Material Studio Tutorial

A introduction for beginner

HU ZHENG

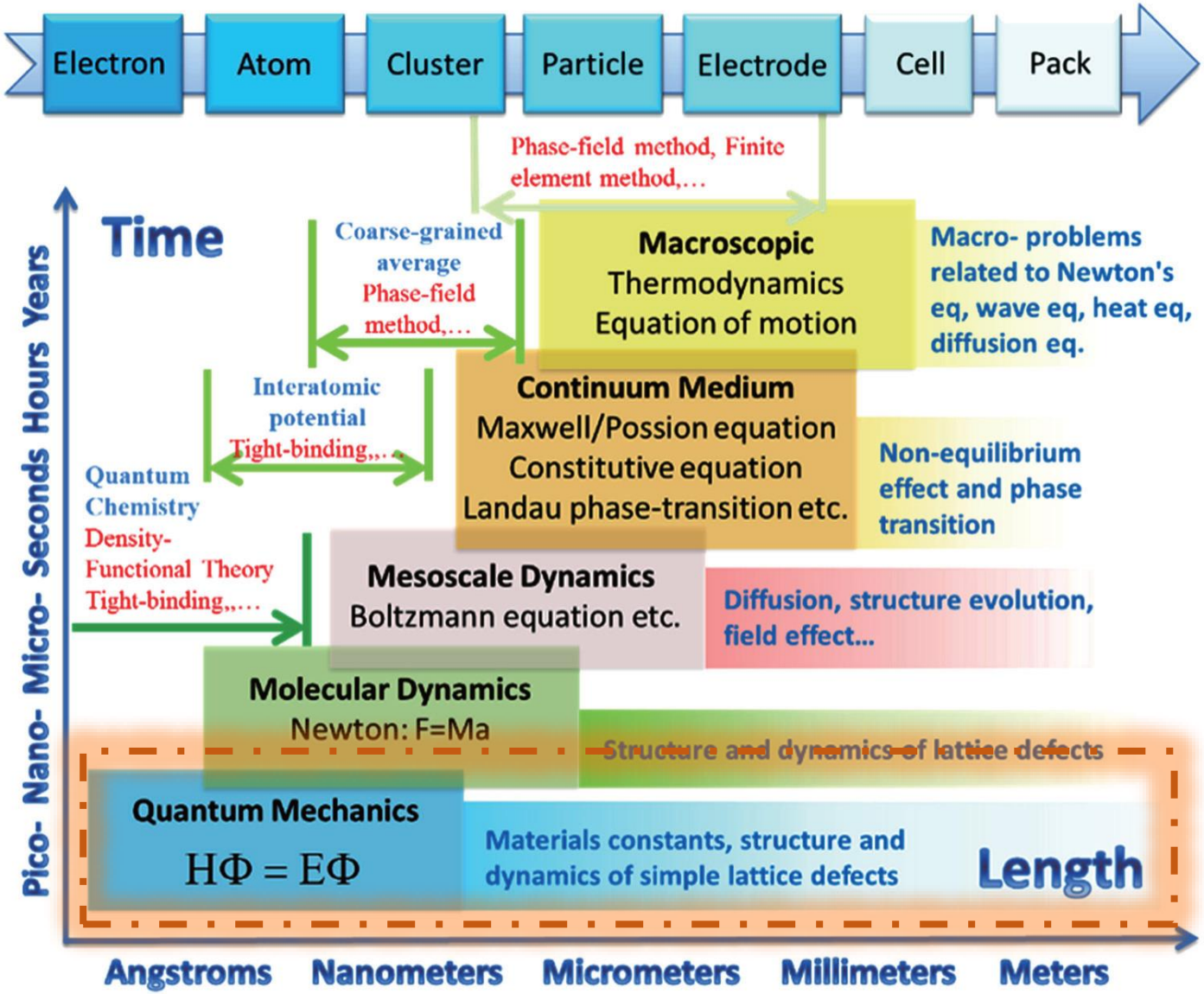
Chemical Engineering Academy

Tianjin University

February 25, 2019

Content

Calculational 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.

$$H\Phi = E\Phi$$

Hydrogen atom (1e)

