

Crystal Builder Insert vacuum

Gold slab

V7.003

X-Ability Co,. Ltd.

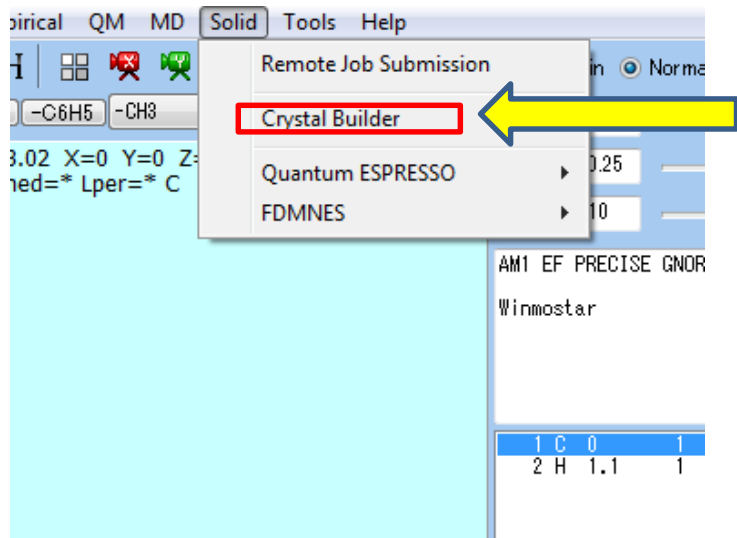
question@winmostar.com

2016/11/01

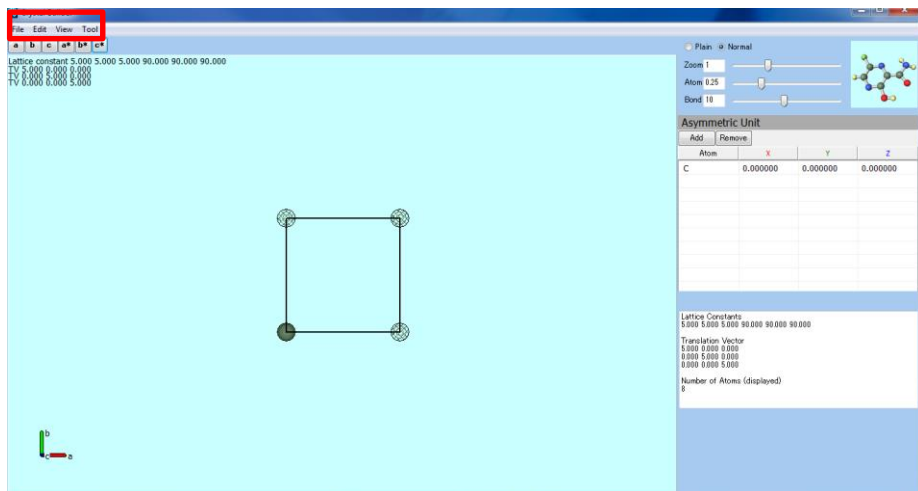
Contents

- I. Define a unit cell
- II. Insert vacuum layer

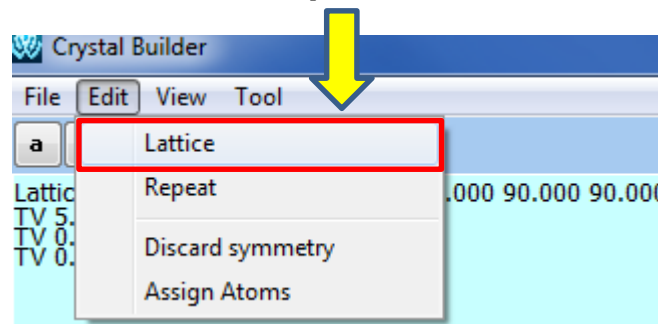
I. Define a unit cell



1. Click **Solid | Crystal Builder**.

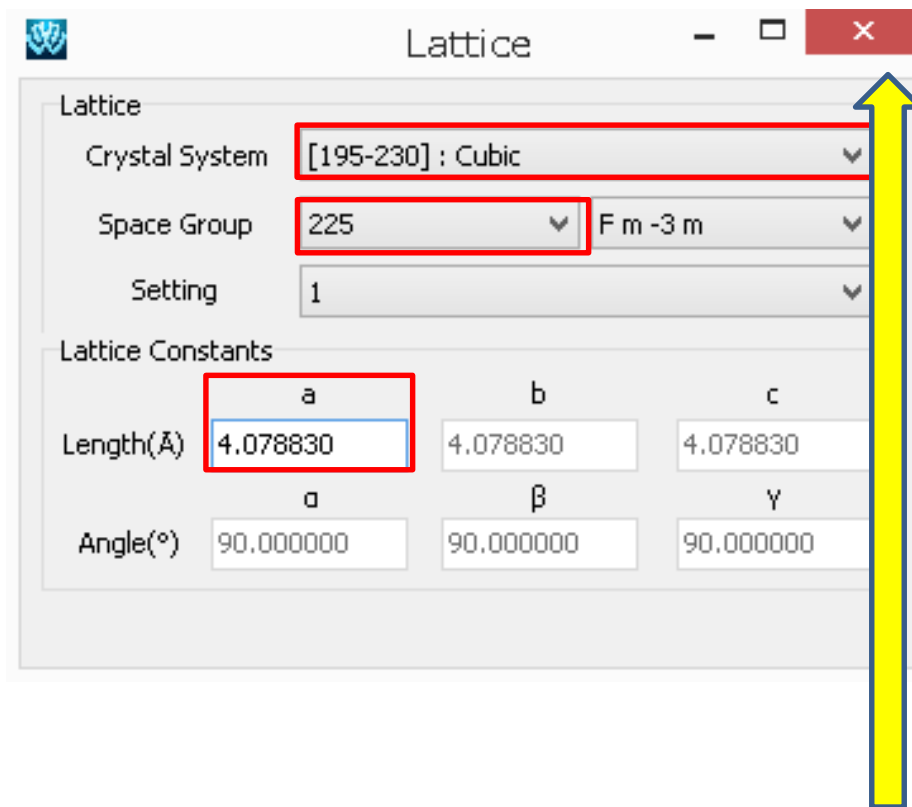


2. Click **Edit | Lattice**.



I. Define a unit cell

1. Set **Crystal System** to **Cubic**.
2. Set **Space Group** to **225**.
3. Set **a** to **4.07883** and push the Enter key.



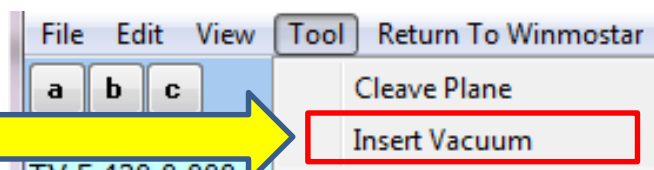
4. Click here to close.

I. Define a unit cell

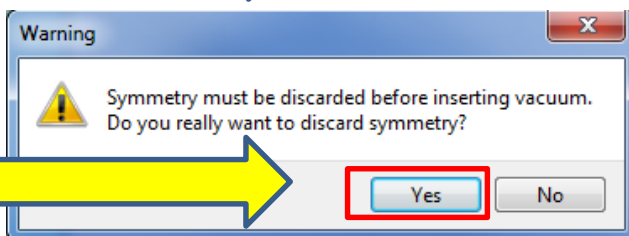
1. Enter **Au.** 

Asymmetric Unit			
Add Remove			
Atom	X	Y	Z
Au	0.000000	0.000000	0.000000

