

# Material Studio Tutorial

A introduction for beginner

HU ZHENG

Chemical Engineering Academy

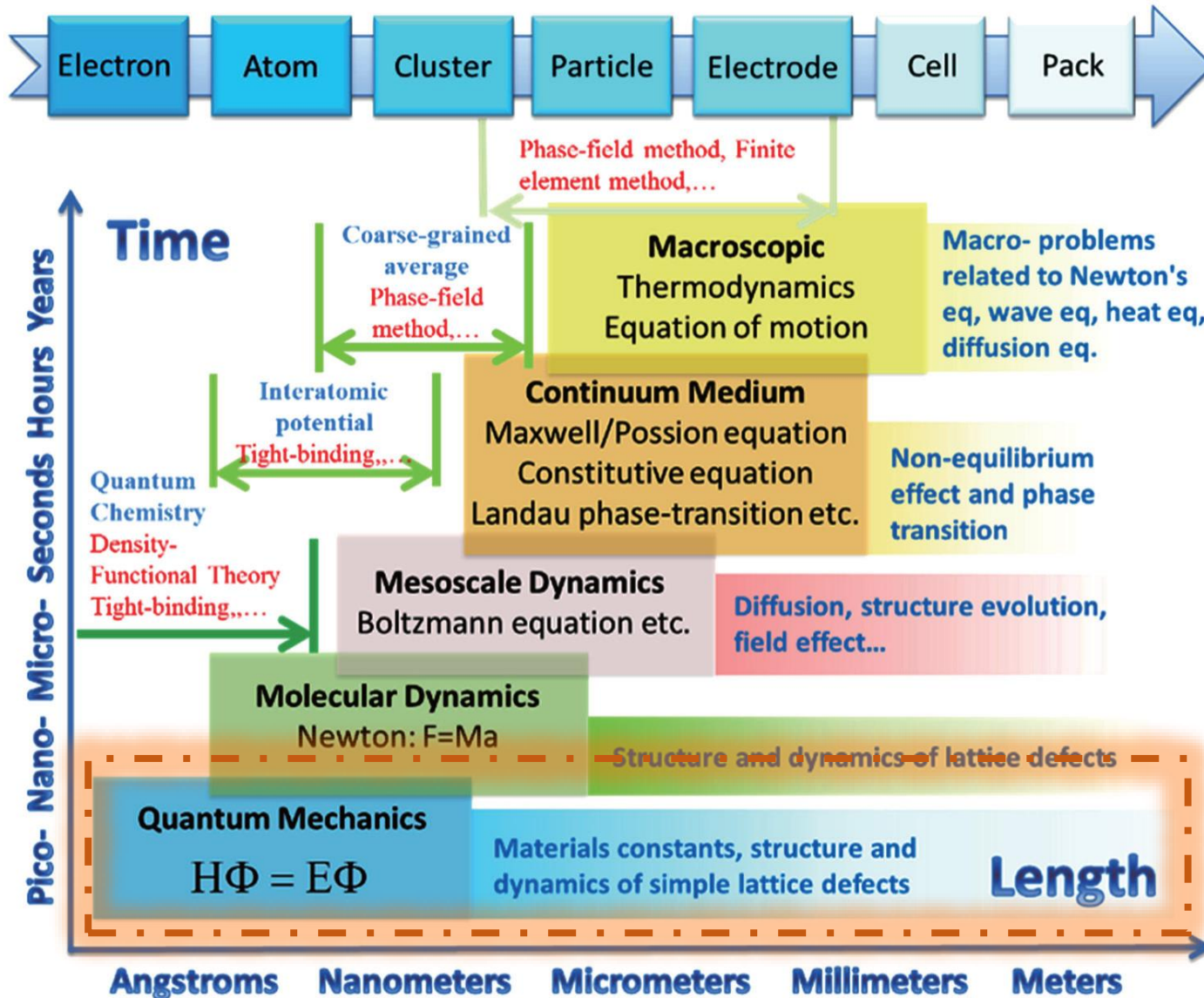
Tianjin University

February 25, 2019

# Content

- 1 Background**
- 2 Material Studio Introduction**
- 3 Castep package**

## Computational Material Science

**Ab initio methods**

- ✓ Schrodinger
- ✓ Hartree-Fock
- ✓ DFT
- ✓ etc.



Scale limit:  
 < 200 atoms  
 Time limit:  
 < 1 ns

## From Schrodinger to post-DFT

**Schrodinger Eq.**

$$H\Phi = E\Phi$$

**Born Oppenheimer Approximation**

$$H = T + W + V$$

- ✓ **Hartree-Fock Methods**  
Rigorously time-consuming
- ✓ **DFT Methods**  
Effectively fast

**Exchange functional approximation:**

- ✓ **LDA**
- ✓ **GGA**
- ✓ **Hybird-GGA**

**Hydrogen atom (1e)**  


- ✓ **Many-body Problem**
- ✓ **One-election like Eq.**

# Content

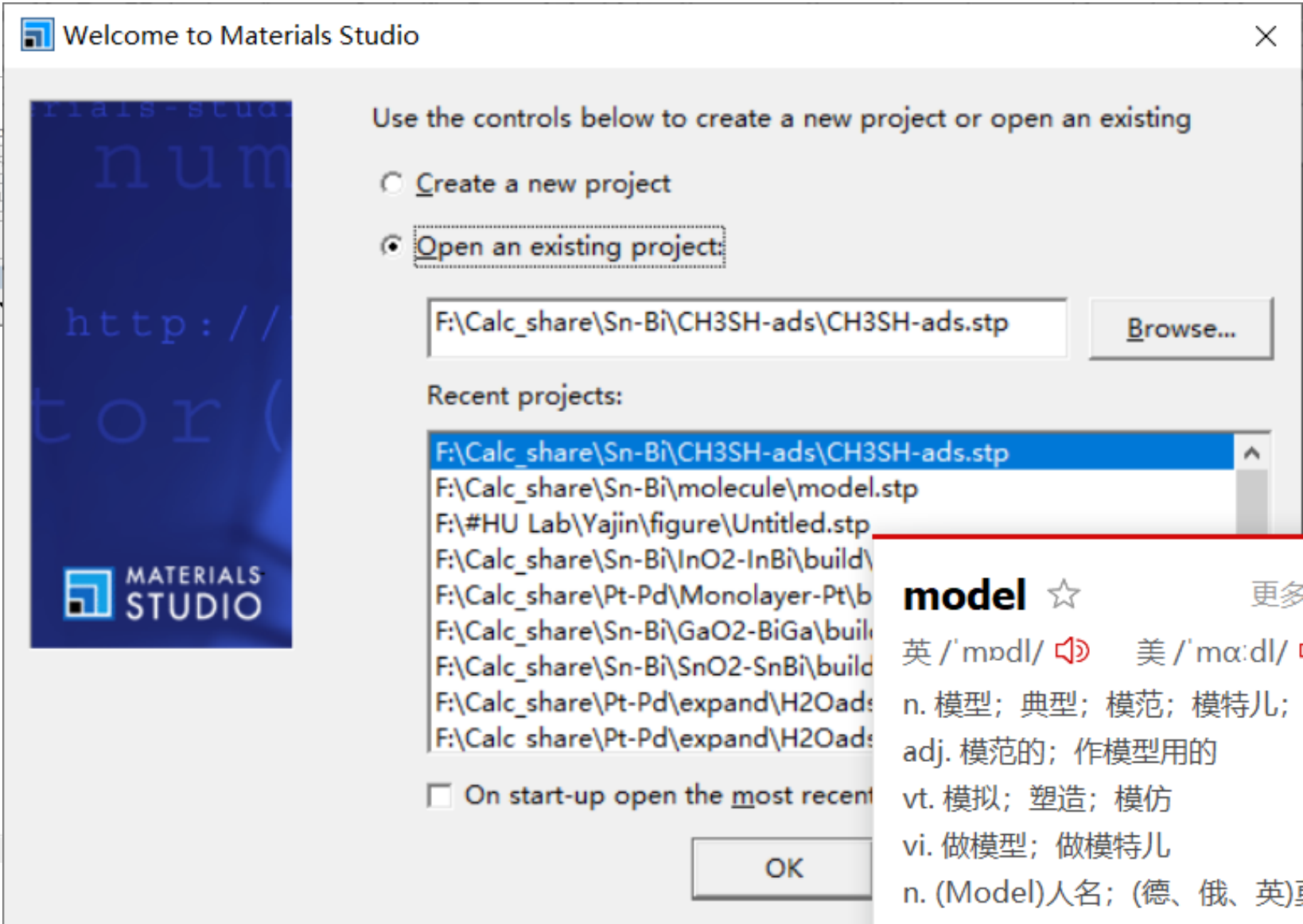
**1** Background

**2** **Material Studio Introduction**

**3** Castep package

## Material Studio

### Start up



Materials Studio

File Edit View Mo

Project

Ready

Welcome to Materials Studio

Use the controls below to create a new project or open an existing

☐ Create a new project

☒ Open an existing project:

F:\Calc\_share\Sn-Bi\CH3SH-ads\CH3SH-ads.stp Browse...

Recent projects:

- F:\Calc\_share\Sn-Bi\CH3SH-ads\CH3SH-ads.stp
- F:\Calc\_share\Sn-Bi\molecule\model.stp
- F:\#HU Lab\Yajin\figure\Untitled.stp
- F:\Calc\_share\Sn-Bi\InO2-InBi\build\
- F:\Calc\_share\Pt-Pd\Monolayer-Pt\b
- F:\Calc\_share\Sn-Bi\GaO2-BiGa\buil
- F:\Calc\_share\Sn-Bi\SnO2-SnBi\build
- F:\Calc\_share\Pt-Pd\expand\H2Oads
- F:\Calc\_share\Pt-Pd\expand\H2Oads

☐ On start-up open the most recent

OK

**model** ☆ 更多

英 /'mɒdl/ 美 /'mɑ:dl/

n. 模型; 典型; 模范; 模特儿;