Born Oppenheimer Approximation

$$H = T + W + V$$

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

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

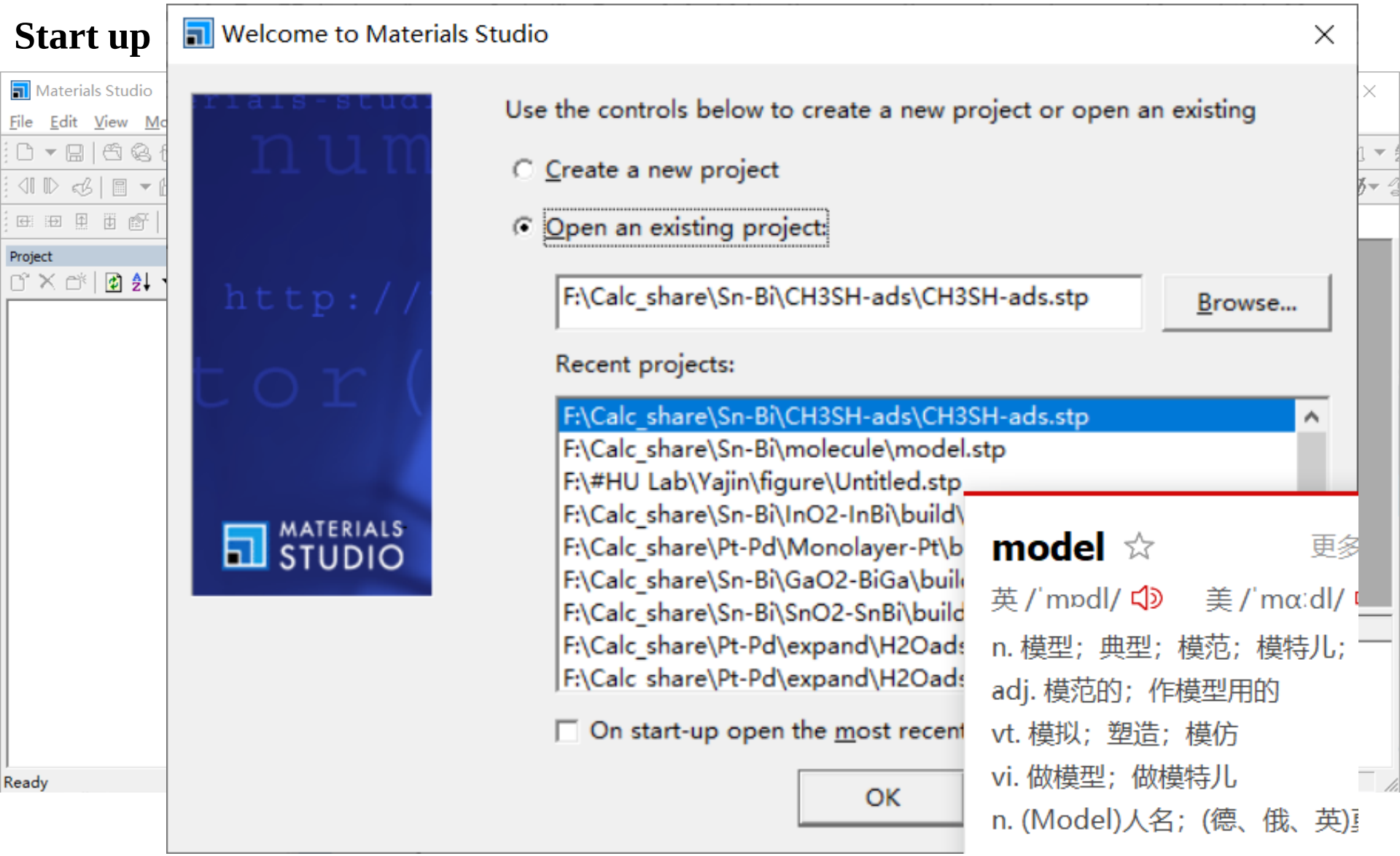
Exchange functional approximation:

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

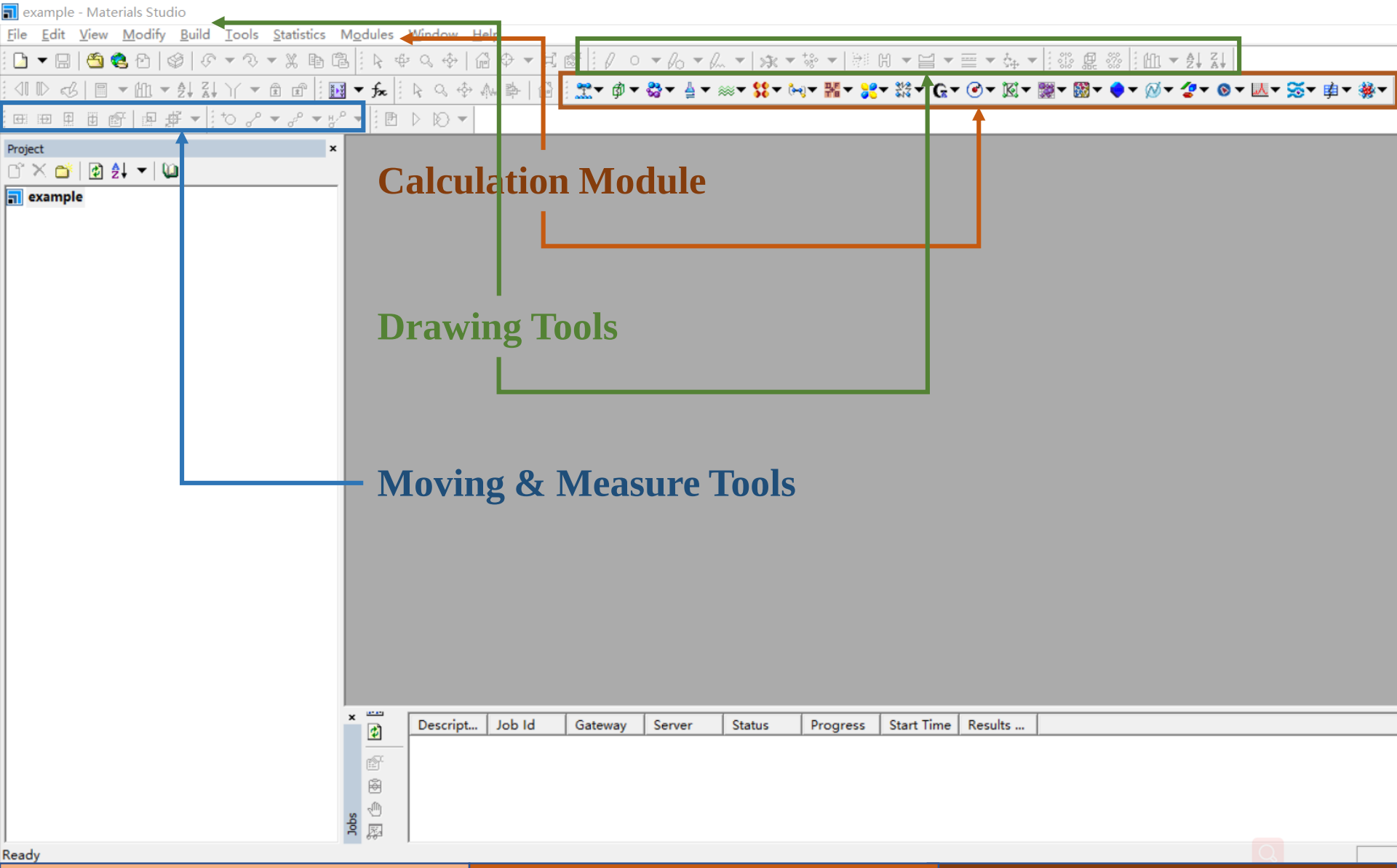
Content

Material Studio

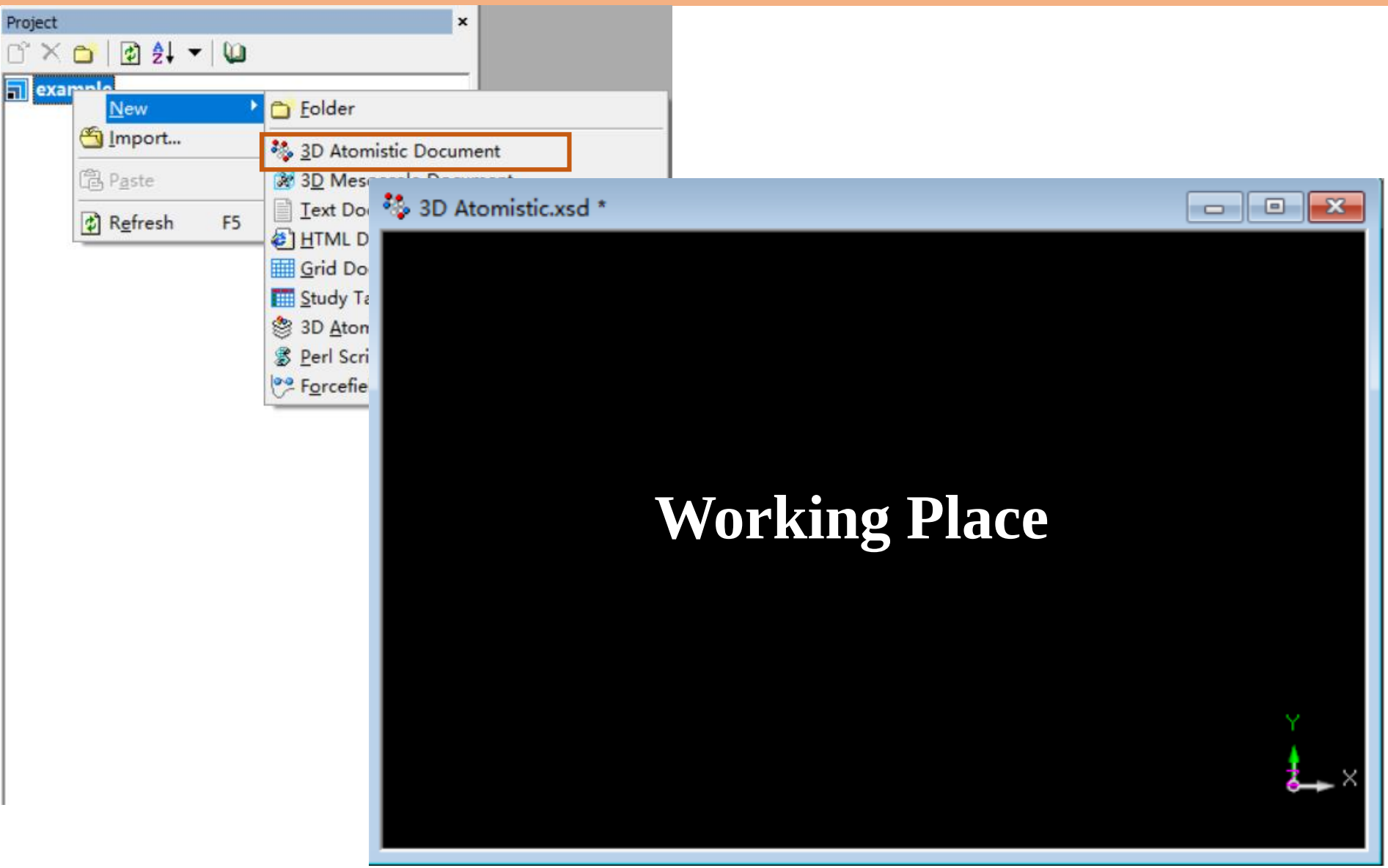
Start up



Status bar


example - Materials Studio
File Edit View Modify Build Tools Statistics Modules Window Help
Project
example
Calculation Module
Drawing Tools
Moving & Measure Tools
Descript... Job Id Gateway Server Status Progress Start Time Results ...
Jobs
Ready