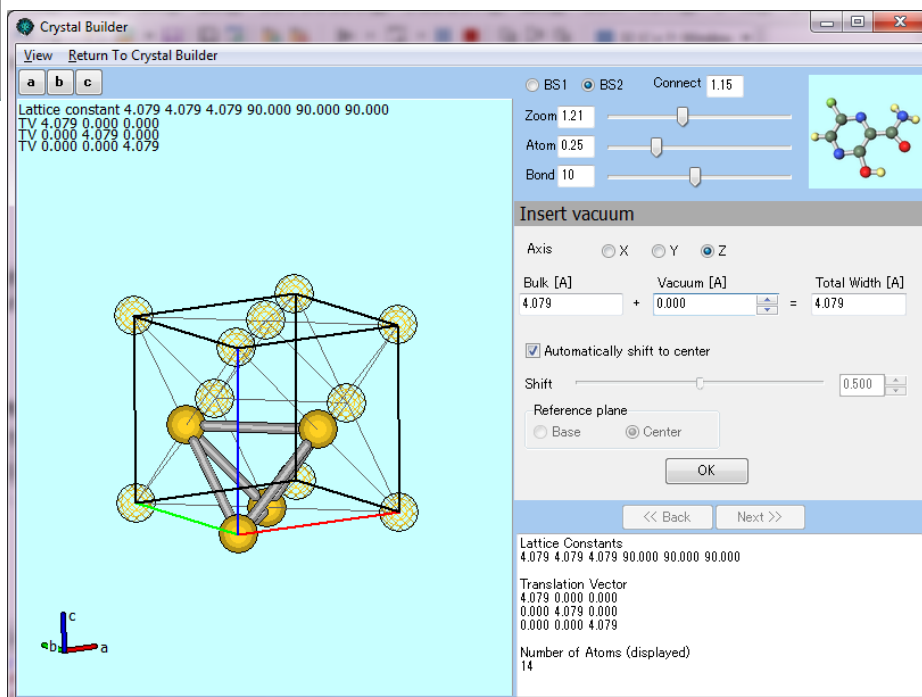
2. Click. 



3. Click. 



Insert vacuum mode will start.

II. Insert vacuum layer

Set **Vacuum** to **25**. It defines the thickness of the vacuum layer.

Click **OK** to quit Insert vacuum mode.

Crystal Builder

View Return To Crystal Builder

a b c

Lattice constant 4.079 4.079 4.079 90.000 90.000 90.000
TV 4.079 0.000 0.000
TV 0.000 4.079 0.000
TV 0.000 0.000 29.079

BS1 BS2 Connect 1.15

Zoom 0.44

Atom 0.25

Bond 10

Insert vacuum

Axis X Y Z

Vacuum [A] 25.000 = Total Width [A] 29.079

Automatically shift to center

Shift 0.500

Reference plane Base Center

OK

<< Back Next >>

Lattice Constants
4.079 4.079 4.079 90.000 90.000 90.000

Translation Vector
4.079 0.000 0.000
0.000 4.079 0.000
0.000 0.000 4.079

Number of Atoms (displayed)
24