Materials Studio/VESTA教程

v1.4

# 前言

Materials Studio、VESTA是优秀的晶体建模软件，文档基于Win7-64位、MS v8.0、VESTA 3.3.8。

更新：<https://www.misaraty.com/2019-04-16_materials-studio-vesta/>。

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# 目录

[前言 1](#_Toc465199211)

[目录 2](#_Toc465199212)

[Materials Studio 3](#_Toc465199213)

[功能简介 3](#_Toc465199214)

[创建晶胞 5](#_Toc465199215)

[苯甲酰胺分子 5](#_Toc465199216)

[尿素晶体 9](#_Toc465199217)

[调整显示晶胞数量 9](#_Toc465199218)

[α石英晶体 11](#_Toc465199219)

[不同晶胞结构对比 11](#_Toc465199220)

[聚甲基丙烯酸甲酯 15](#_Toc465199221)

[超晶胞 16](#_Toc465199222)

[界面 17](#_Toc465199223)

[界面加真空层 18](#_Toc465199224)

[VESTA 19](#_Toc465199225)

[下载 19](#_Toc465199226)

[创建晶胞 19](#_Toc465199227)

[导出600dpi tif 21](#_Toc465199228)

[截取晶面 22](#_Toc465199229)

[调整晶胞边界 22](#_Toc465199230)

[查看unit cell中atoms nums 22](#_Toc465199231)

[创建supercell 23](#_Toc465199232)

[设置真空层 23](#_Toc465199233)

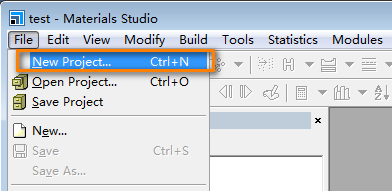
[导出POSCAR 24](#_Toc465199234)

[参考 25](#_Toc465199235)

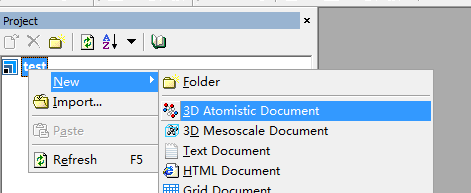
# Materials Studio

## 功能简介

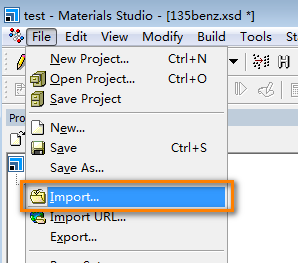
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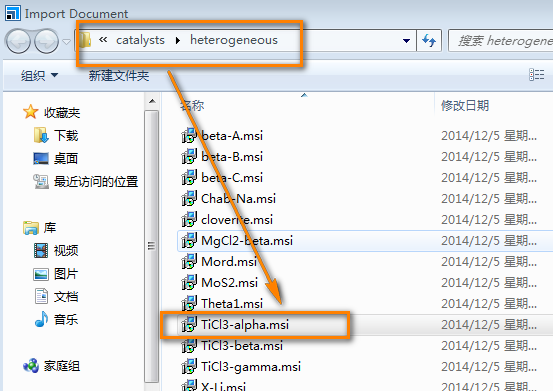


新建晶体文件，

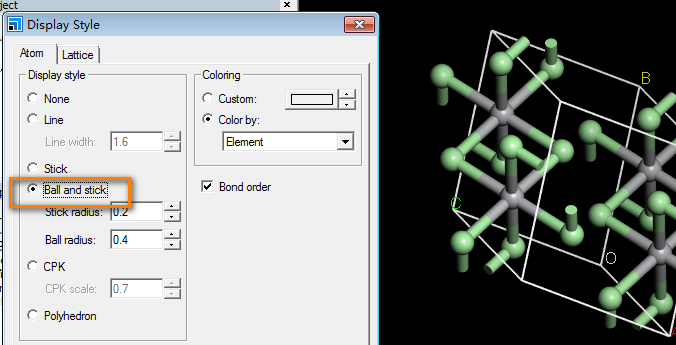


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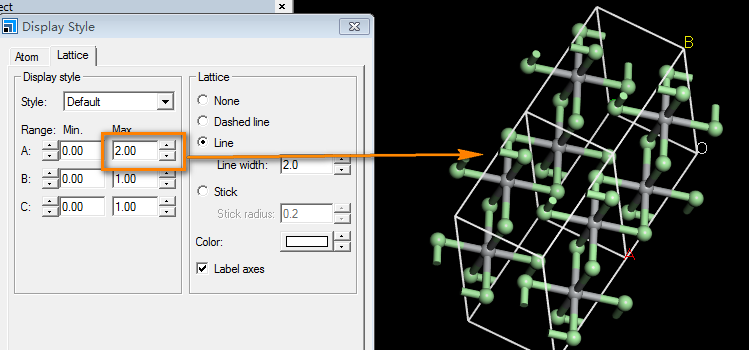




调整显示方式，



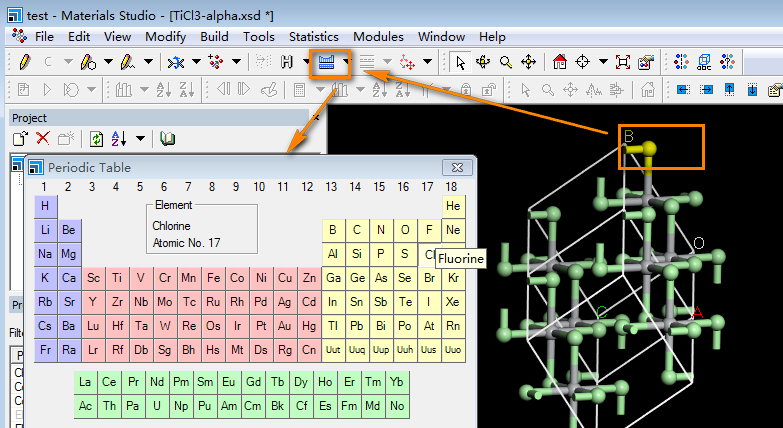
调整晶界，



快捷键，

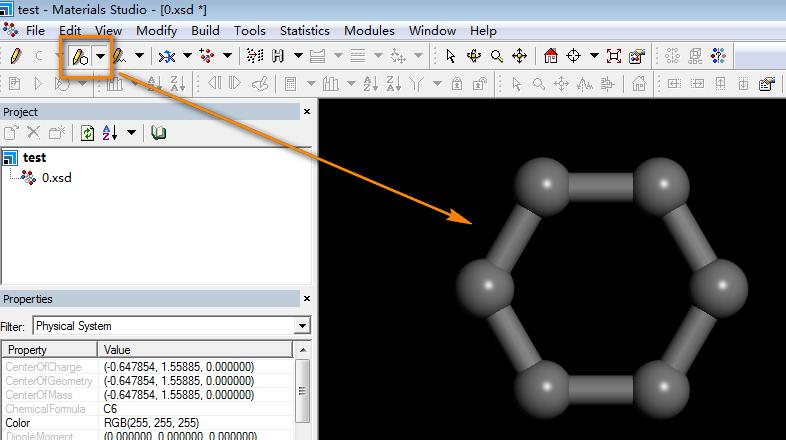
鼠标左键：选择；鼠标右键：旋转；滚轮固定：拖动；滚轮滚动：缩放；ctrl+z撤销。