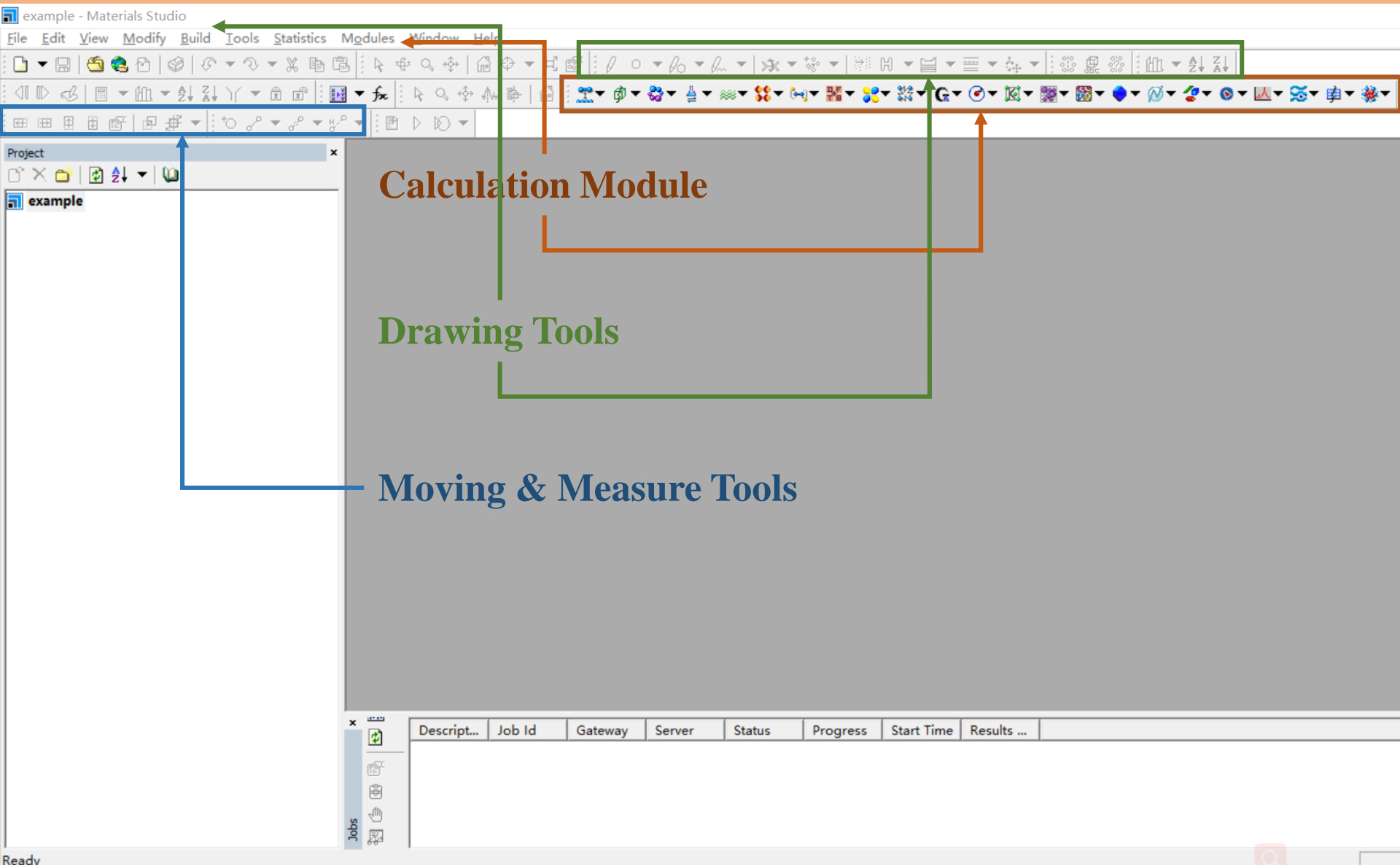
adj. 模范的; 作模型用的

vt. 模拟; 塑造; 模仿

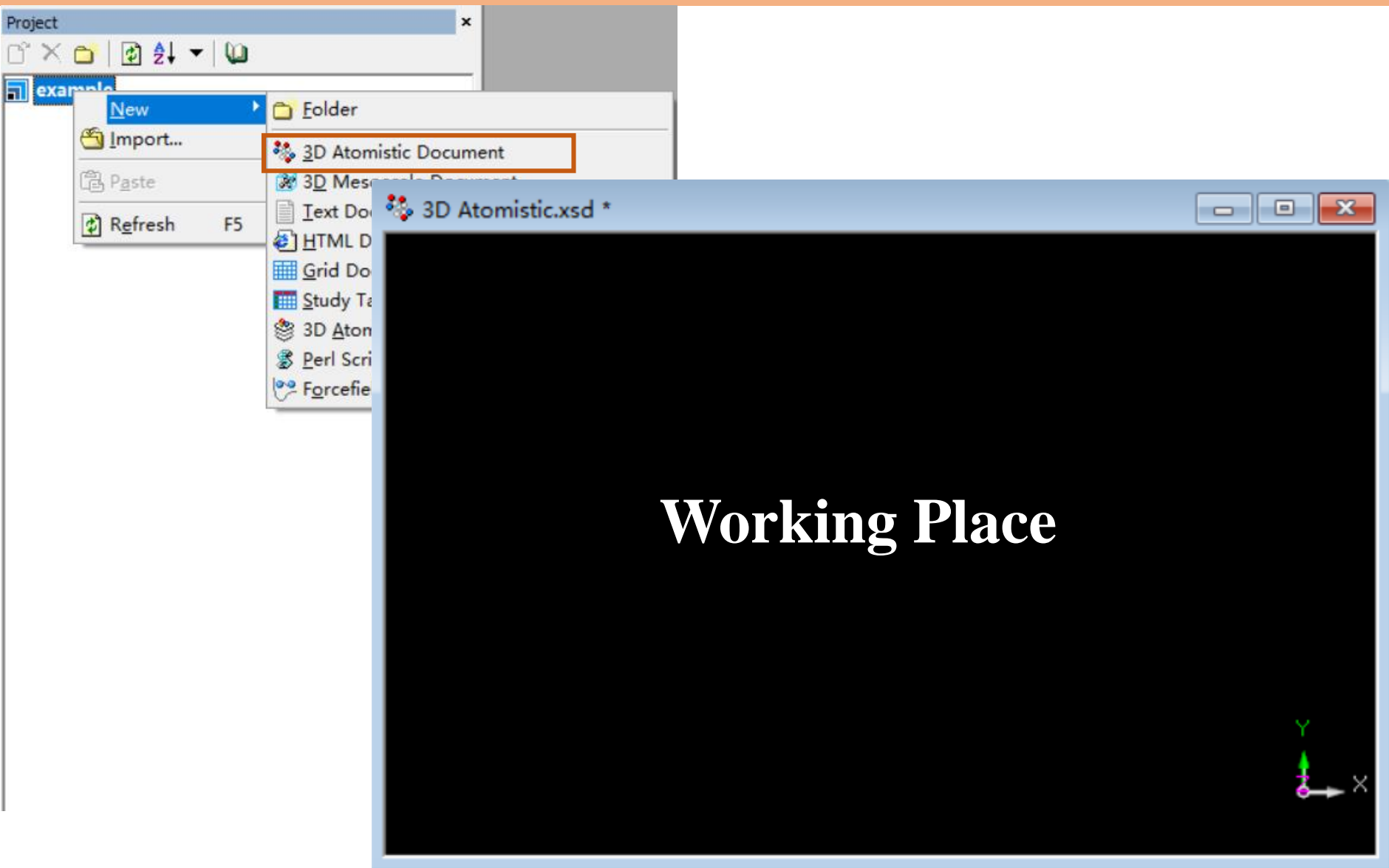
vi. 做模型; 做模特儿

n. (Model)人名; (德、俄、英)

## Status bar



## Modeling

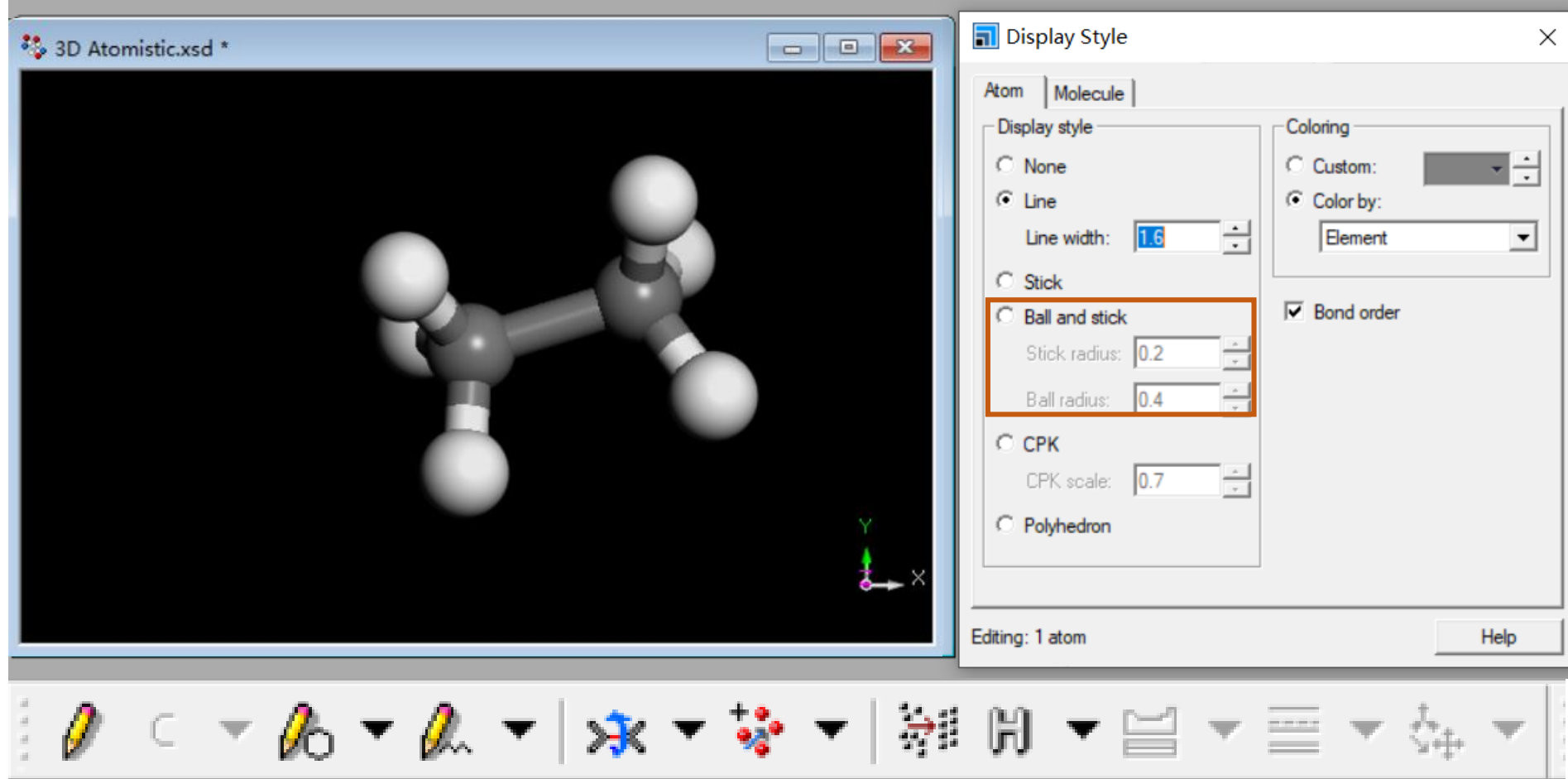




## Modeling ~ Organic Molecules

### ethane model

### Single molecule



The screenshot displays the Material Studio interface. The main window, titled "3D Atomistic.xsd \*", shows a 3D ball-and-stick model of an ethane molecule (CC) against a black background. The molecule consists of two carbon atoms (grey) and six hydrogen atoms (white). To the right, the "Display Style" dialog box is open, with the "Molecule" tab selected. Under the "Display style" section, the "Ball and stick" option is chosen and highlighted with a red rectangle. The "Stick radius" is set to 0.2 and the "Ball radius" is set to 0.4. The "Coloring" section shows "Color by" set to "Element". The "Bond order" checkbox is checked. At the bottom of the dialog, it says "Editing: 1 atom" and there is a "Help" button. Below the main window is a toolbar with various icons for building and editing the molecular model.