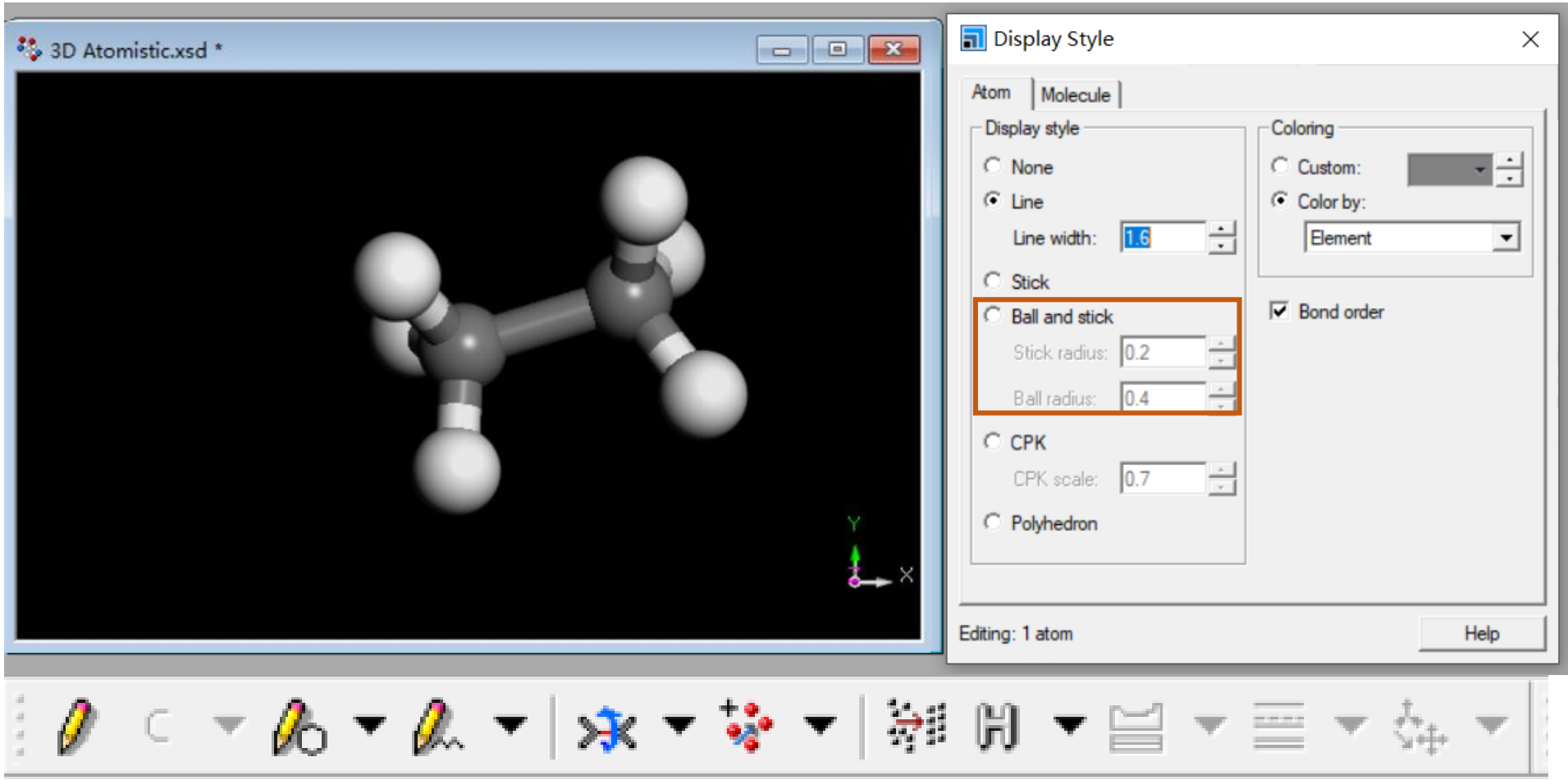
Modeling


Project
example
New
Import...
Paste
Refresh F5
Folder
3D Atomistic Document
Text Do
HTML D
Grid Do
Study Ta
3D Aton
Perl Scri
Forcefie
3D Atomistic.xsd *
Working Place
Y
X

Modeling ~ Organic Molecules

ethane model

Single molecule



Sketch atoms, bonds, cycles, etc.