替换原子，

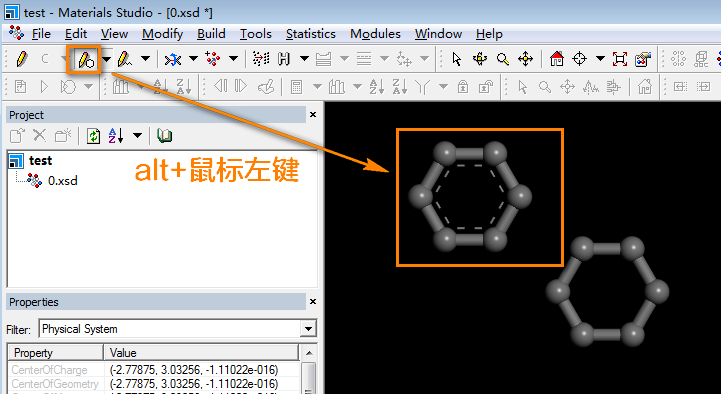


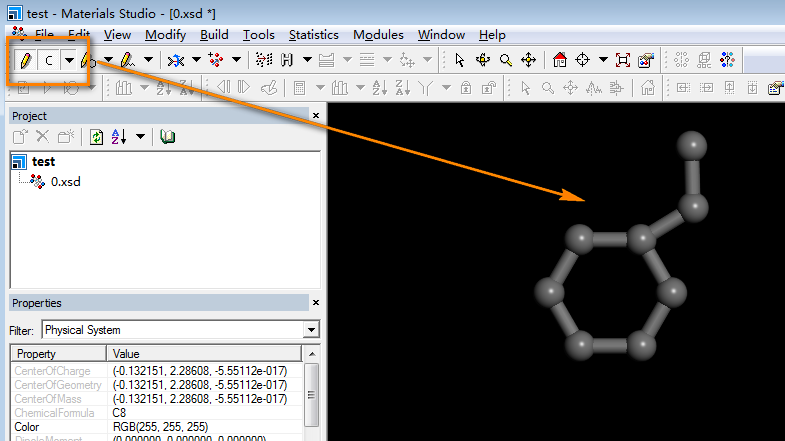
## 创建晶胞

### 苯甲酰胺分子

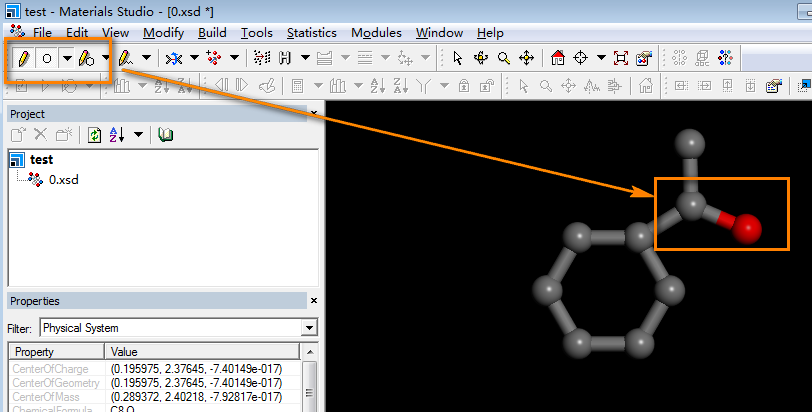


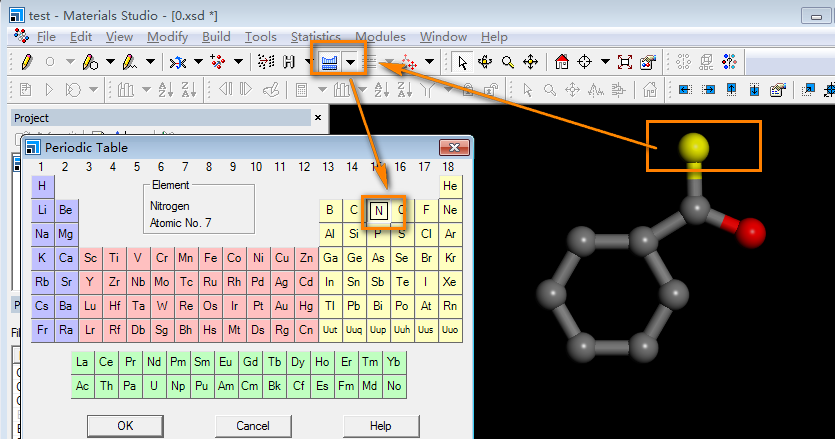
在数字键中键入数字改变环的大小。

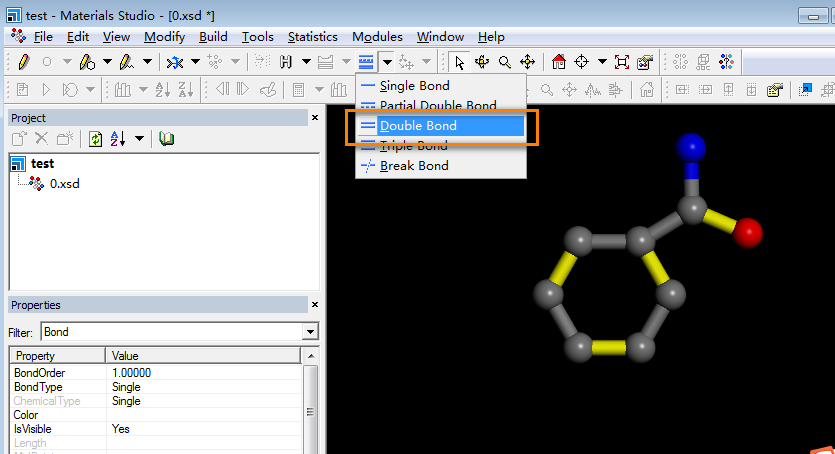


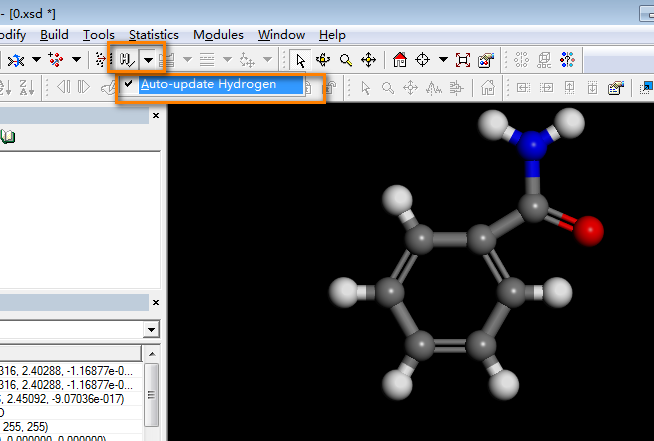


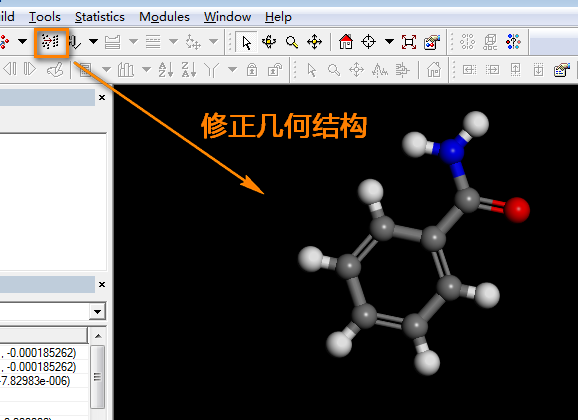
按esc取消创键。

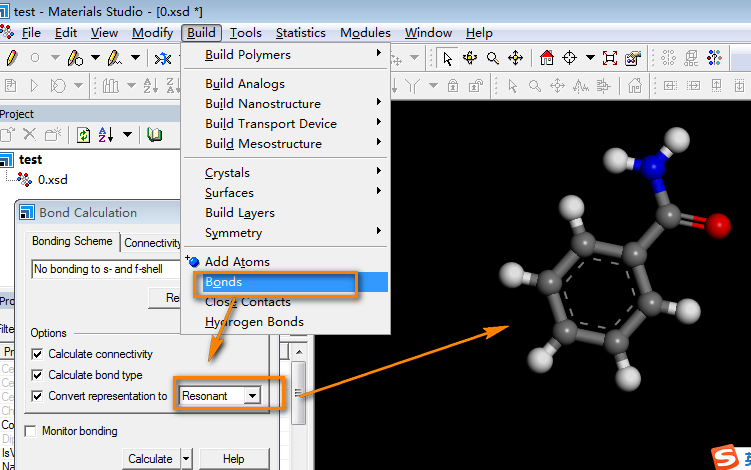


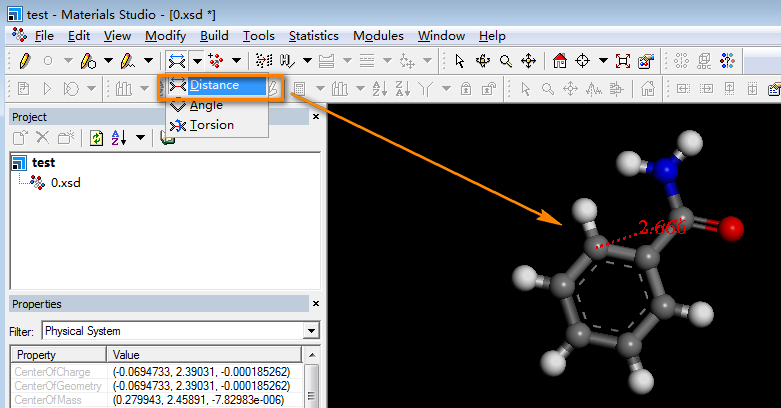


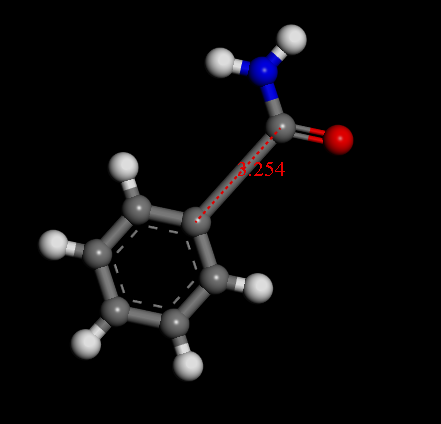






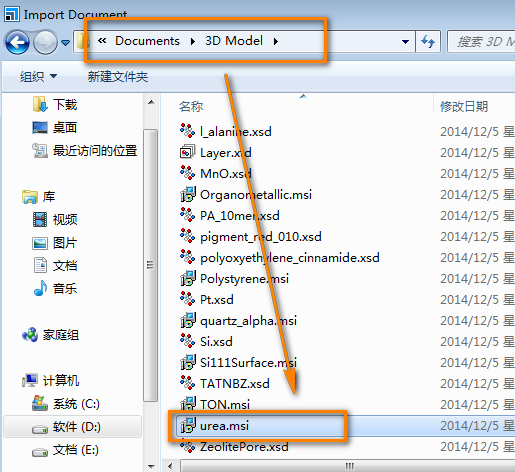


