

# Crystal Builder Insert vacuum

Gold slab

V8.007

X-Ability Co.,. Ltd.

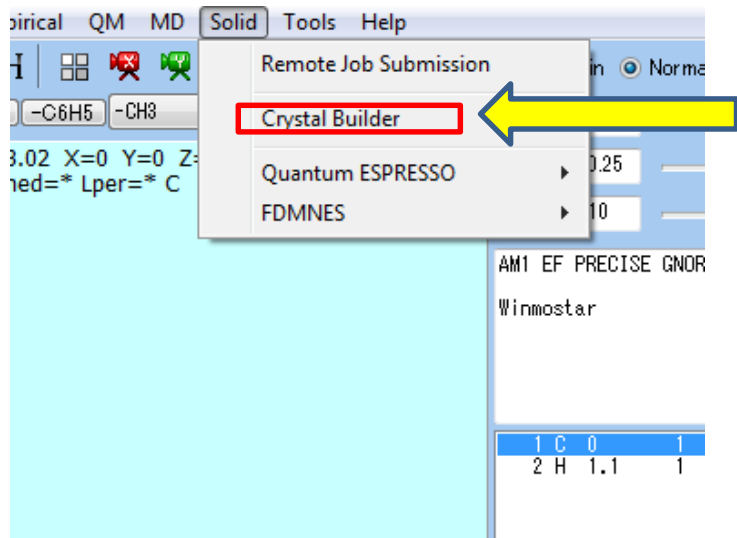
[question@winmostar.com](mailto:question@winmostar.com)

2018/01/15

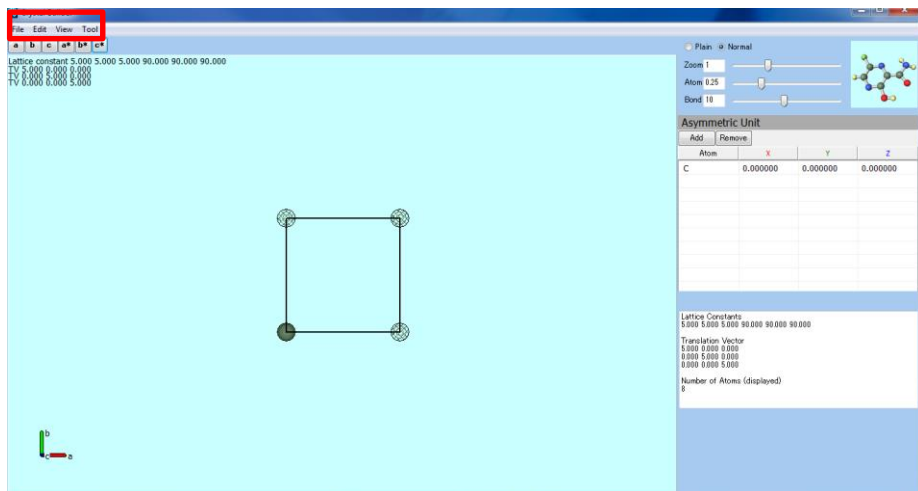
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- I. Define a unit cell
- II. Insert vacuum layer