Sketch atoms, bonds, cycles, etc.

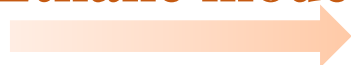
Auto-add H atoms

Change atoms/bonds

## Modeling ~ Organic Molecules

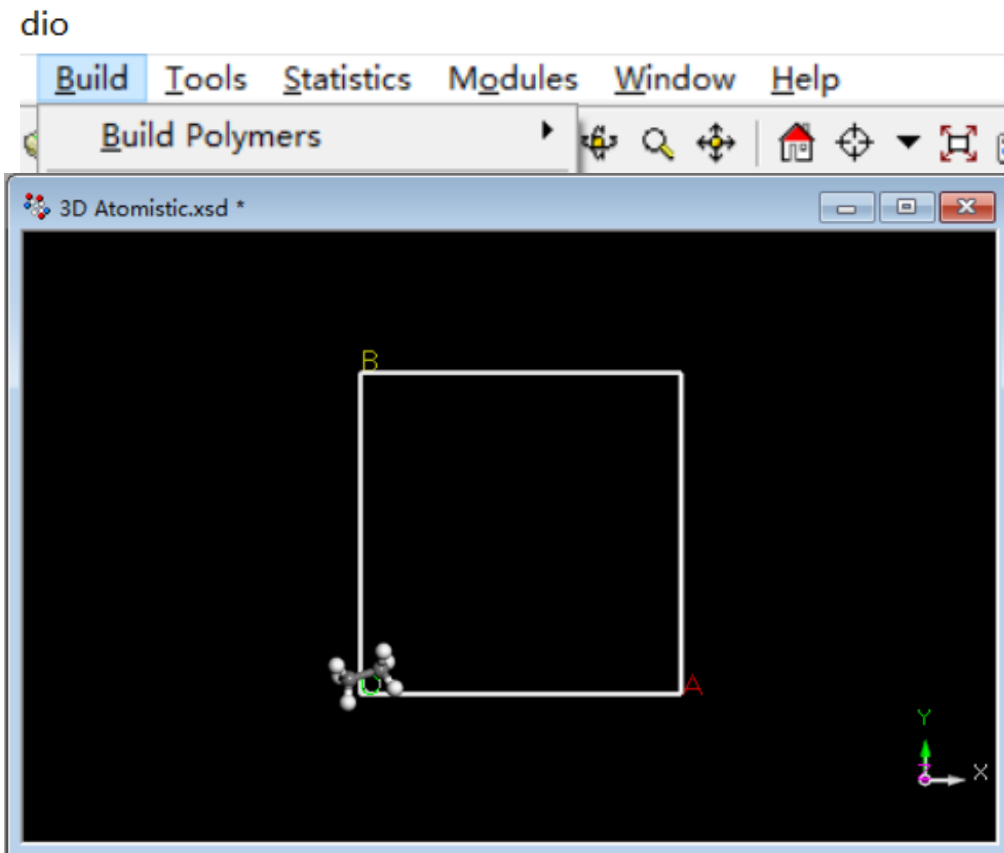
Single molecule

Ethane model



Molecule system

- ✓ Gas
- ✓ Liquid
- ✓ Solid
  - Crystal
  - Amorphous



Build Crystal

Space Group Lattice Parameters Options

Lattice type: 3D Triclinic

Lengths (Å)

a: 15.000 b: 15.000 c: 15.000

Symmetry constraints: None

Angles (degrees)

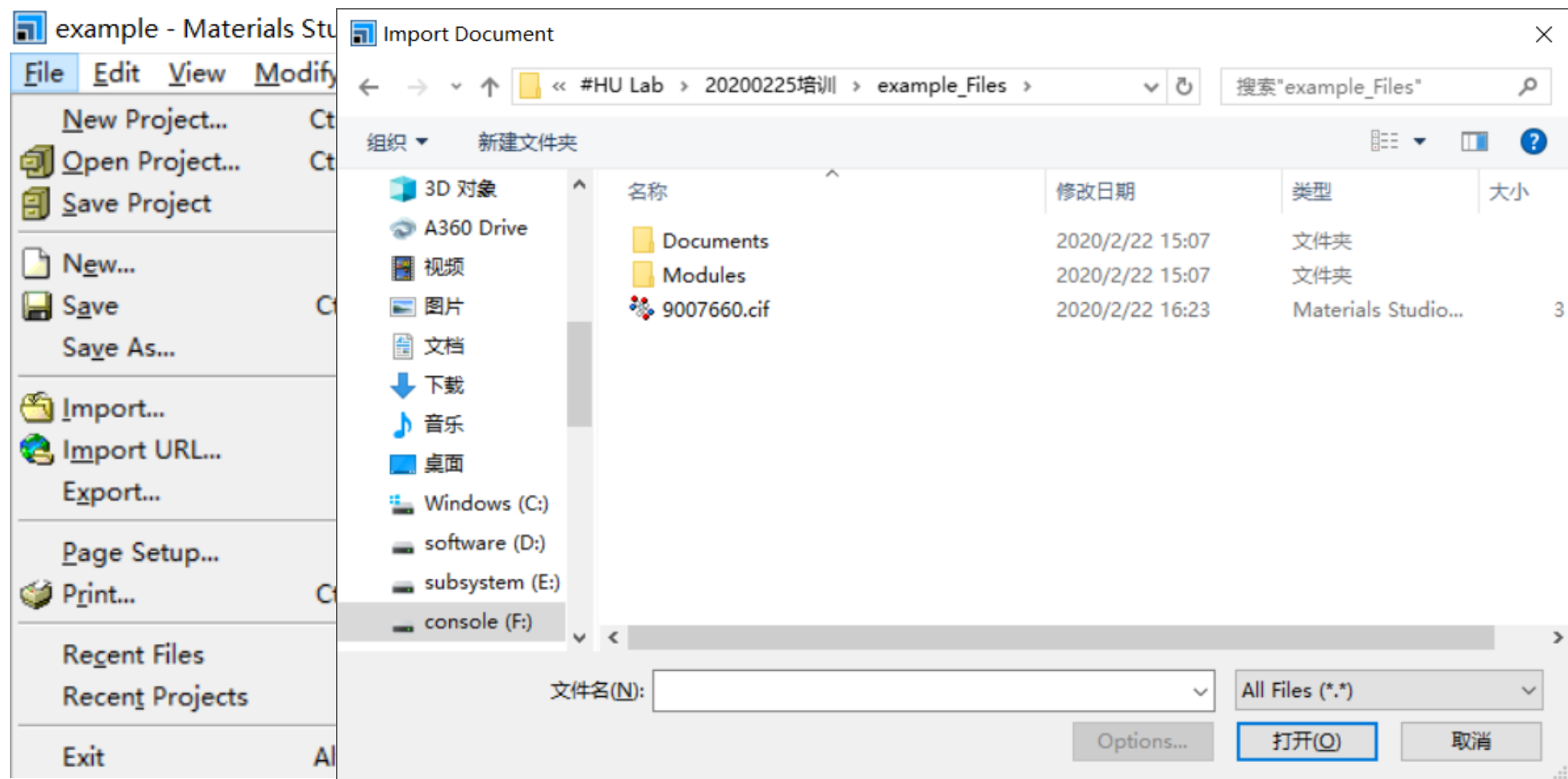
$\alpha$ : 90.000  $\beta$ : 90.000  $\gamma$ : 90.000

Symmetry constraints: None

Build Apply Cancel Help

## Modeling ~ Metal &amp; Other Crystals

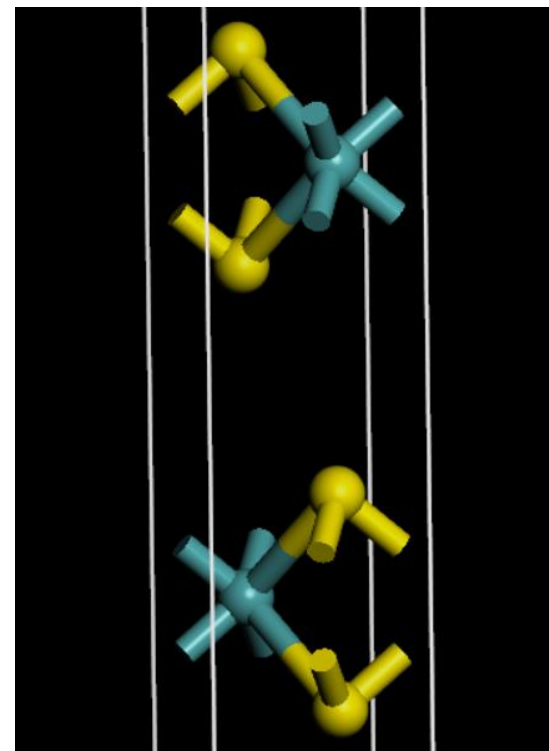
## “import” operation



# Modeling ~ Metal & Other Crystals

text (1 or 2 words)	MoS2
journal	
year	
volume	
issue	
DOI	
<u>Z</u> (min, max)	
<u>Z'</u> (min, max)	
chemical formula (in Hill notation)	
1 to 8 elements	
NOT these elements	
volume min and max	
number of distinct elements min and max	
	<input type="checkbox"/> has E...