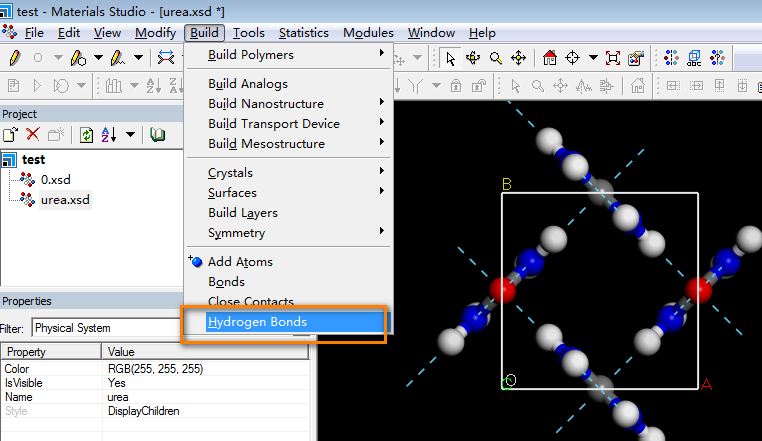




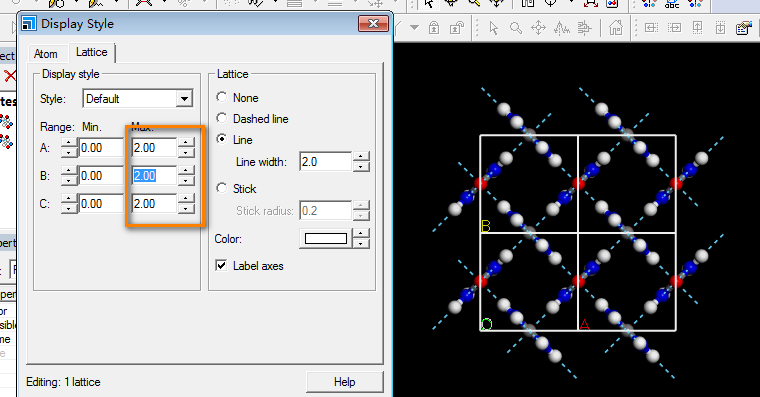
分子外，鼠标左键，向上拖动，则C-O伸长。

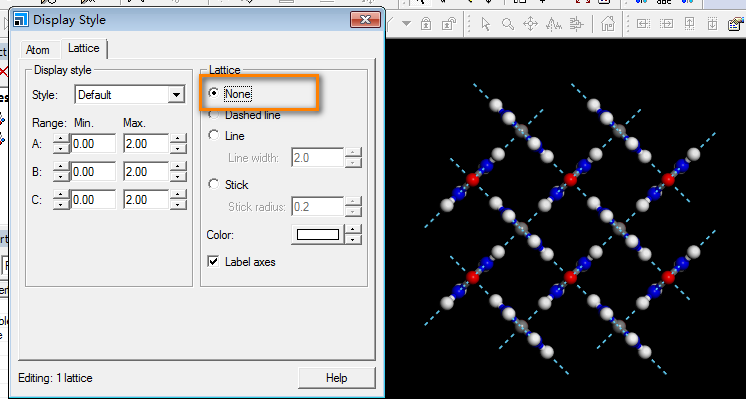
### 尿素晶体





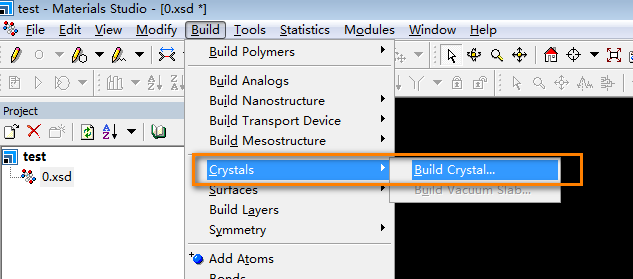
#### 调整显示晶胞数量

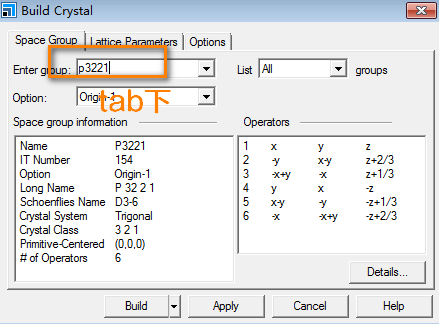


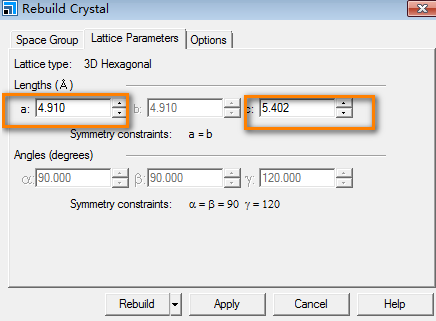


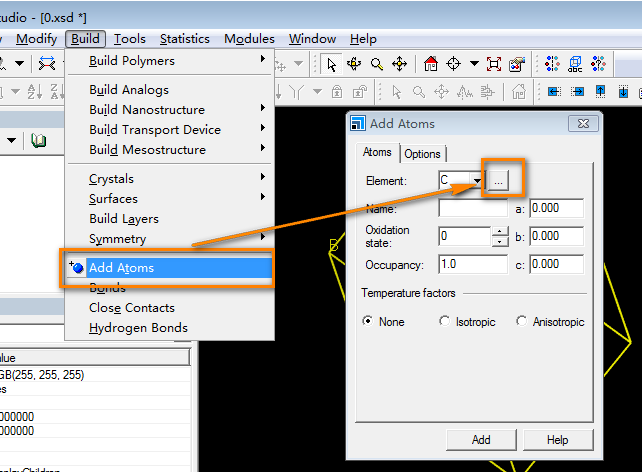
### α石英晶体

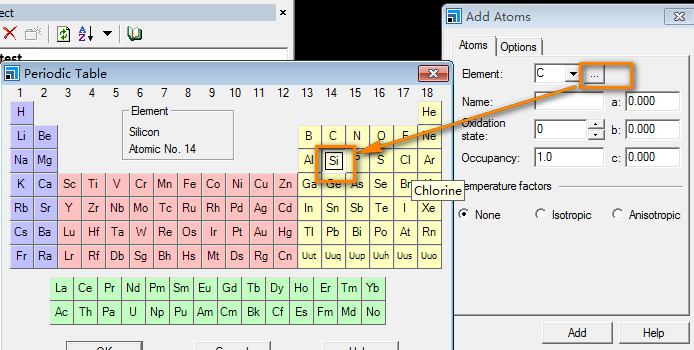
#### 不同晶胞结构对比

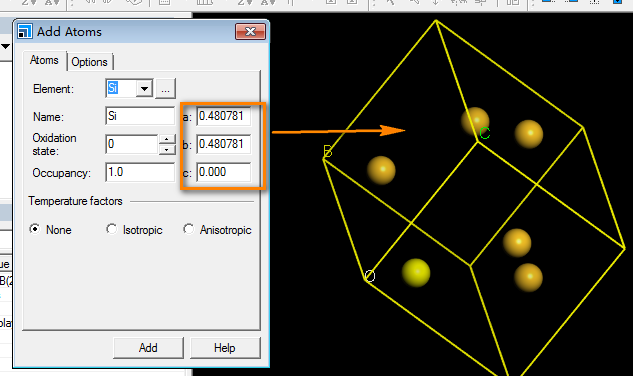


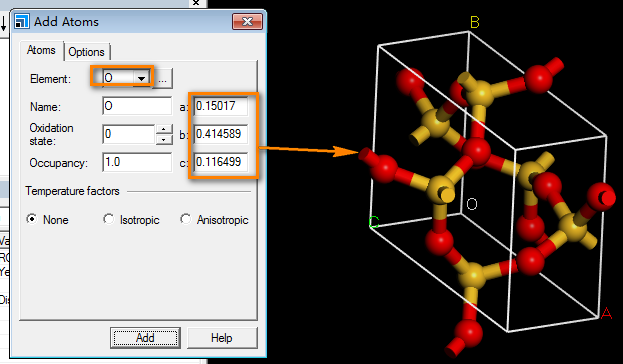