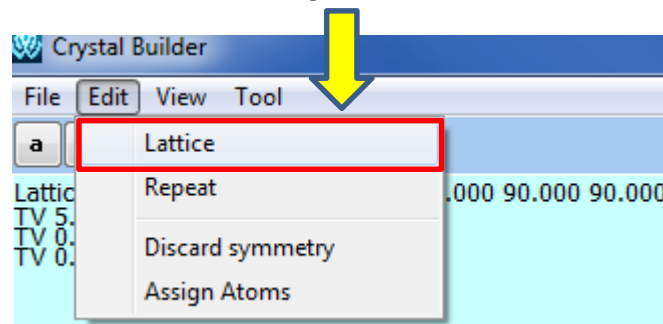
# I. Define a unit cell



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

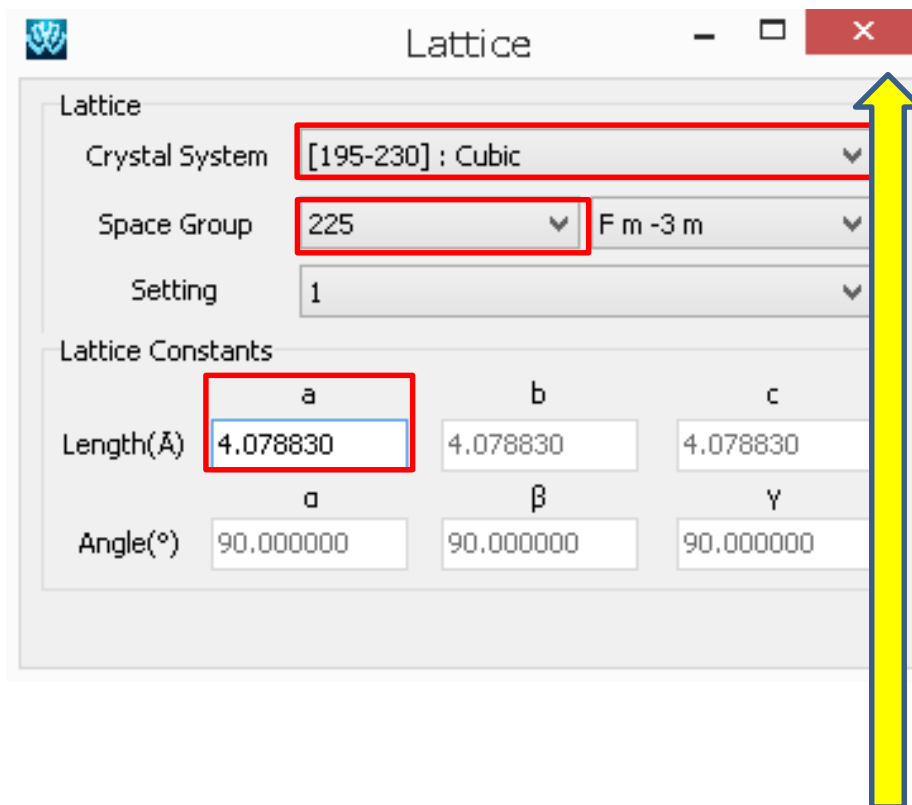


2. Click **Edit | Lattice**.



# 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.



Lattice			
Crystal System	[195-230] : Cubic		
Space Group	225	F m -3 m	
Setting	1		
Lattice Constants			
	a	b	c
Length(Å)	4.078830	4.078830	4.078830
	α	β	γ
Angle(°)	90.000000	90.000000	90.000000

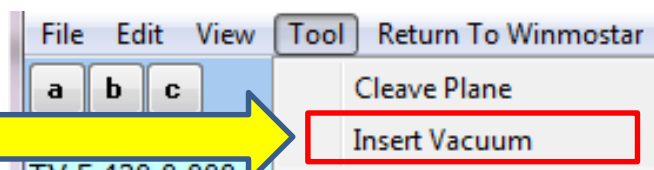
4. Click here to close.

# I. Define a unit cell

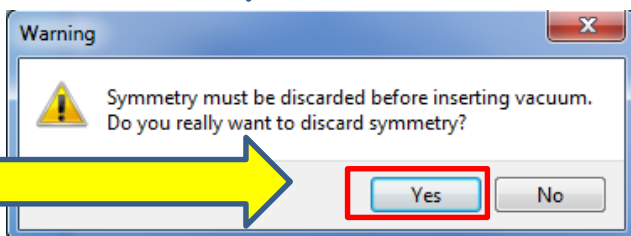
1. Enter **Au.** 

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

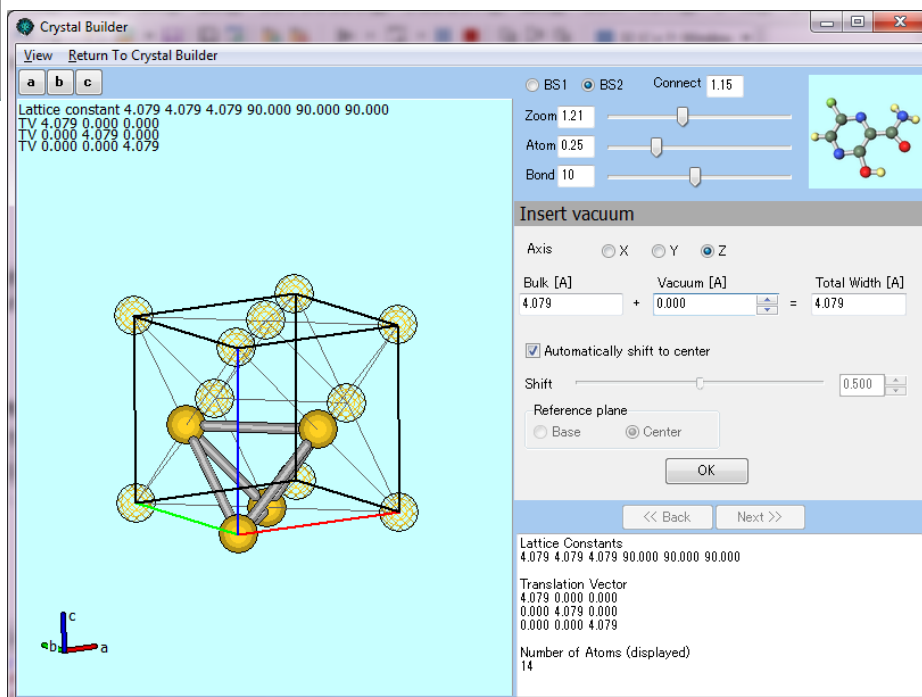
2. Click. 



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 [Å] = Total Width [Å]  
 25.000 = 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