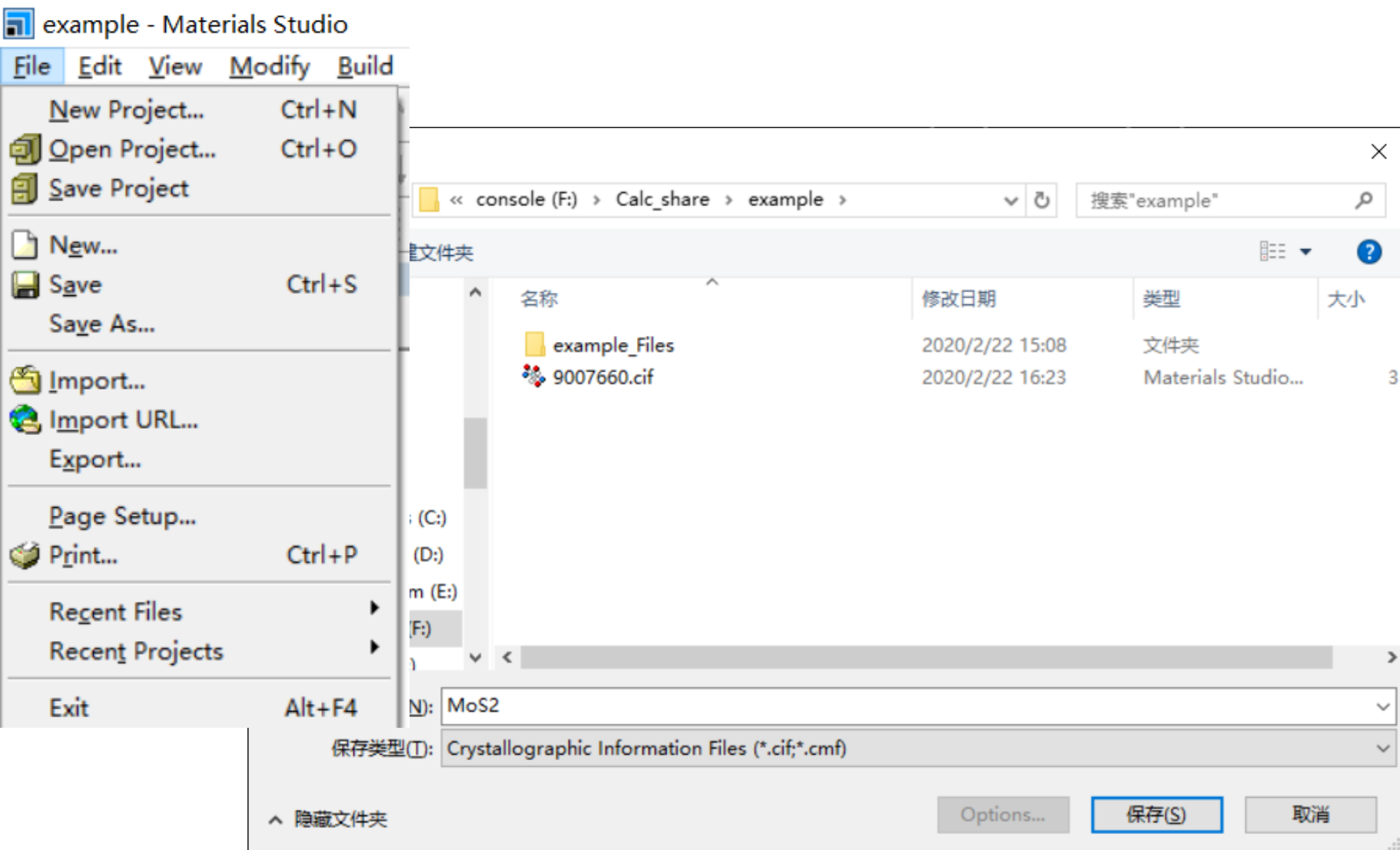
## cif file database



COD ID ▲	Links	Formula ▲	Space group ▲	Cell parameters	Cell volume ▲	Bibliography
<a href="#">9007660</a>	<a href="#">CIF</a>	Mo S2	<a href="#">P 63/m m c</a>	3.161; 3.161; 12.295 90; 90; 120	106.392	Schonfeld, B.; Huang, J. J.; Moss, S. C. Anisotropic mean-square displacements (MSD) in single crystals of 2H- and 3R-MoS2 Note: 2H polytype, this is the most common in nature Locality: synthetic <a href="#">Acta Crystallographica, Section B, 1983, 39</a> , 404-407
<input type="button" value="Reset"/>			<input type="button" value="Send"/>			

<http://crystallography.net/cod/search.html>

## Modeling ~ Export file



# Content

**1** Background

**2** Material Studio Introduction

**3** Castep package

## 关于CASTAP



**CASTAP是特别为固体材料学而设计的一个现代的量子力学基本程序，其使用了密度泛函(DFT) 平面波赝势方法，进行第一性原理量子力学计算，以探索如半导体，陶瓷，金属，矿物和沸石等材料的晶体和表面性质。**

**典型的应用包括表面化学，键结构，态密度和光学性质等研究，CASTAP也可用于研究体系的电荷密度和波函数的3D形式。此外，CASTAP可用于有效研究点缺陷（空位，间隙和置换杂质）和扩展缺陷（如晶界和位错）的性质。**

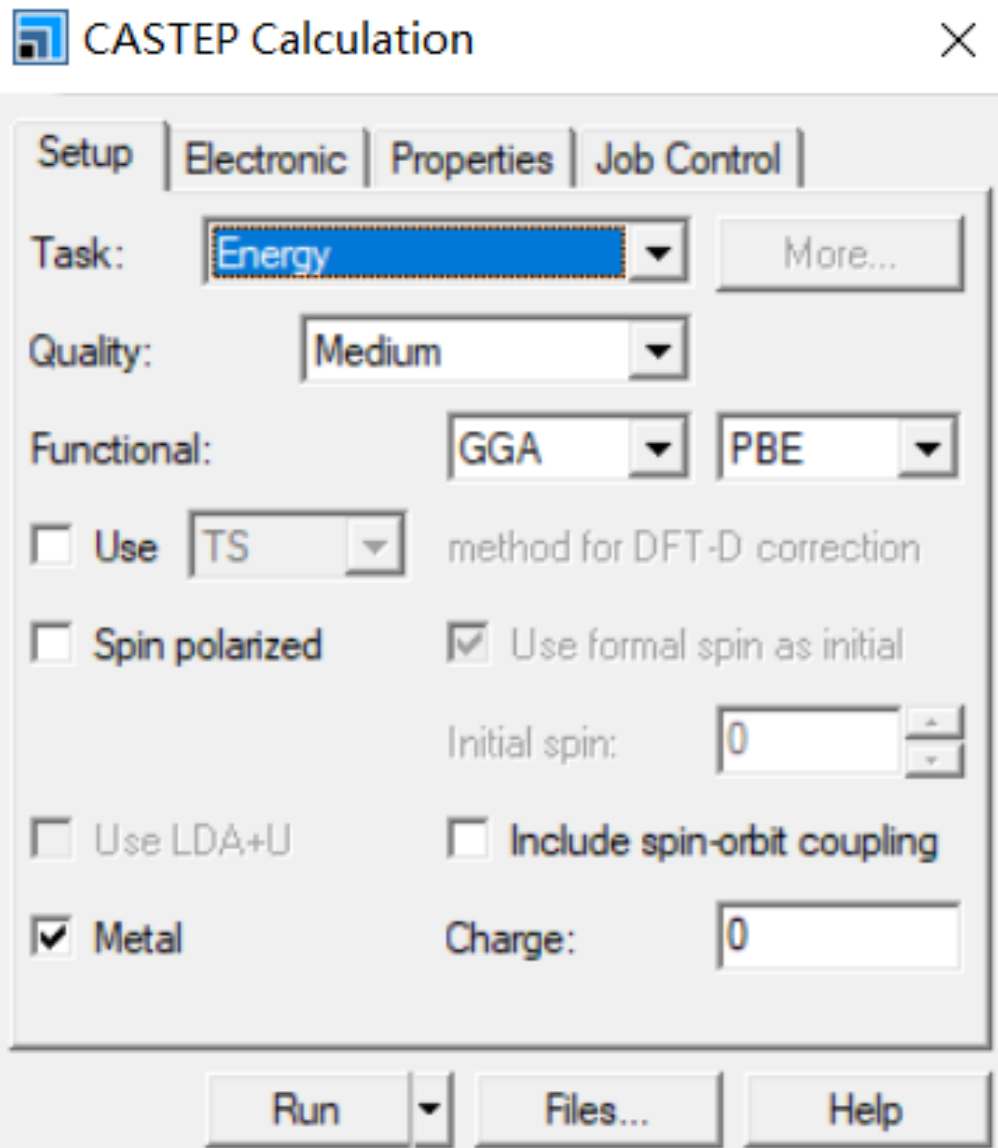
**Material Studio使用组件对话框中的CASTAP选项允许准备，启动，分析和监测CASTAP服役工作。**