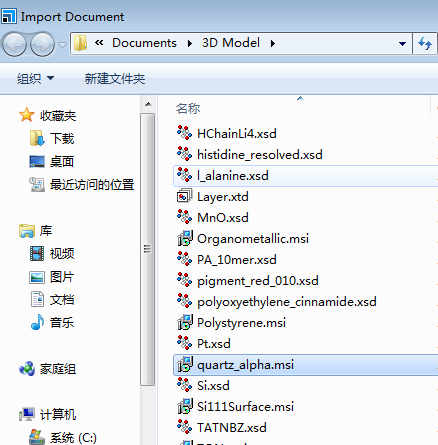


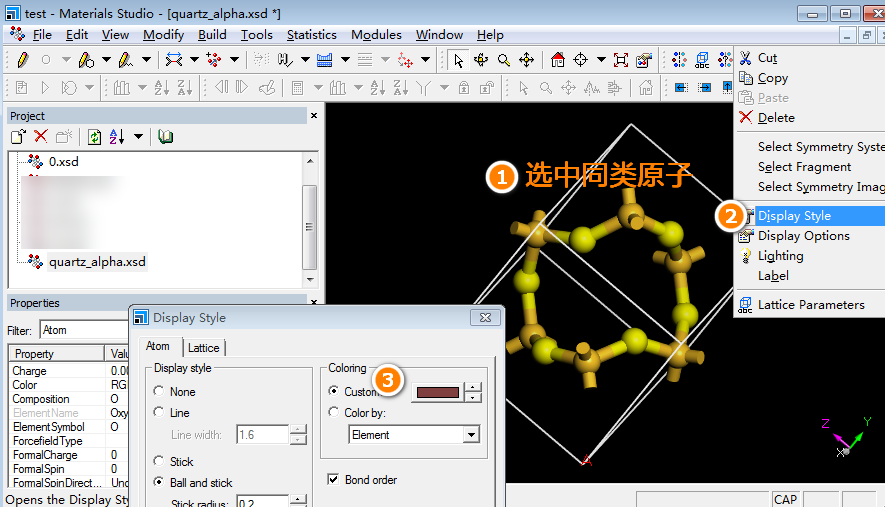


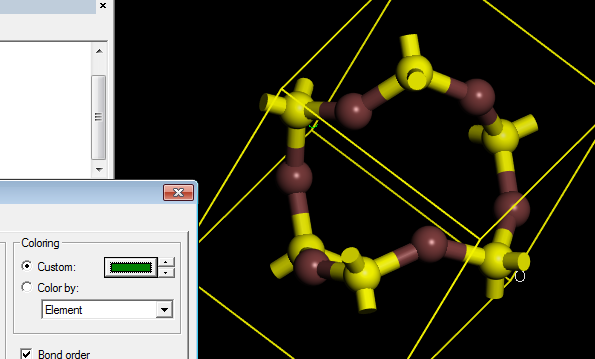


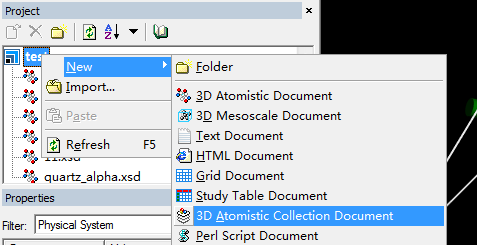


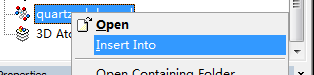


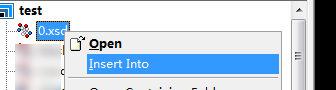


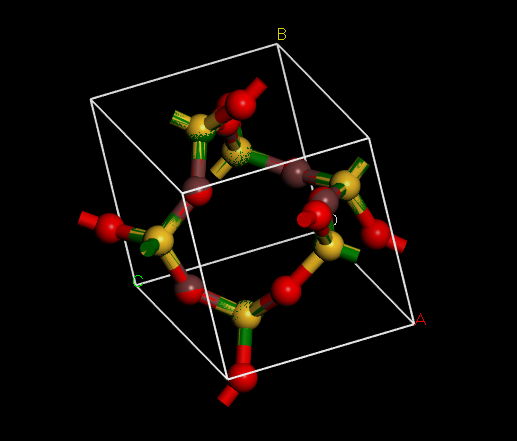




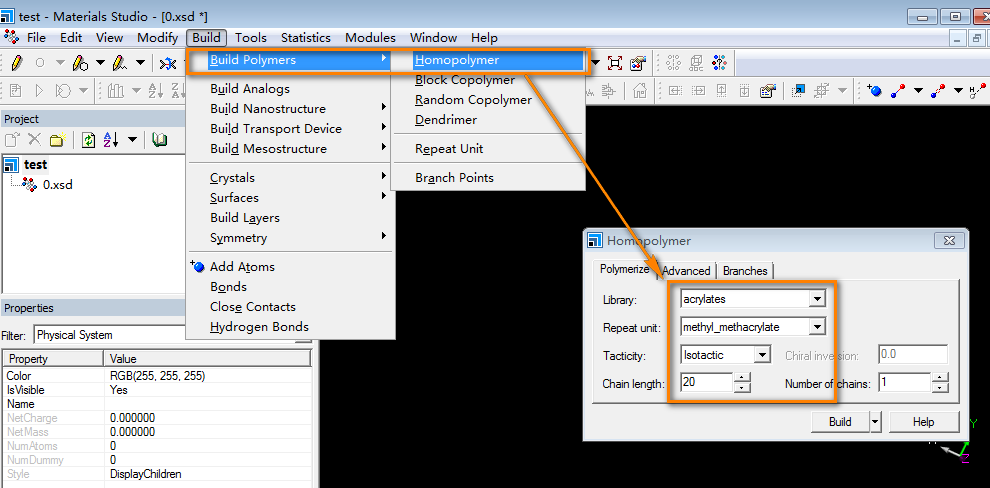


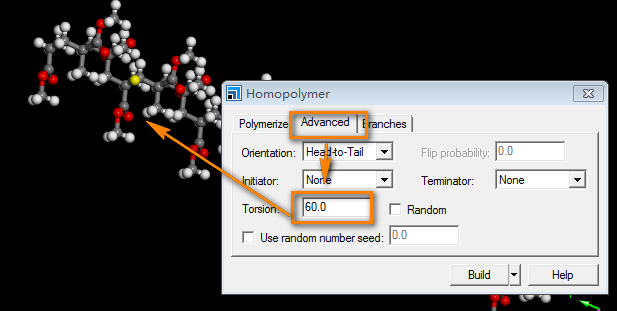


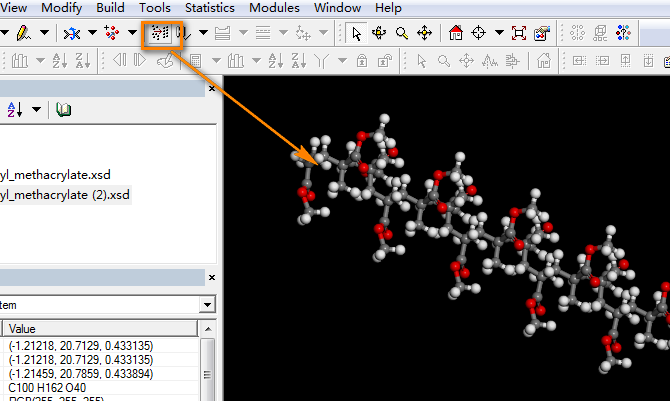




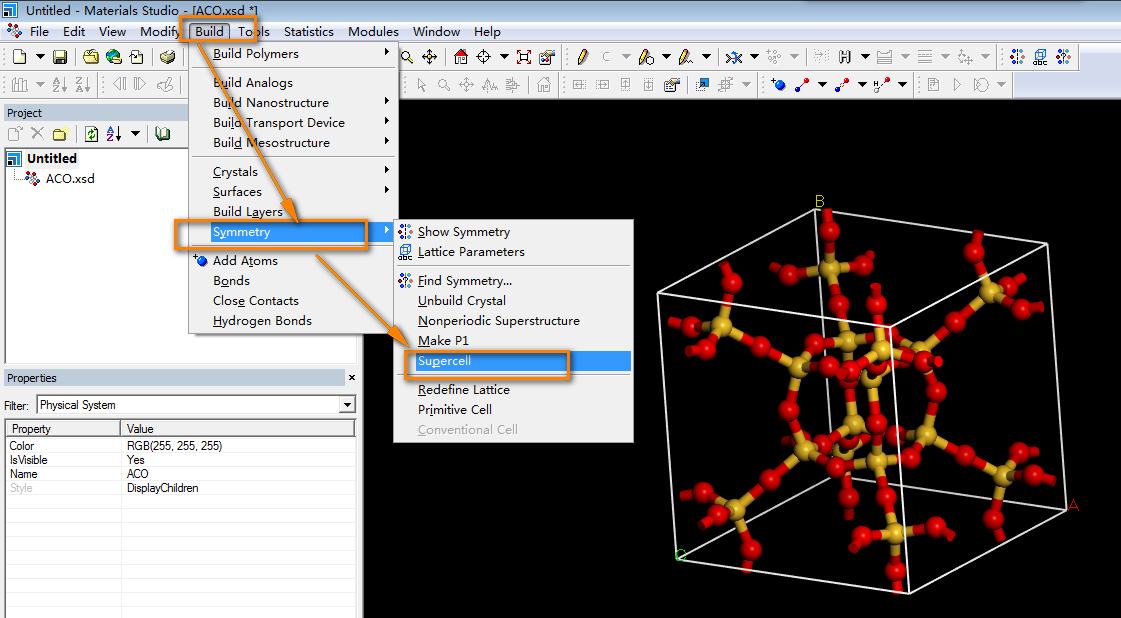
### 聚甲基丙烯酸甲酯

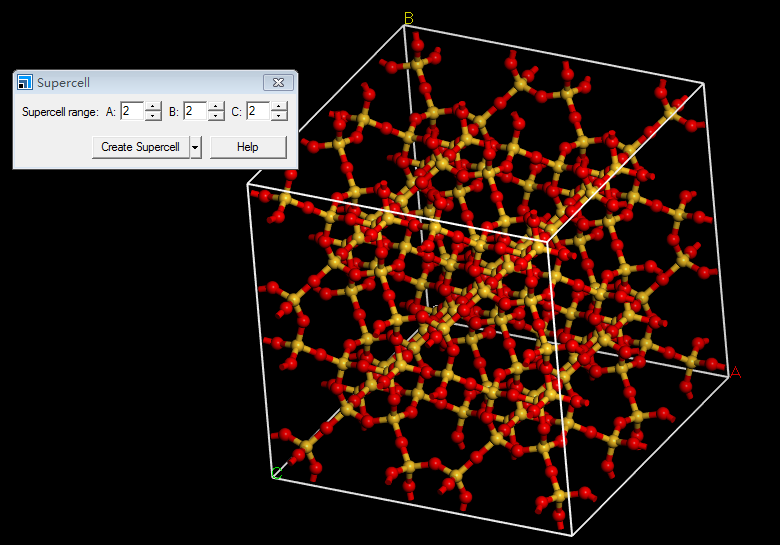