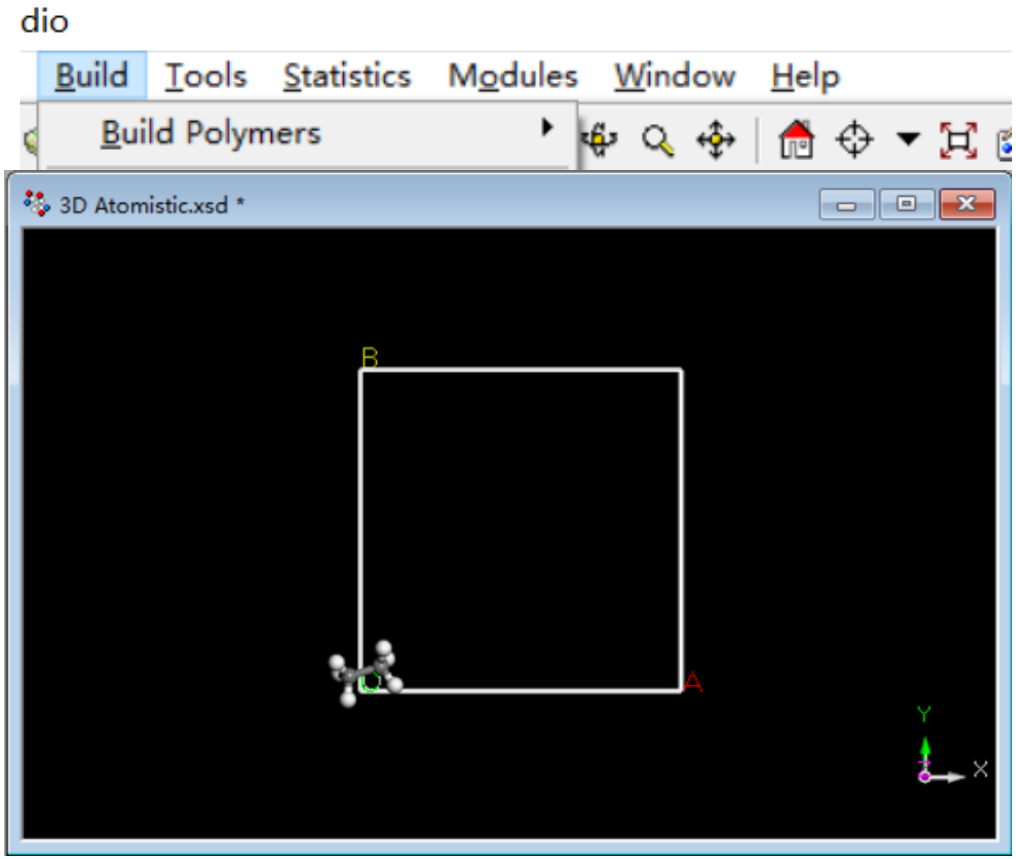
Auto-add H atoms

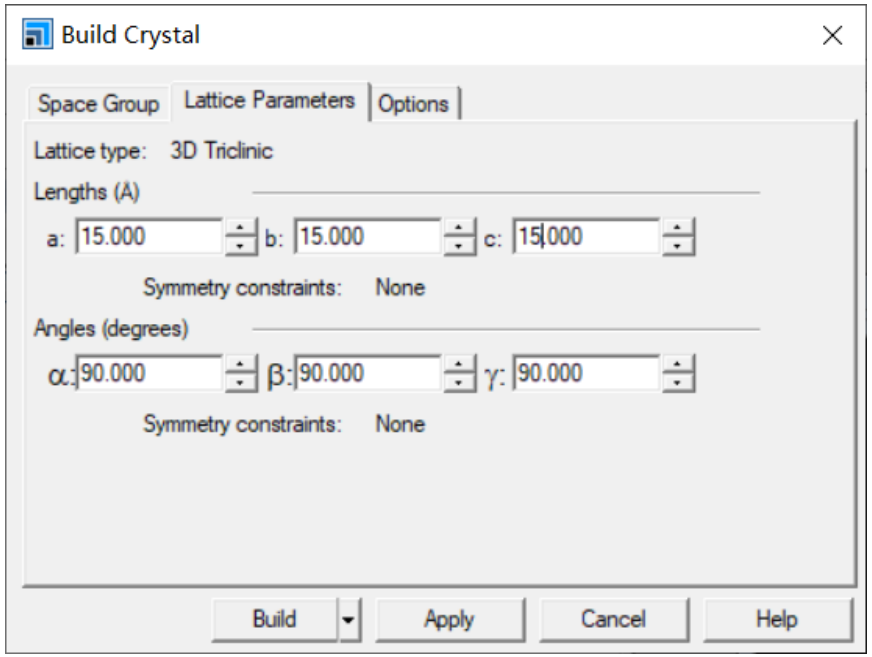
Change atoms/bonds

Modeling ~ Organic Molecules

Single molecule → **Ethane model** → **Molecule system**

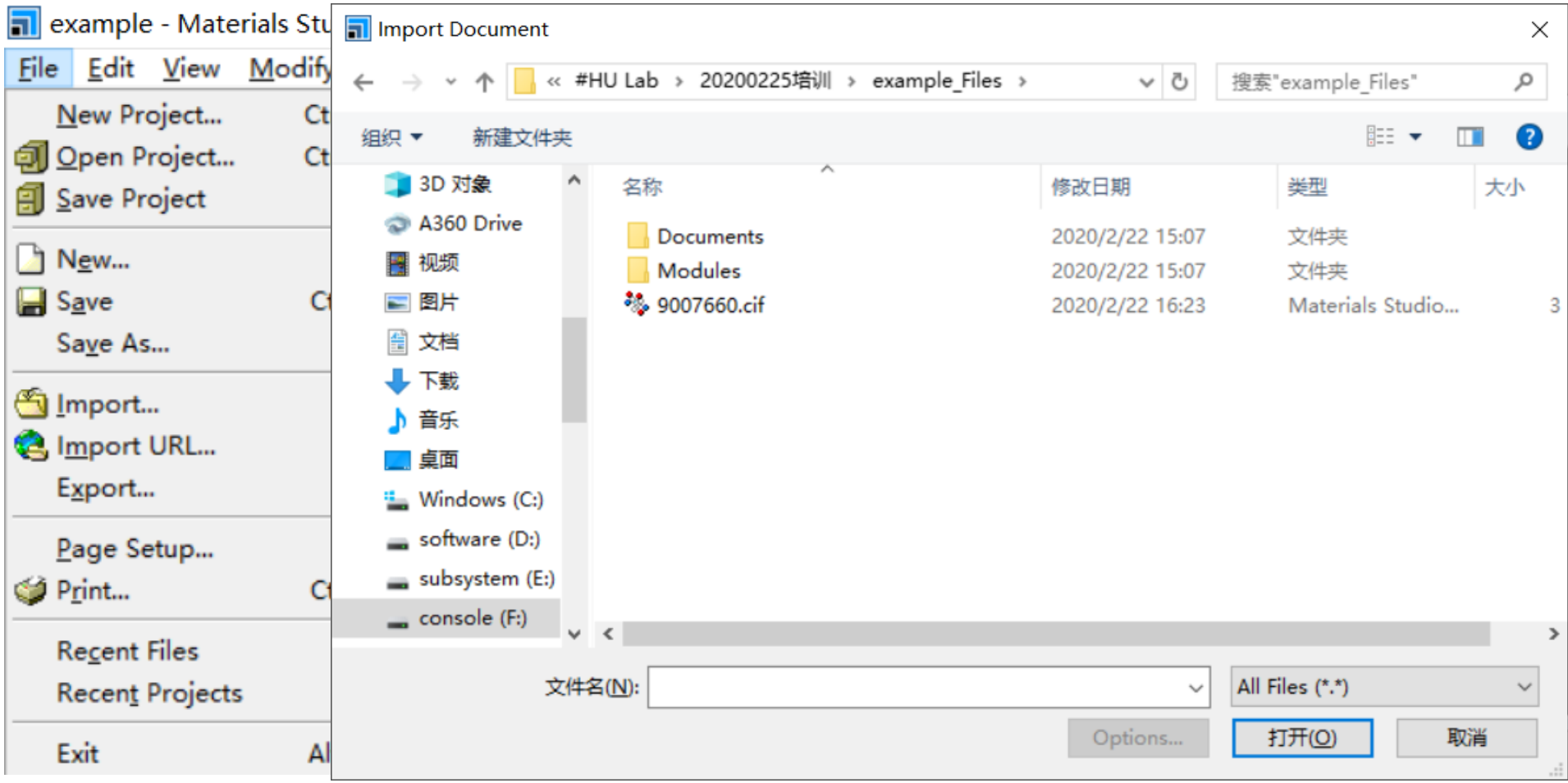
- ✓ **Gas**
- ✓ Liquid
- ✓ Solid
  - ➢ Crystal