**计算：允许选择计算选项（如基集，交换关联势和收敛判据），作业控制和文档控制。**

**分析：允许处理和演示CASTAP计算结果。这一工具提供加速整体直观化以及键结构图，态密度图形和光学性质图形。**

<http://www.castep.org/>

## Castep package



### ✓ Task

- Energy
- Geometry Optimization
- Dynamics

### ✓ Quality

- Coarse
- Medium
- Fine
- Ultra-fine

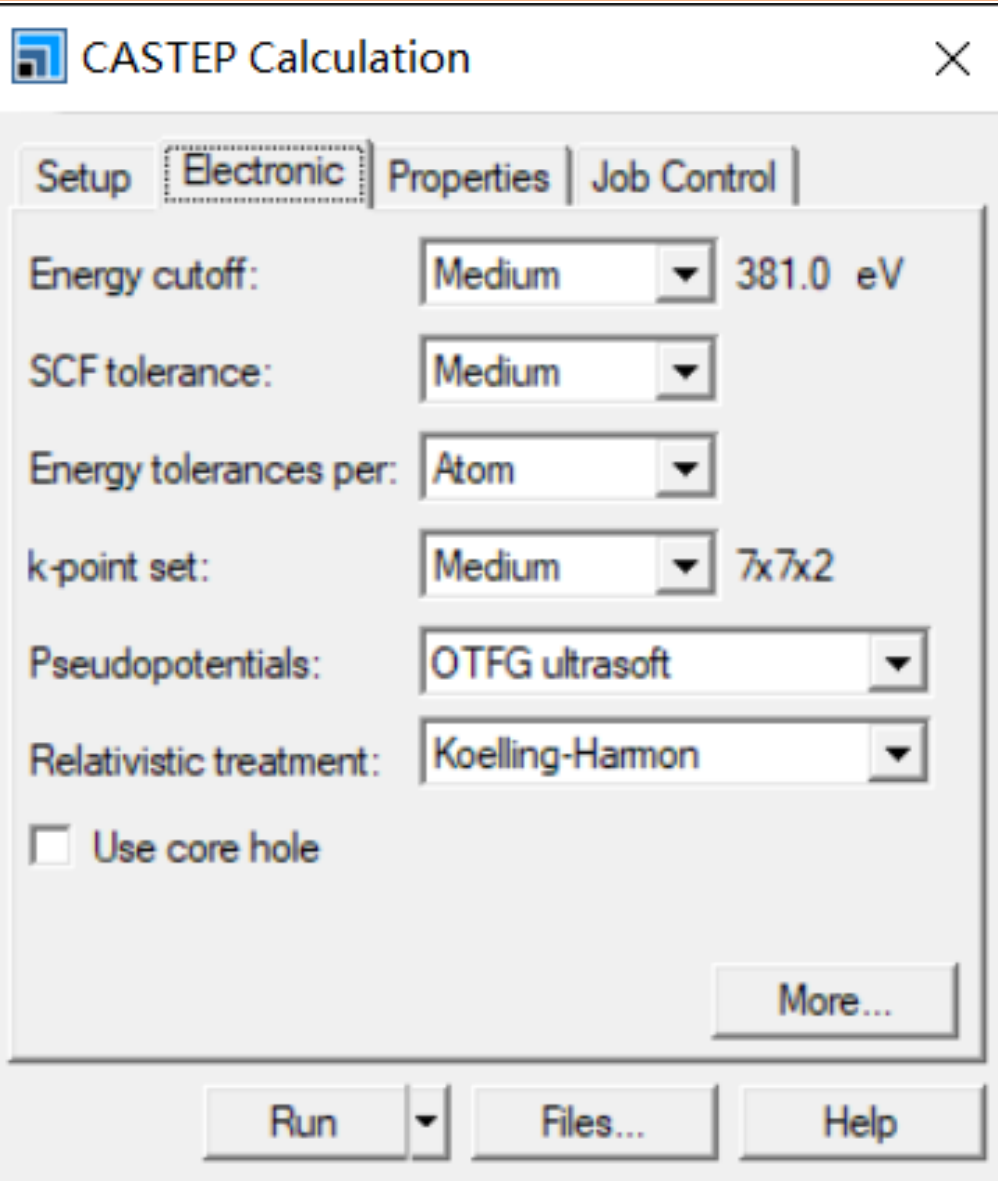
### ✓ Functional

- GGA-PBE
- LDA-CA-PZ

### ✓ Metal options

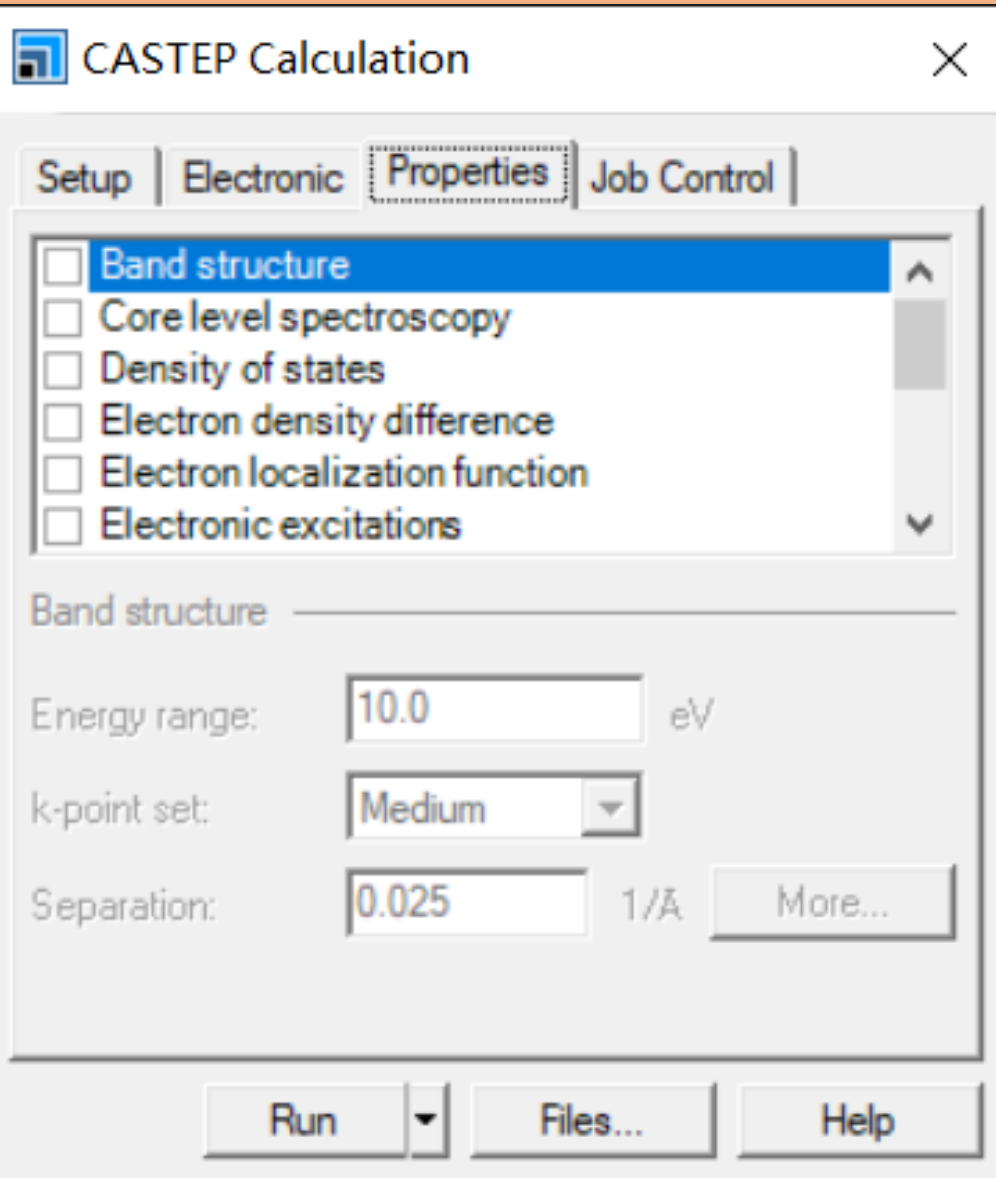


## Castep package ~ Calculation quality control



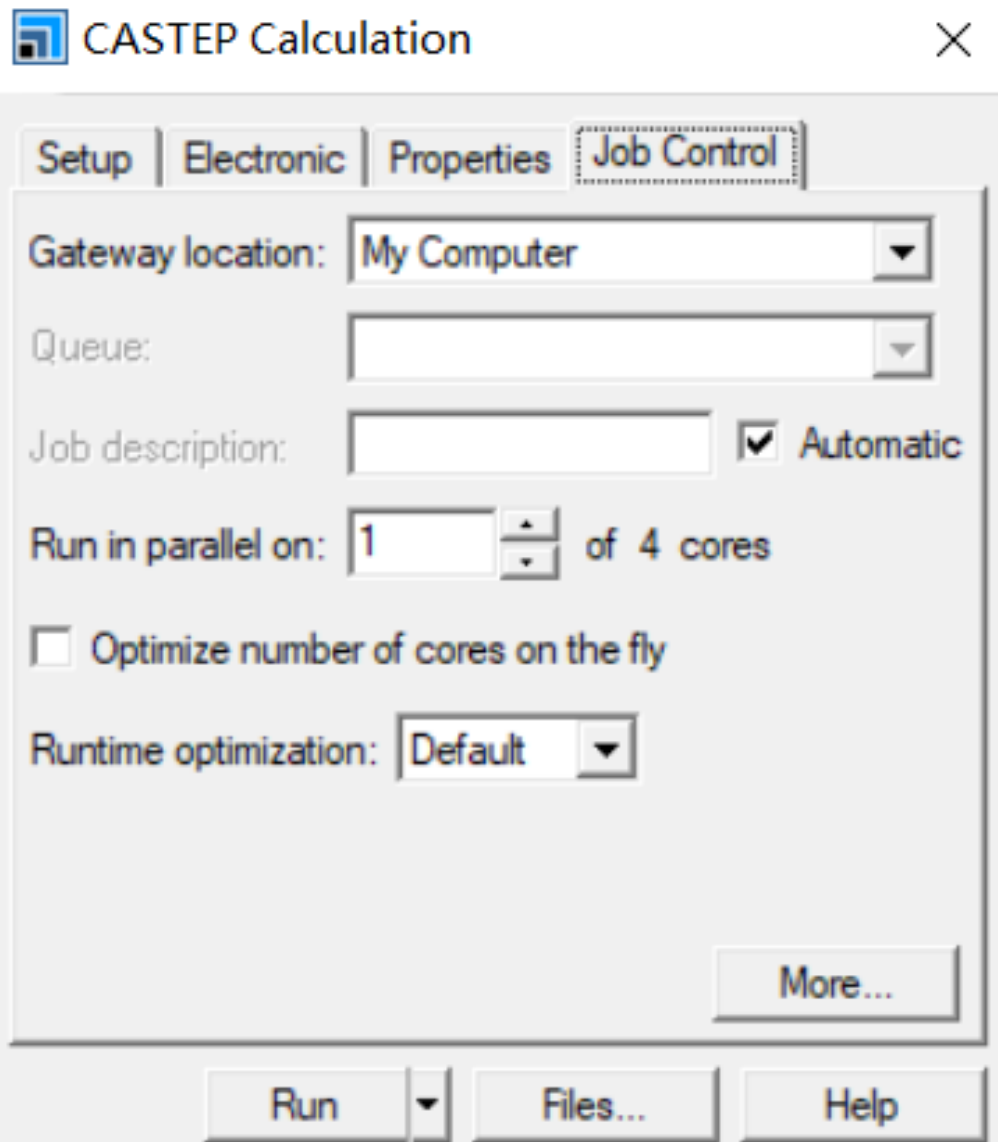
- ✓ **Energy cutoff**
  - Coarse
  - Medium
  - Fine
  - Ultra-fine
- ✓ **SCF tolerance**
  - Medium
- ✓ **k-points**
  - Gamma
  - Coarse
  - Medium
  - Fine
- ✓ **Pseudopotentials**

## Castep package ~ Calculation results control



- ✓ **Band structure**
- ✓ **Density of State**
- ✓ **Electron density difference**
- ✓ **Spectrum**

## CasteP package ~ Job Control



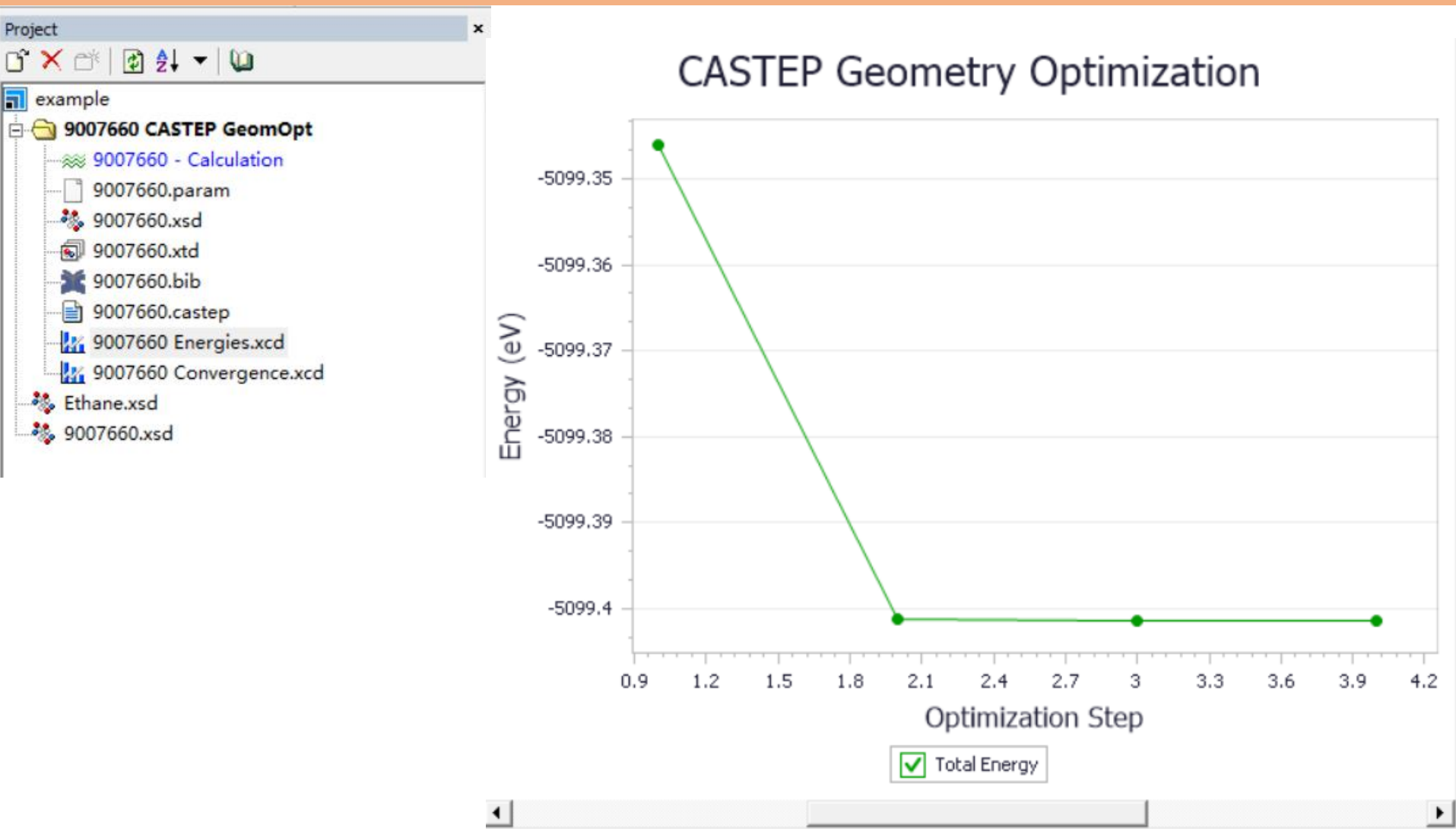
- ✓ **Parallel Setting**
  - Maximum: 4 (for most personal computer)
- ✓ **Runtime optimization**