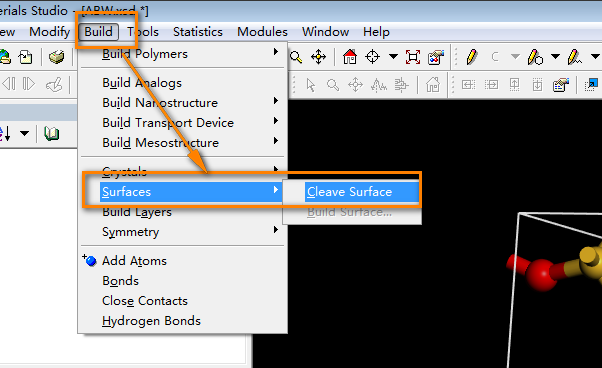


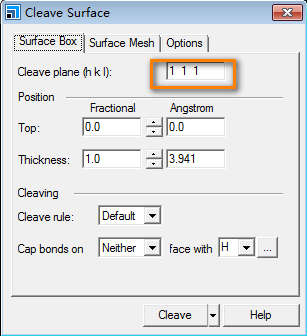
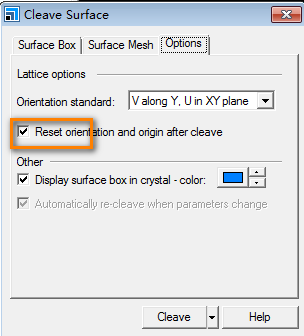
## 超晶胞



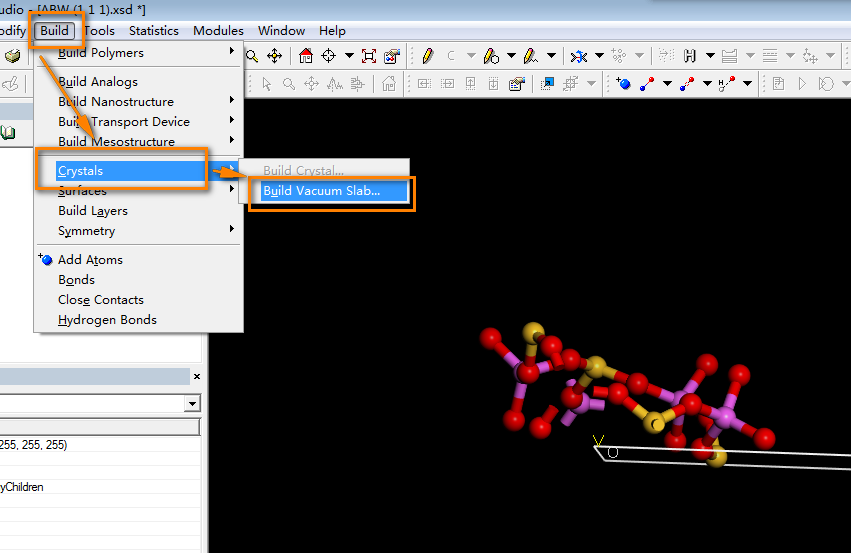


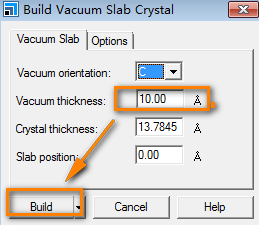
## 界面





## 界面加真空层





# VESTA

## 下载

VESTA 3.3.8[下载](http://jp-minerals.org/vesta/en/download.html)。

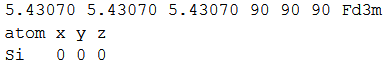
Win7-64位，直接解压打开即可，绿色免安装。

## 创建晶胞

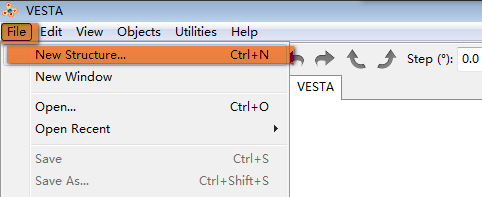
si.cif[下载](http://rruff.geo.arizona.edu/AMS/minerals/Silicon)，