  - ➢ Amorphous





Modeling ~ Metal & Other Crystals

“import” operation

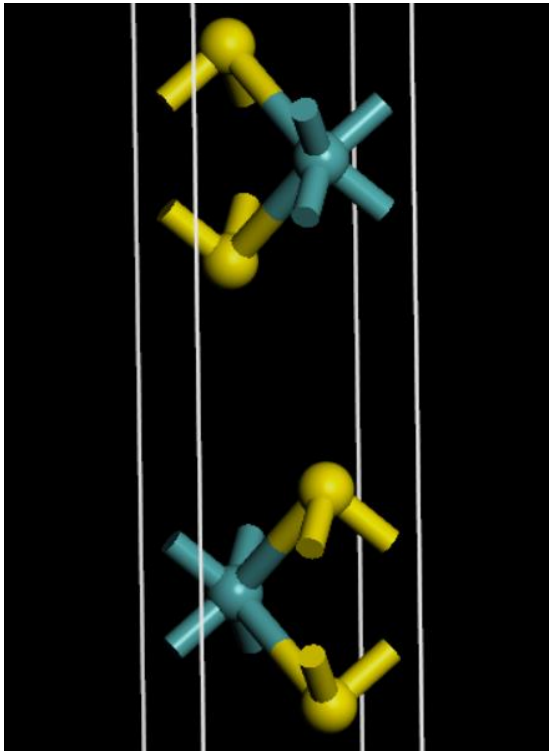


Modeling ~ Metal & Other Crystals

text (1 or 2 words)	MoS2
journal	
year	
volume	
issue	
DOI	
Z (min, max)	
Z' (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	
	has E...

