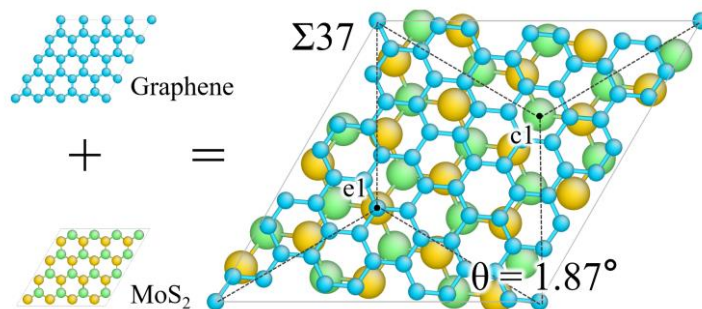
These commands will generate mismatch.csv under current folder and transform Graphene.POSCAR (left) to S8011.POSCAR (right).

For example: (run.sh in exp/Graphene-MoS2 folder) for heterostructure

Surfkit --match GRAPHENE.POSCAR MoS2.POSCAR mlen 50 mbox 50 mtwi

10 mvec 0.02 magm 125 migm 115 mang 0.1

Surfkit --twist GRAPHENE.POSCAR MoS2.POSCAR S37.POSCAR 1.871770



These commands will generate mismatch.csv under current folder and transform

Graphene.POSCAR and MoS₂ (left) to S37.POSCAR (right).

Adjust spacing of slabs

Surfkit --space [file1(Slab)] [file2(Output)] [Height] {[Max step] [Distance/auto]}

This command will change distance between layer above Height and beyond Height to Distance in file1, and dump the result to file2. If auto is used, distance will be set to average bond length among both layers. Max step is used to limit calculation. In most conditions, 1000 steps are sufficient.

For example: (run.sh in exp/Graphene-MoS2 folder) for heterostructure

Surfkit --space S37.POSCAR S37.POSCAR 3 1000 auto

Search for adsorption site

Surfkit --site2D [file1(Slab)] [file2(Site List)] [Distance(2D)] [Max multiplicity]

This command will search any possible adsorption site in ab plane under limitation from POSCAR file named [file1] in 2D search mode (more definition in paper). Sites will be saved to POSCAR file named [file2]. Status of possible sites will be saved to “**Status.csv**” which contains three columns: **Type**, **Name** and **Sum**. **Type** is used to locate adsorption site in the following step. In most condition, the smaller type is, the smaller the multiplicity is. **Name** is the Wyckoff symbol of current site. **Sum** is how many sites in current model of current type. Distance (2D) is the distance between current site list and the top of surface slab along c axis. Max multiplicity is the maximum multiplicity of searched result.

Surfkit --site3D [file1(Slab)] [file2(Site List)] [Distance(3D)] [Max multiplicity]

This command will search any possible adsorption site in ab plane under limitation from POSCAR file named [file1] in 3D search mode (more definition in paper). Sites will be saved to POSCAR file named [file2]. Status of possible sites will be saved to “**Status.csv**” which contains three columns: **Type**, **Name** and **Sum**. **Type** is used to locate adsorption site in the following step. In most condition, the smaller type is, the smaller the multiplicity is. **Name** is the Wyckoff symbol of current site. **Sum** is how many sites in current model of current type. Site whose distance between the top of surface slab along c axis above Distance(3D) will be deleted. Max multiplicity is the maximum multiplicity of searched result.

Absorb molecule to site

Surfkit --adsorb -ele [file1(Slab)] [file2(Site List)] [file3(Output)] [Type] [ID] [Element]

This command will adsorb one atom to surface slab POSCAR file named [file1], [file2] is the output of *Search for adsorption site*. [Type] can be referenced from “**Status.csv**”. [ID] is the nth site of [Type]. [Element] is the output element of added atom.

Surfkit --adsorb -file [file1(Slab)] [file2(Site List)] [file3(Output)] [Type] [ID] [file4(Molecular)] [Element] [Element ID] [M11] [M12] [M13] [M21] [M22] [M23] [M31] [M32] [M33]

Surfkit --adsorb -file [file1(Slab)] [file2(Site List)] [file3(Output)] [Type] [ID]

[file4(Molecular)] [Element] [Element ID]

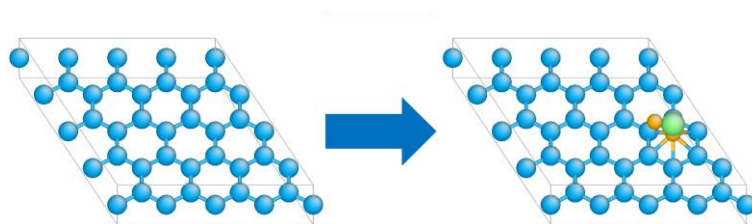
This command will adsorb atoms defined in POSCAR file [file4] to surface slab POSCAR file named [file1], [file2] is the output of *Search for adsorption site*. [Type] can be referenced from **“Status.csv”**. [ID] is the nth site of [Type]. [Element] is the element of atom which will be overlayed on adsorption site. [Element ID] is the nth atom of [Element]. [Mxx] is the element of 3x3 rotation matrix, which is not needed to be unitized.

For example: (run.sh in exp/Adsorption_Graphene folder)

Surfkit --site2D Graphene.POSCAR 2D.POSCAR 1 3

Surfkit.exe --adsorb -file Graphene.POSCAR 2D.POSCAR Slab.POSCAR 1 5

H2O.poscar H 1 0 1 0 1 0 0 0 1

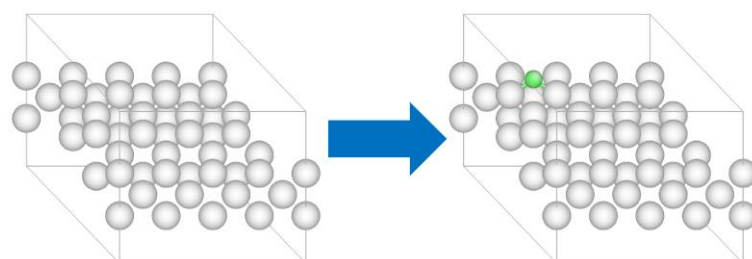


These commands will generate status.csv under current folder and transform Graphene.POSCAR and H2O.POSCAR (left) to Slab.POSCAR (right).

For example: (run.sh in exp/Adsorption_Pt folder)

Surfkit.exe --site3D Pt211.POSCAR 3D.POSCAR 1 9

Surfkit.exe --adsorb -ele Pt211.POSCAR 3D.POSCAR Slab.POSCAR 3 1 H



These commands will generate status.csv under current folder and transform Pt211.POSCAR(left) to Slab.POSCAR (right).