# Example 1: Predict MoS<sub>2</sub> lattice parameter using castep

## Parameter Setting:

- ✓ **Task**
  - Geometry Optimization
- ✓ **Quality**
  - Medium
- ✓ **Functional**
  - GGA-PBE
- ✓ **Metal options**
  - Selected
- ✓ **Energy cutoff**
  - Medium
- ✓ **SCF tolerance**
  - Medium
- ✓ **k-points**
  - Medium
- ✓ **Pseudopotentials**
- ✓ **Parallel Setting**
  - Maximum: 4 (for most personal computer)
- ✓ **Runtime optimization**
  - default

## Example 1: Predict $\text{MoS}_2$ lattice parameter using castep



## Example 1: Predict MoS<sub>2</sub> lattice parameter using castep

The screenshot displays the CASTEP software interface. The top window, titled "9007660 CASTEP GeomOpt\9007660.xsd", shows a 3D model of a MoS<sub>2</sub> lattice structure. A context menu is open over the model, listing options: Cut (Ctrl+X), Copy (Ctrl+C), Paste (Ctrl+V), Delete, Display Style, Display Options, Lighting, Label, and Lattice Parameters. The "Lattice Parameters" option is highlighted. An orange arrow points from this option to the "Lattice Parameters" dialog box in the bottom-left corner.

The "Lattice Parameters" dialog box is open, showing the "Advanced" tab. It displays the following parameters:

- Lattice type: 3D Hexagonal
- Lengths (Å):
  - a: 3.161
  - b: 3.161
  - c: 12.295
- Symmetry constraints:  $a = b$
- Angles (degrees):
  - $\alpha$ : 90.000
  - $\beta$ : 90.000
  - $\gamma$ : 120.000
- Symmetry constraints:  $\alpha = \beta = 90$   $\gamma = 120$

The top-left window shows the project tree with the following files:

- example
  - 9007660 CASTEP GeomOpt
    - 9007660 - Calculation
      - 9007660.param
      - 9007660.xsd (highlighted)
      - 9007660.xtd
      - 9007660.bib
      - 9007660.castep
      - 9007660 Energies.xcd
      - 9007660 Convergence.xcd
    - Ethane.xsd
    - 9007660.xsd

## Example 2: Predict MoS<sub>2</sub> lattice parameter using castep

The screenshot displays the CASTEP software interface. The top window, titled "9007660 CASTEP GeomOpt\9007660.xsd", shows a 3D model of a MoS<sub>2</sub> lattice structure. A context menu is open over the model, listing options: Cut (Ctrl+X), Copy (Ctrl+C), Paste (Ctrl+V), Delete, Display Style, Display Options, Lighting, Label, and Lattice Parameters. The "Lattice Parameters" option is highlighted. An orange arrow points from this option to the "Lattice Parameters" dialog box in the bottom-left corner.

The "Lattice Parameters" dialog box is open, showing the "Advanced" tab. It displays the following parameters:

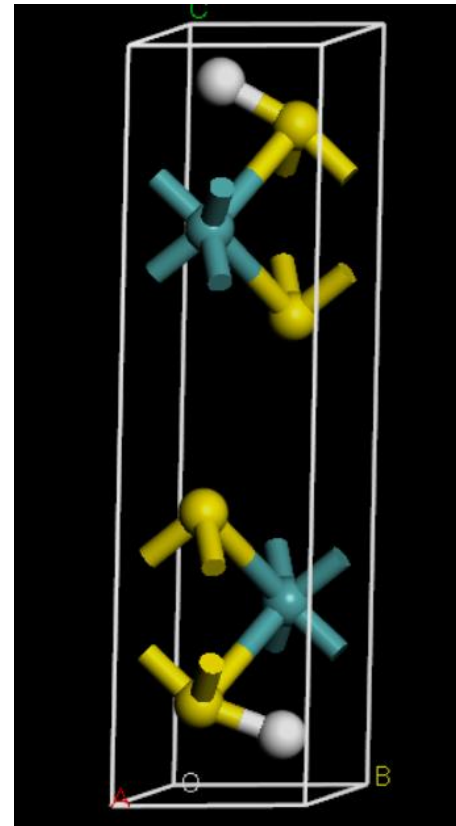
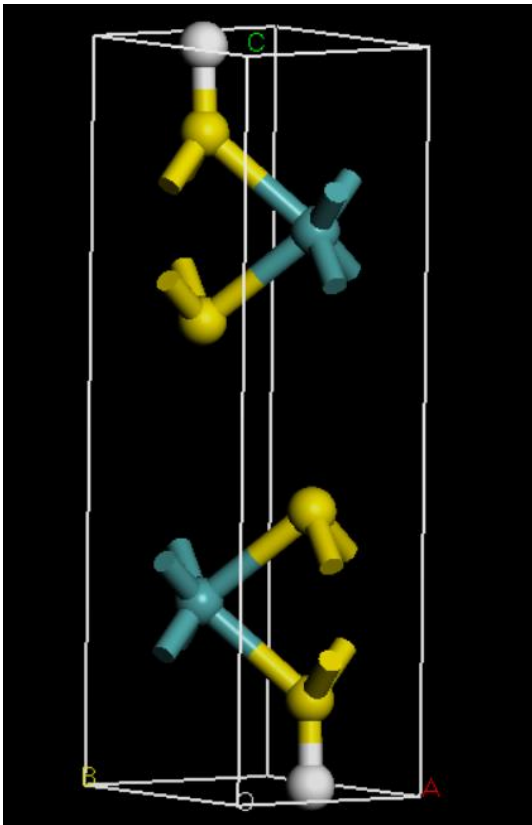
- Lattice type: 3D Hexagonal
- Lengths (Å):
  - a: 3.161
  - b: 3.161
  - c: 12.295
- Symmetry constraints:  $a = b$
- Angles (degrees):
  - $\alpha$ : 90.000
  - $\beta$ : 90.000
  - $\gamma$ : 120.000
- Symmetry constraints:  $\alpha = \beta = 90$   $\gamma = 120$

The top-left pane shows the project tree with the following files:

- example
  - 9007660 CASTEP GeomOpt
    - 9007660 - Calculation
      - 9007660.param
      - 9007660.xsd (highlighted)
      - 9007660.xtd
      - 9007660.bib
      - 9007660.castep
      - 9007660 Energies.xcd
      - 9007660 Convergence.xcd
    - Ethane.xsd
    - 9007660.xsd

# Test 1: Predict H@MoS<sub>2</sub> structure

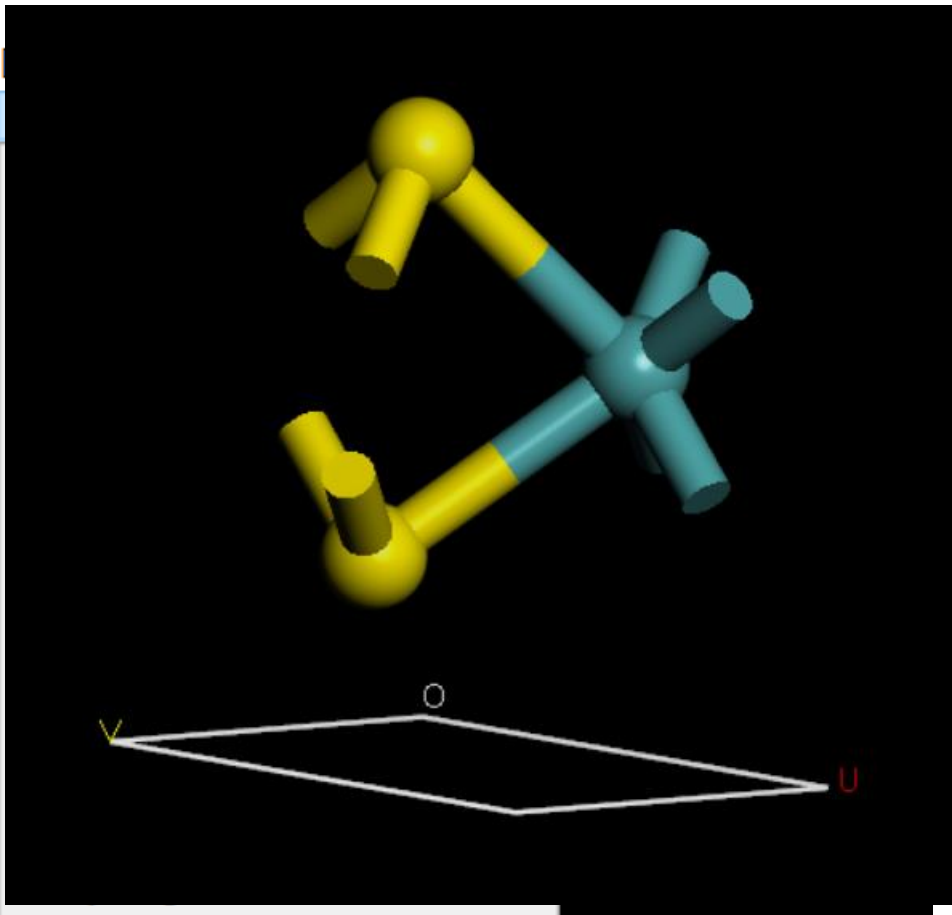
- ✓ Use **drawer tools** add H atoms
- ✓ Use **optimized** MoS<sub>2</sub> structure as template
- ✓ Try **top and bridge** adsorption site





Example 2: Predict H@monolayer-MoS<sub>2</sub> structure**Slab Model**

- ✓ Select facet (here is (001))
- ✓ Cleave face



**Cleave Surface** [X]

Surface Box | Surface Mesh | Options

Cleave plane (h k l):