Reset Send

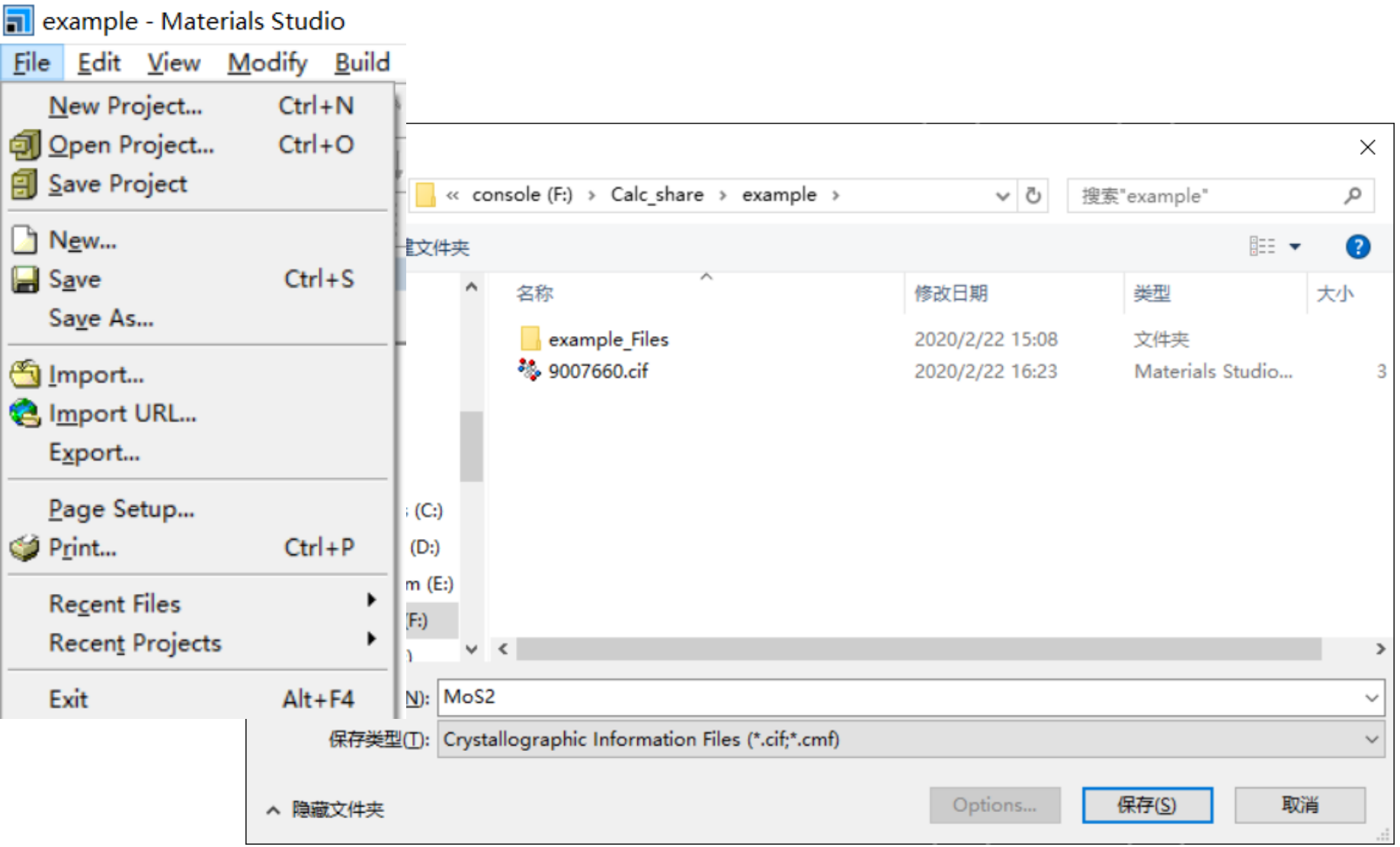
cif file database



COD ID ▲	Links	Formula ▲	Space group ▲	Cell parameters	Cell volume ▲	Bibliography
9007660	CIF	Mo S2	P 63/m m c	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 *Acta Crystallographica, Section B*, **1983**, *39*, 404-407

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

Modeling ~ Export file



Content

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。

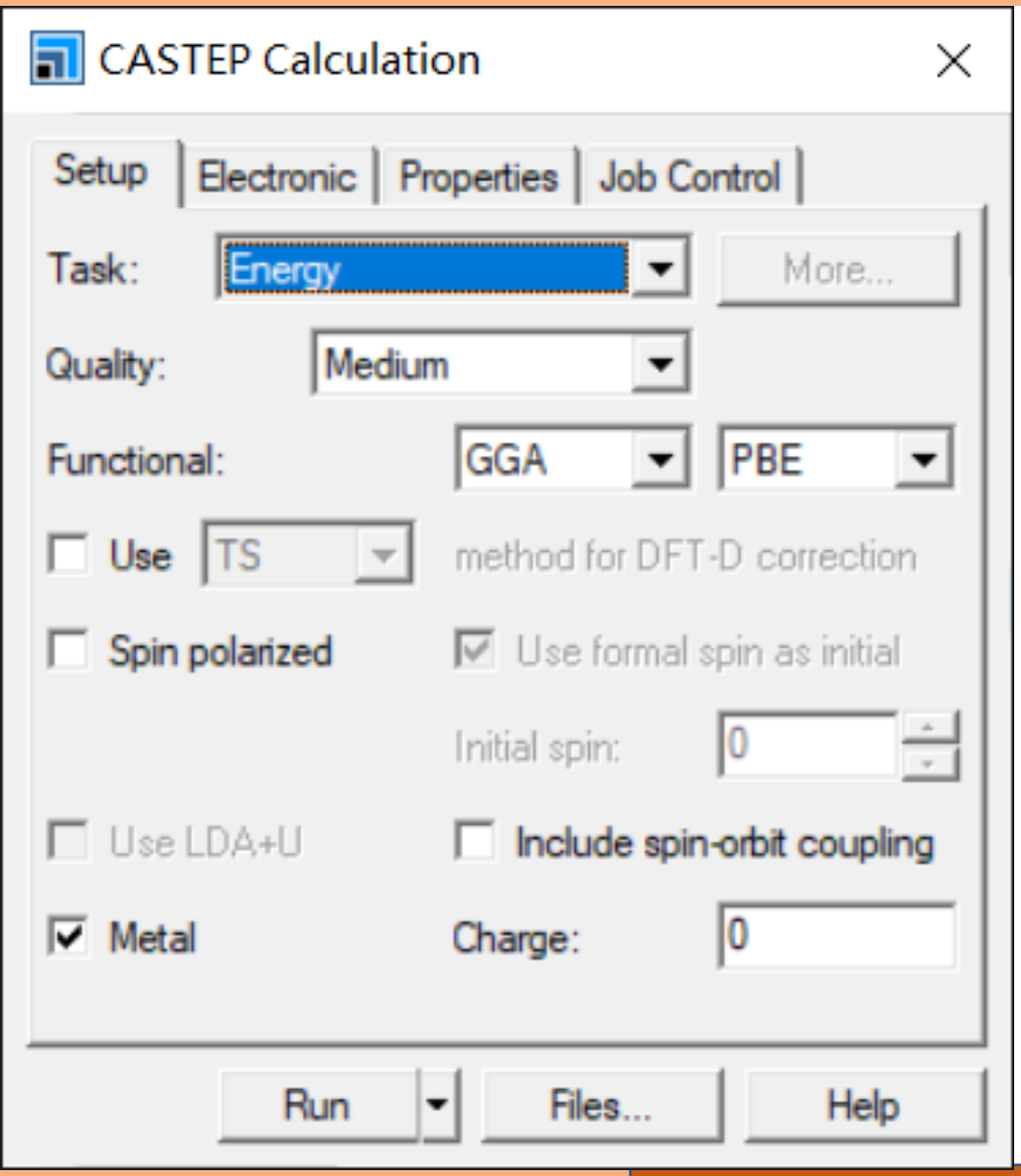
Material Studio使用组件对话框中的CASTAP选项允许准备，启动，分析和监测CASTAP服役工作。