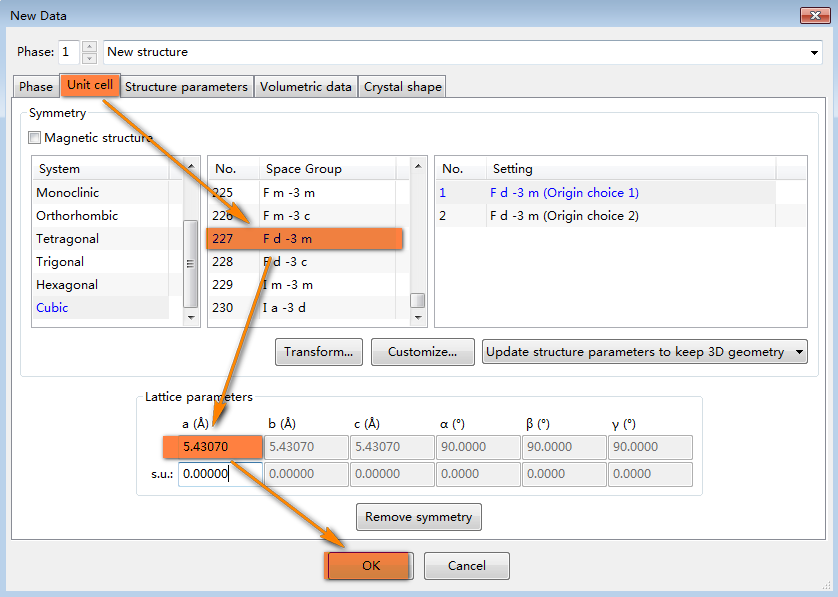
*Wyckoff R W G*

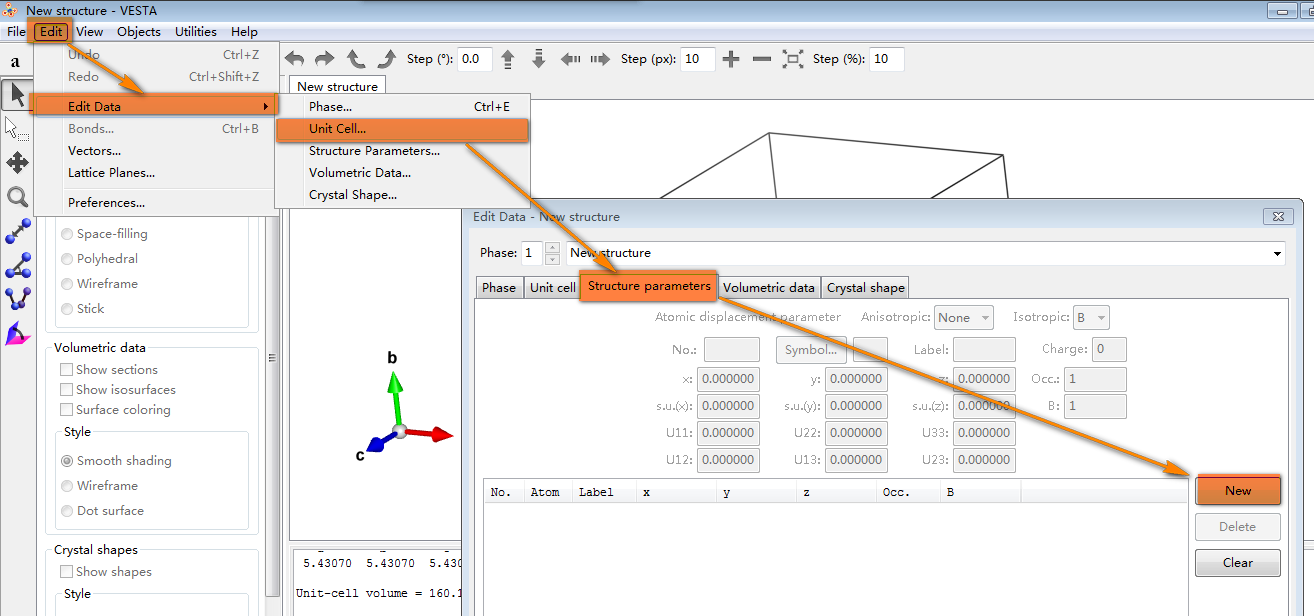
*Crystal Structures 1 (1963) 7-83*

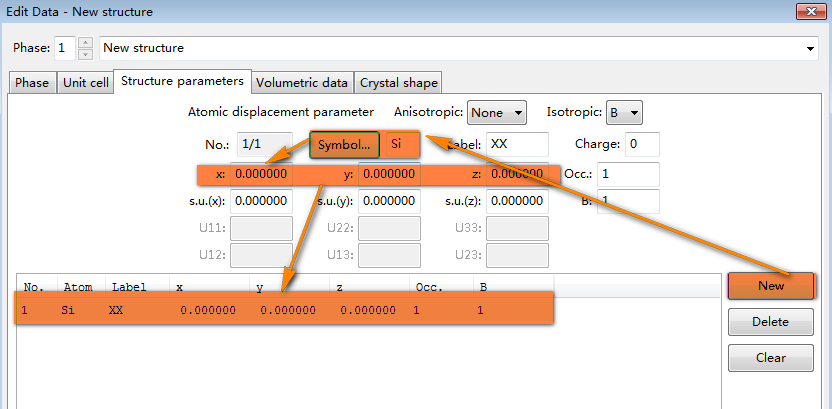


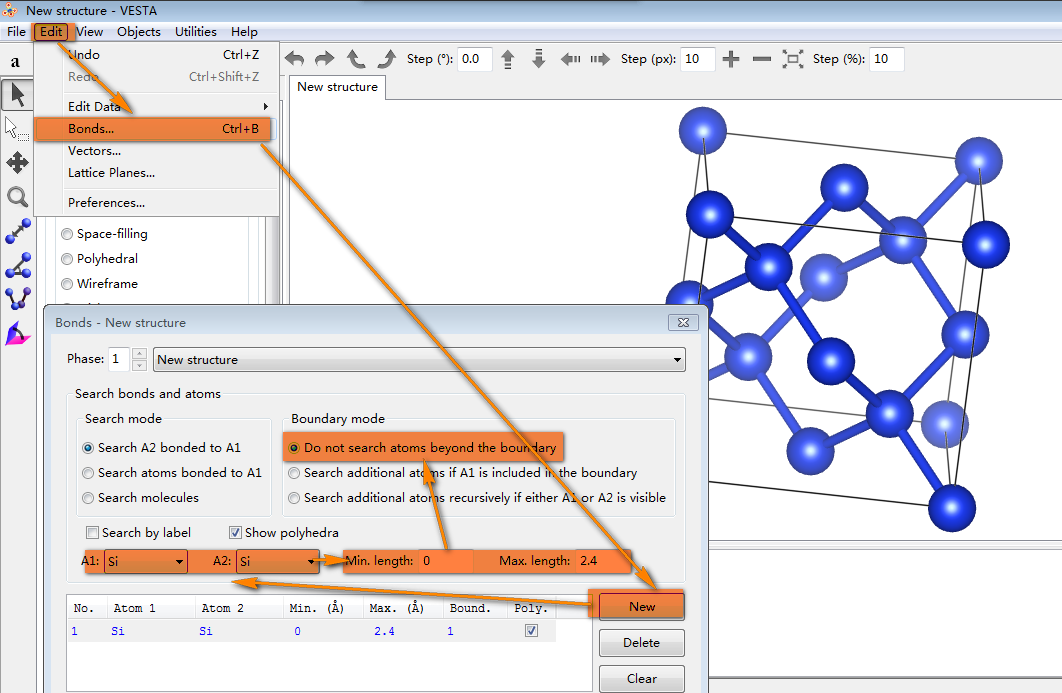
在<http://www.cryst.ehu.es/cgi-bin/cryst/programs/nph-table>，查找空间群序号，227。