Position

	Fractional	Angstrom
Top:	<input type="text" value="0.0"/>	<input type="text" value="0.0"/>
Thickness:	<input type="text" value="0.5"/>	<input type="text" value="6.147"/>

Cleaving

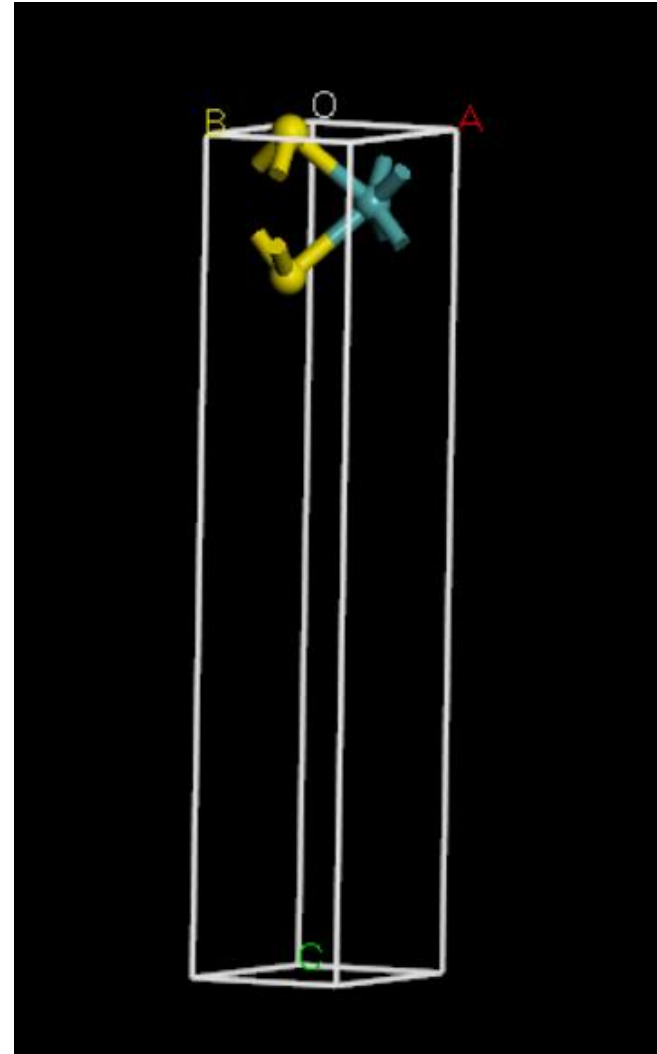
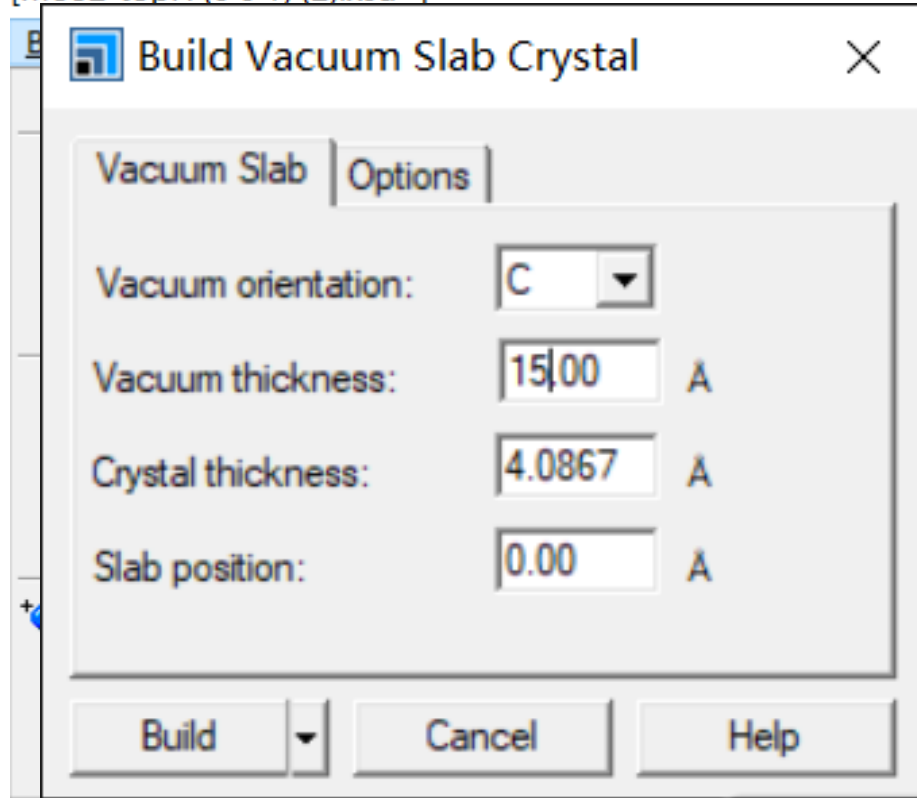
Cleave rule:

Cap bonds on  face with

Example 2: Predict H@monolayer-MoS<sub>2</sub> structure**Slab Model**

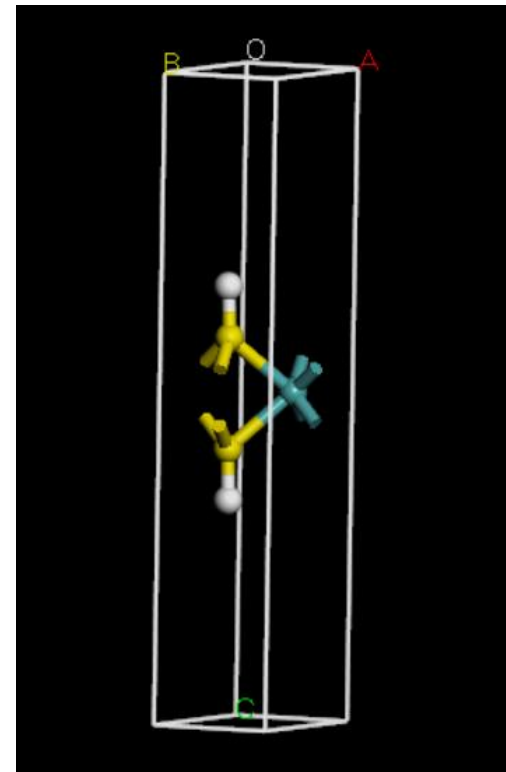
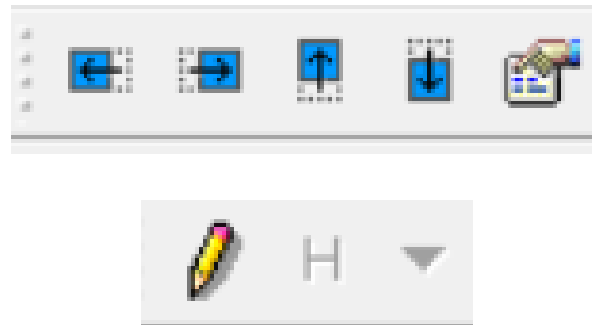
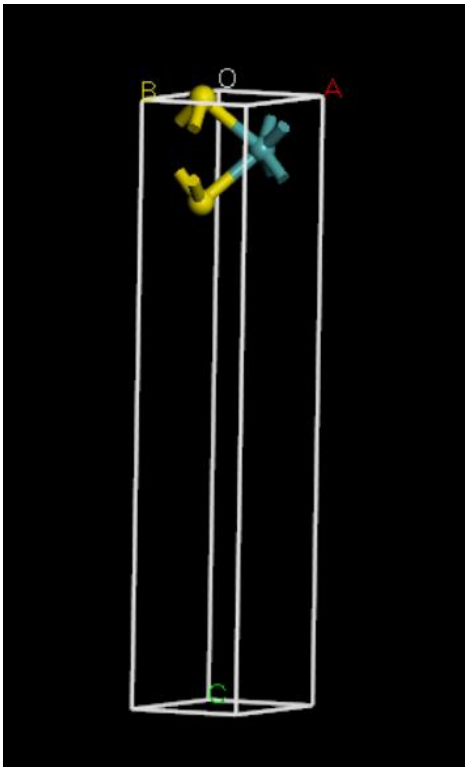
- ✓ Build vacuum layer

[MoS2-topH (0 0 1) (2).xsd \*]



Example 2: Predict H@monolayer-MoS<sub>2</sub> structure**Slab Model**

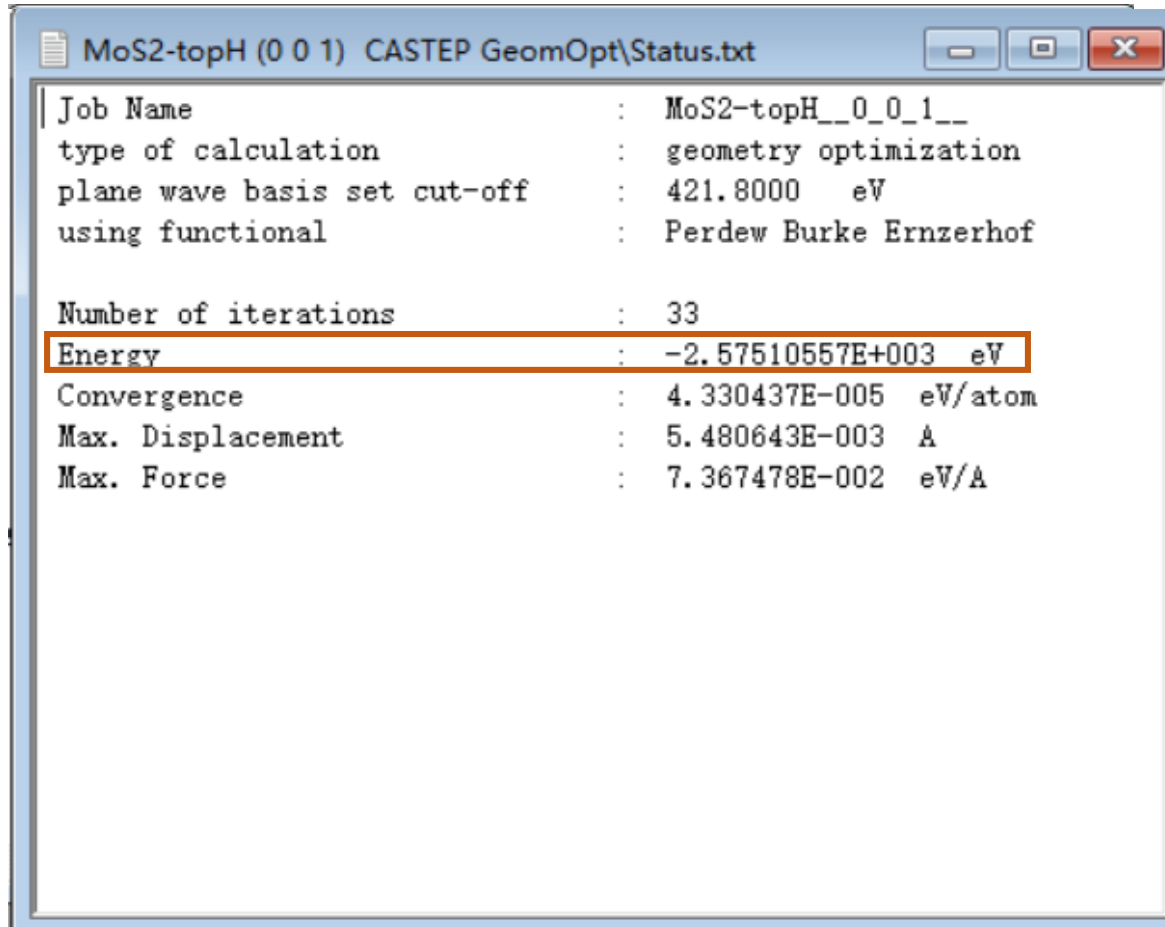
- ✓ Move MoS<sub>2</sub>
- ✓ Add H atom



Example 2: Predict H@monolayer-MoS<sub>2</sub> structure**CasteP module**

- ✓ **Task**
  - Geometry Optimization
- ✓ **Quality**
  - Medium
- ✓ **Functional**
  - GGA-PBE
- ✓ **Metal options**
  - Selected
- ✓ **Parallel Setting**
  - Maximum: 4 (for most personal computer)
- ✓ **Runtime optimization**
  - default
- ✓ **Energy cutoff**
  - Medium
- ✓ **SCF tolerance**
  - Medium
- ✓ **k-points**
  - Medium
- ✓ **Pseudopotentials**

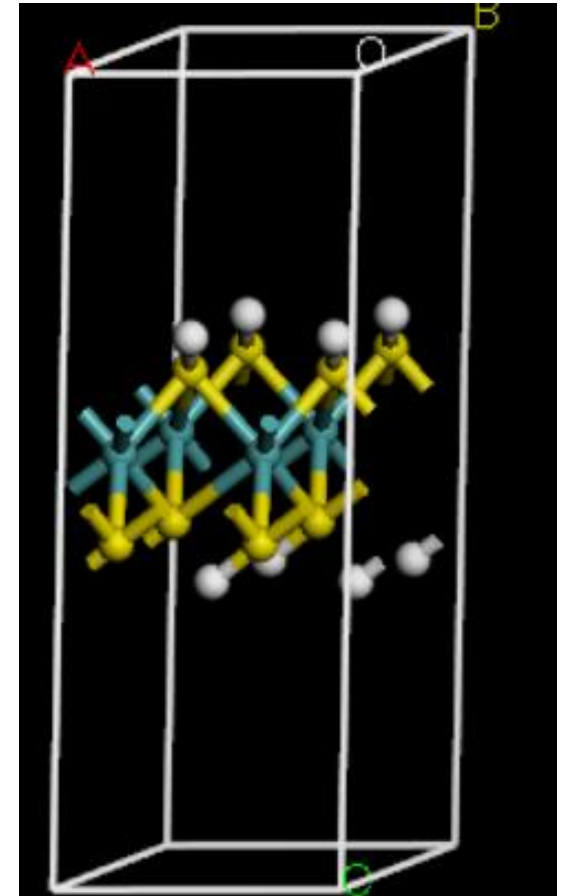
**Same Parameters**

Example 2: Predict H@monolayer-MoS<sub>2</sub> structureResults

```
MoS2-topH (0 0 1) CASTEP GeomOpt\Status.txt

Job Name           : MoS2-topH__0_0_1__
type of calculation : geometry optimization
plane wave basis set cut-off : 421.8000 eV
using functional    : Perdew Burke Ernzerhof

Number of iterations : 33
Energy              : -2.57510557E+003 eV
Convergence         : 4.330437E-005 eV/atom
Max. Displacement   : 5.480643E-003 A
Max. Force          : 7.367478E-002 eV/A
```



Example 2: Predict H@monolayer-MoS<sub>2</sub> structureAdsorption energy

$$\Delta E_{\text{H}} = \frac{1}{n} [E(\text{surf} + n\text{H}) - E(\text{surf}) - \frac{n}{2} E(\text{H}_2)]$$

$E(\text{surf} + n\text{H})$       **MoS<sub>2</sub> energy**

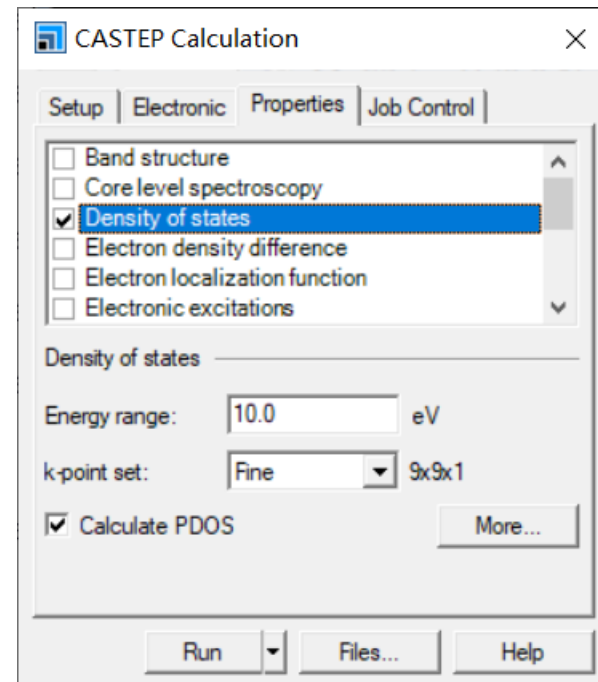
$E(\text{surf})$       **H@MoS<sub>2</sub> energy**

$E(\text{H}_2)$       **H energy**

Example 3: MoS<sub>2</sub> Density of State

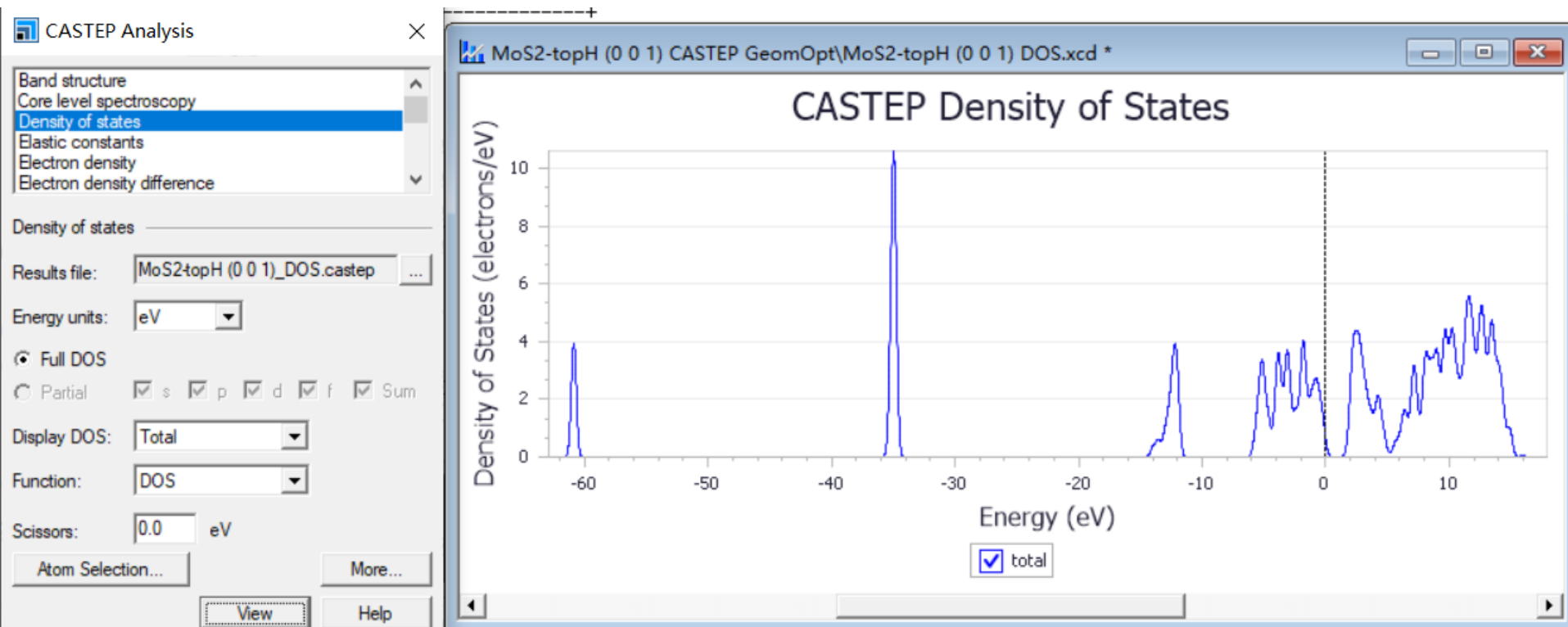
## CasteP module

- ✓ **Task**
  - Geometry Optimization
- ✓ **Quality**
  - High
- ✓ **Functional**
  - GGA-PBE
- ✓ **Metal options**
  - Selected
- ✓ **Parallel Setting**
  - Maximum: 4 (for most personal computer)
- ✓ **Runtime optimization**
  - default
- ✓ **Energy cutoff**
  - High
- ✓ **SCF tolerance**
  - Medium
- ✓ **k-points**
  - High
- ✓ **Pseudopotentials**



# Example 3: MoS<sub>2</sub> Density of State

## Results



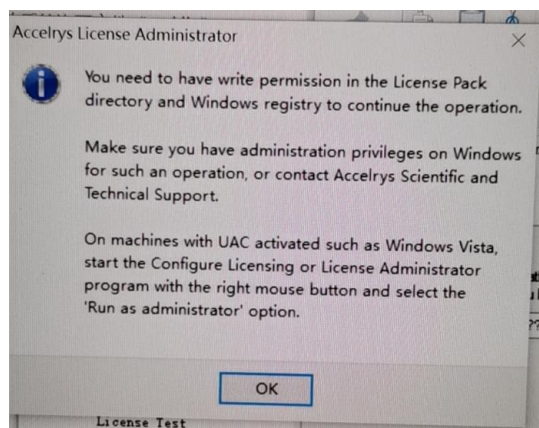


# Installation Question Collection

Q: Lic文件在哪里?



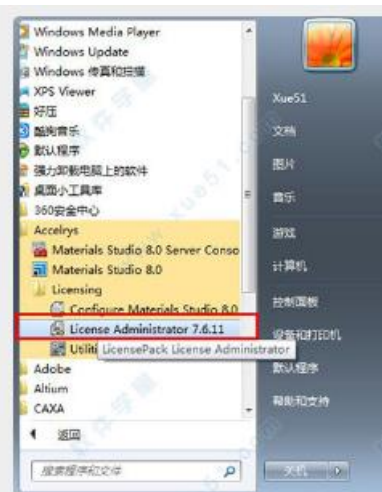
Q:



A:

2020-02-20 12:37

74KB



选择那一步，右键管理员身份运行，

**Thanks for your attention!**