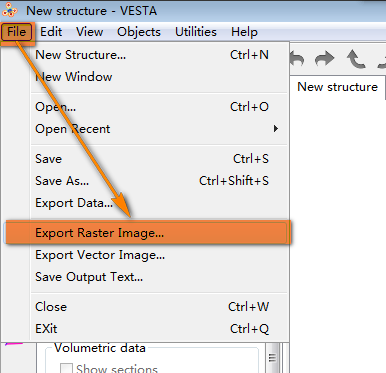


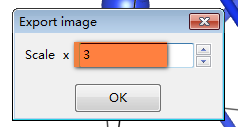




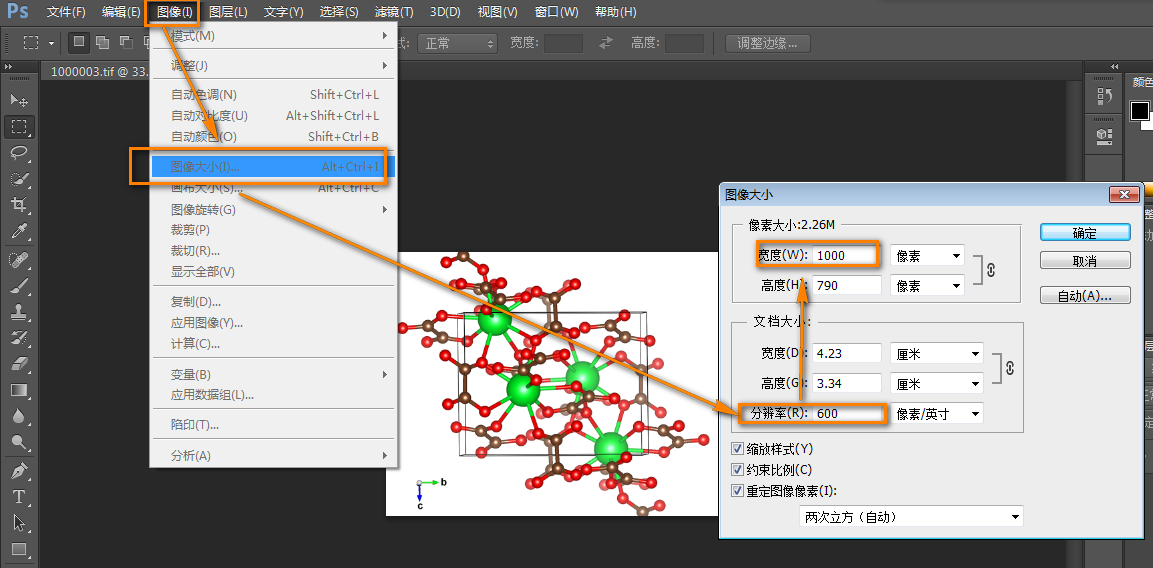


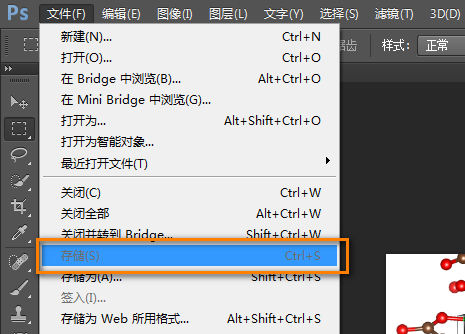
## 导出600dpi tif



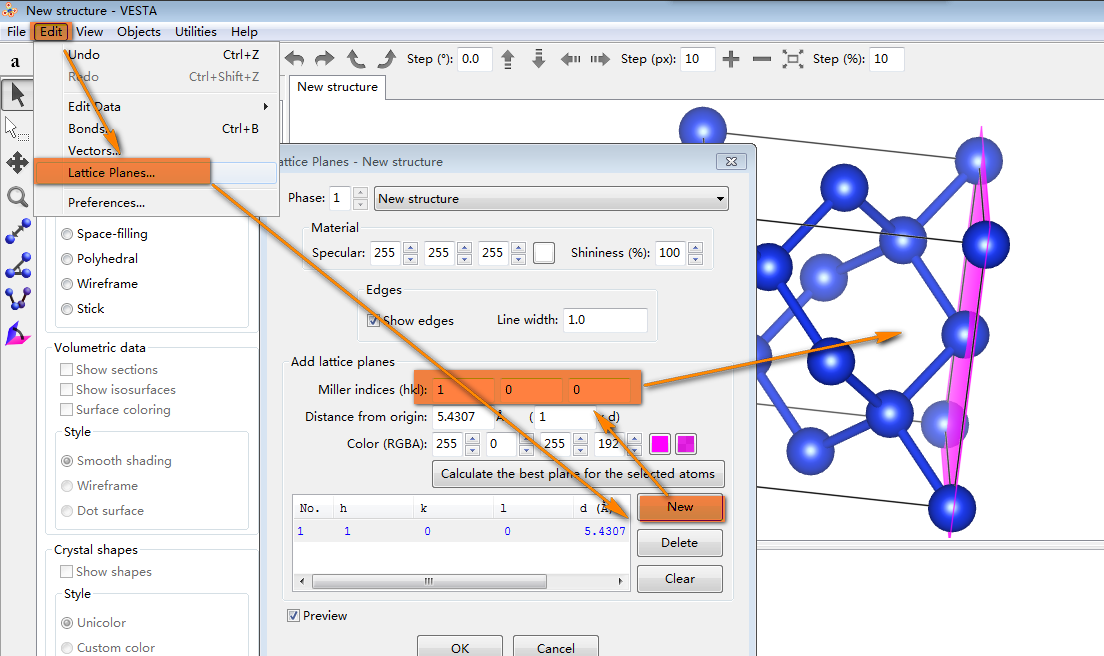


打开Adobe Photoshop CS6，

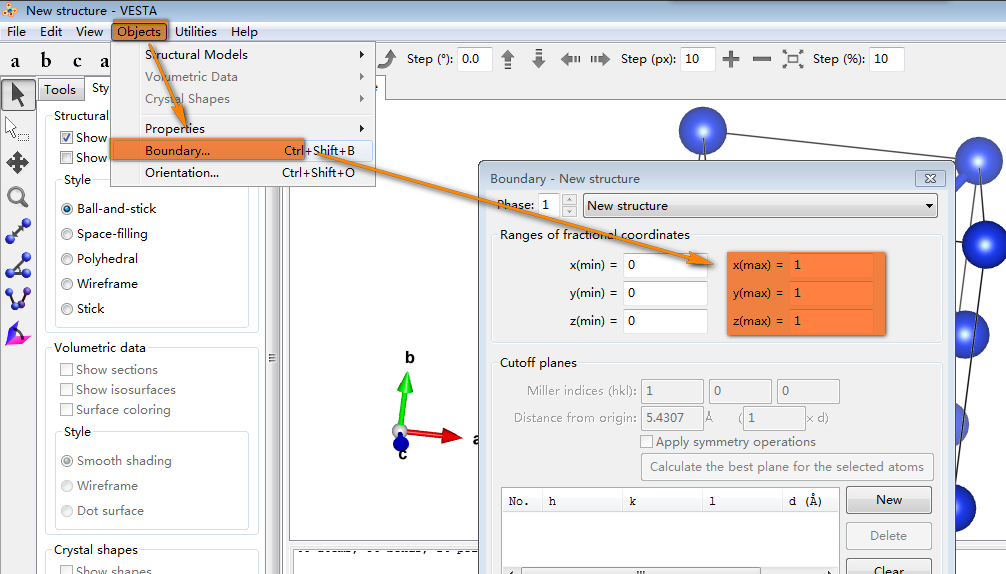




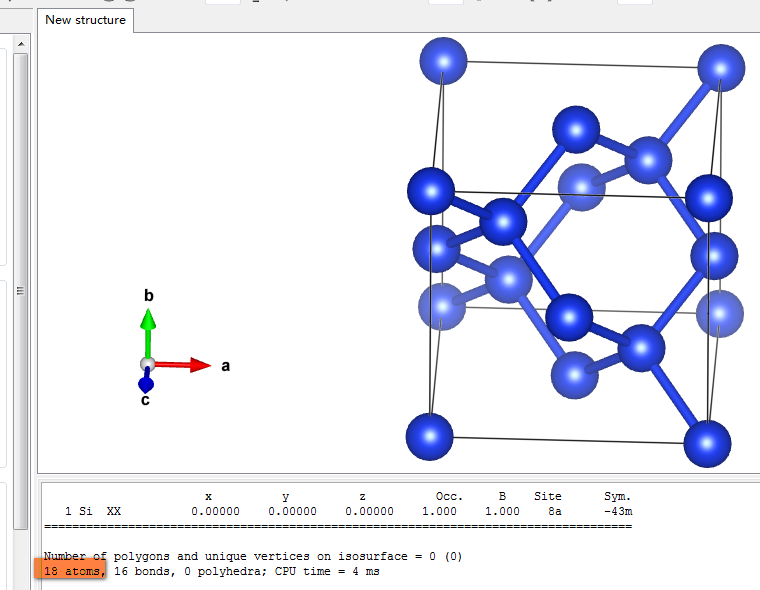
## 截取晶面



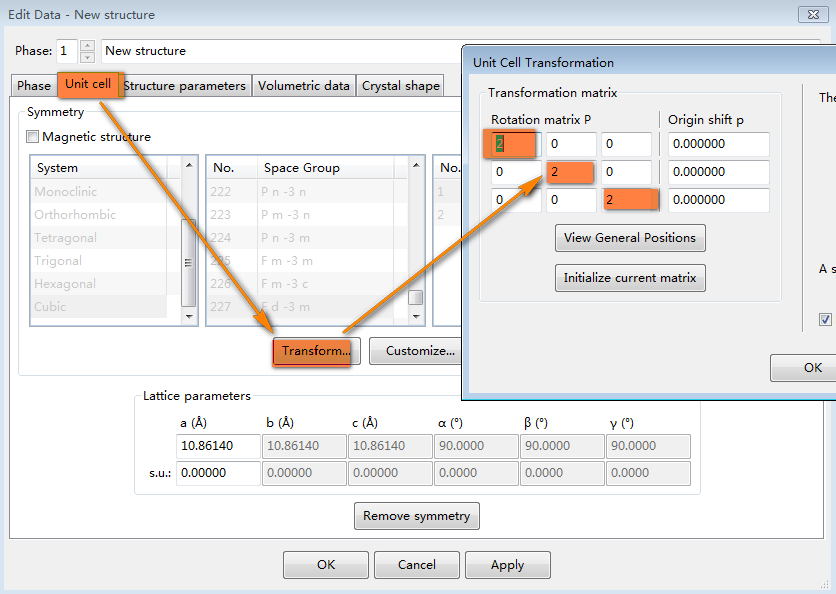
## 调整晶胞边界



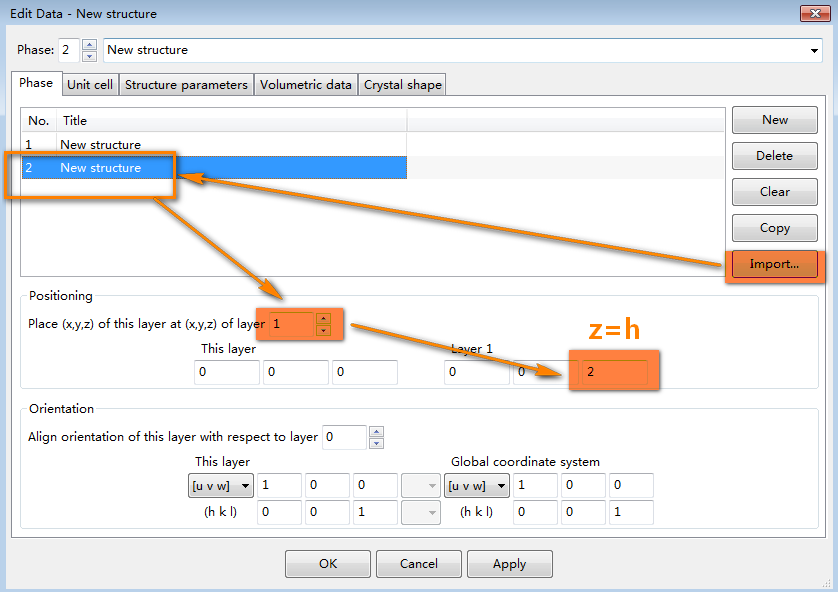
## 查看unit cell中atoms nums

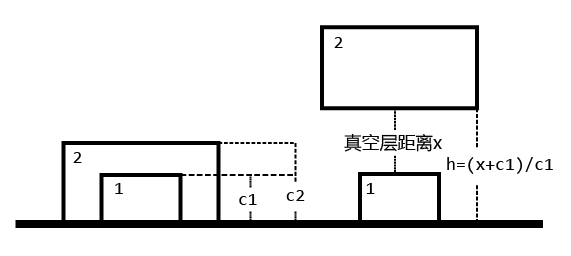


## 创建supercell



## 设置真空层

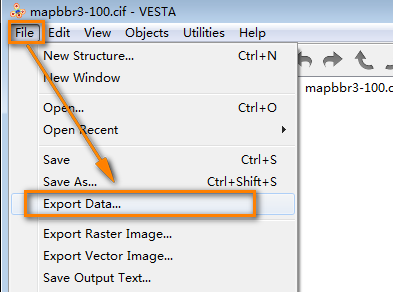


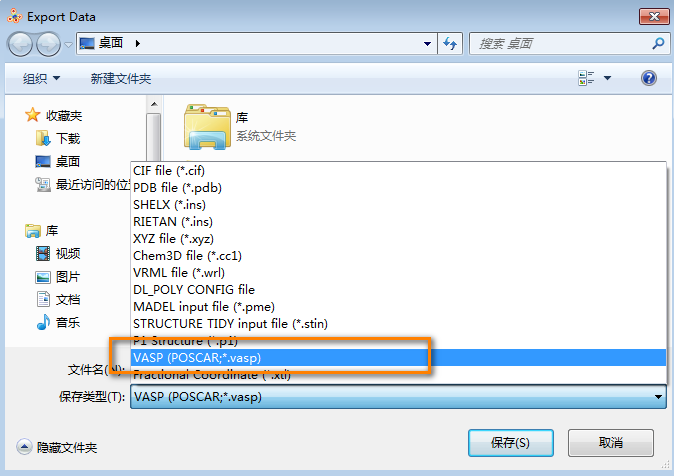


若真空层为c1 Å，

z=h=(x+c1)/c1=2

## 导出POSCAR





# 参考

**Materials studio**

* Class 1--Materials Studio 快速入门教程.ppt

**VESTA**

* [请大家交流一下VESTA软件的用法](http://muchong.com/bbs/viewthread.php?tid=6422652&fpage=1&target=blank)
* [Surface slabs with VESTA](https://compuphys.wordpress.com/2015/02/10/surface-slabs-mit-vesta/)
* [如何从六角晶胞构建立方晶胞](http://www.52souji.net/how-to-convert-hexagonal-cell-to-cubic-cell/)
* [Drawing Crystal Structures](http://profex.doebelin.org/?page_id=559)
* [VESTA官方文档](http://www.geocities.jp/kmo_mma/crystal/download/VESTA_Manual.pdf)
* [How to Prepare an Input File for Surface Calculations](http://www.emresururi.com/physics/?cat=54)
* [请教一个用vesta建超晶包的问题](http://emuch.315955.com/html/201309/6376825.html)
* [Building slab geometries for catalysis with VESTA](http://hjklol.mit.edu/content/building-slab-geometries-catalysis-vesta)