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。

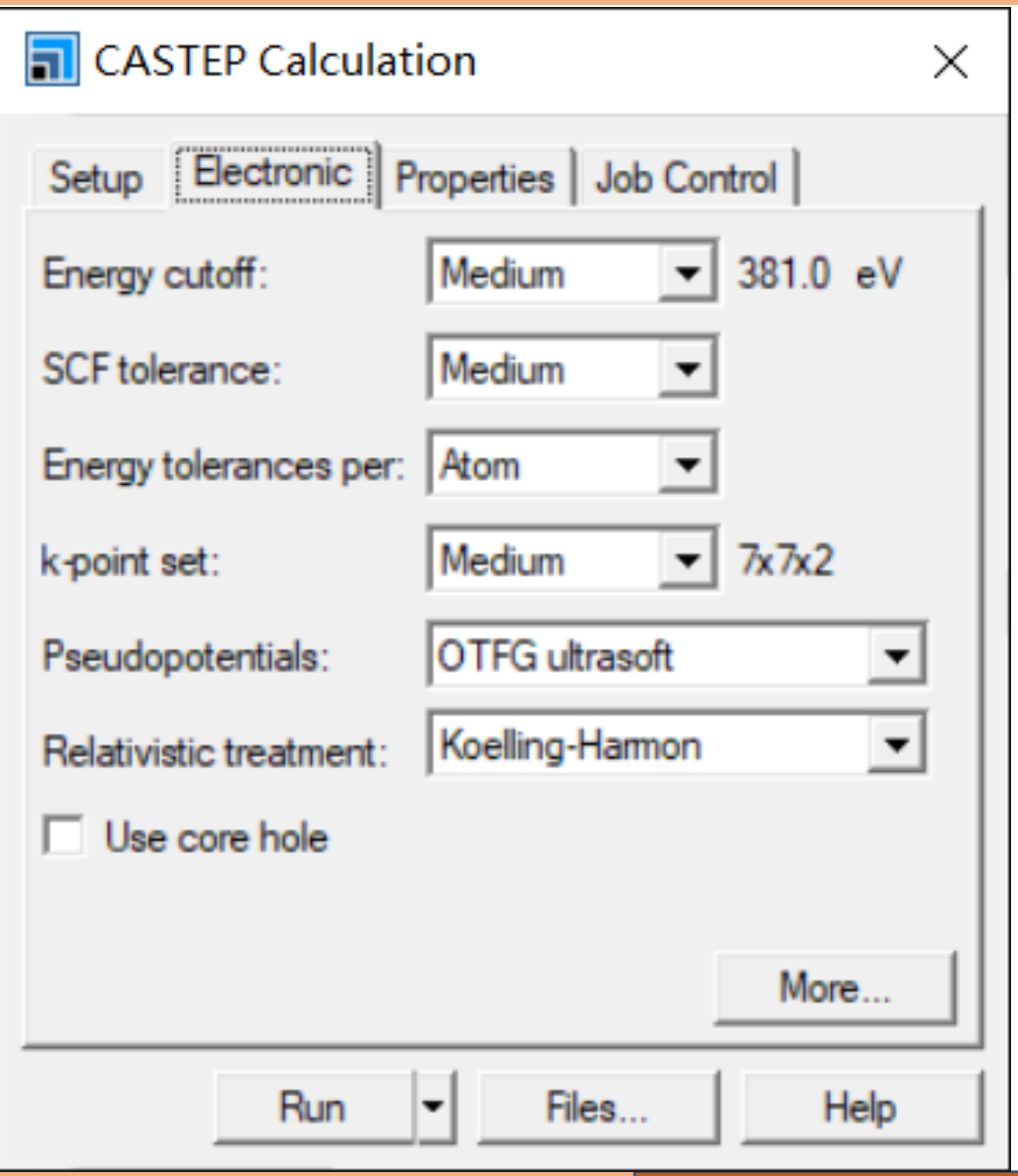
http://www.castep.org/

Castep package



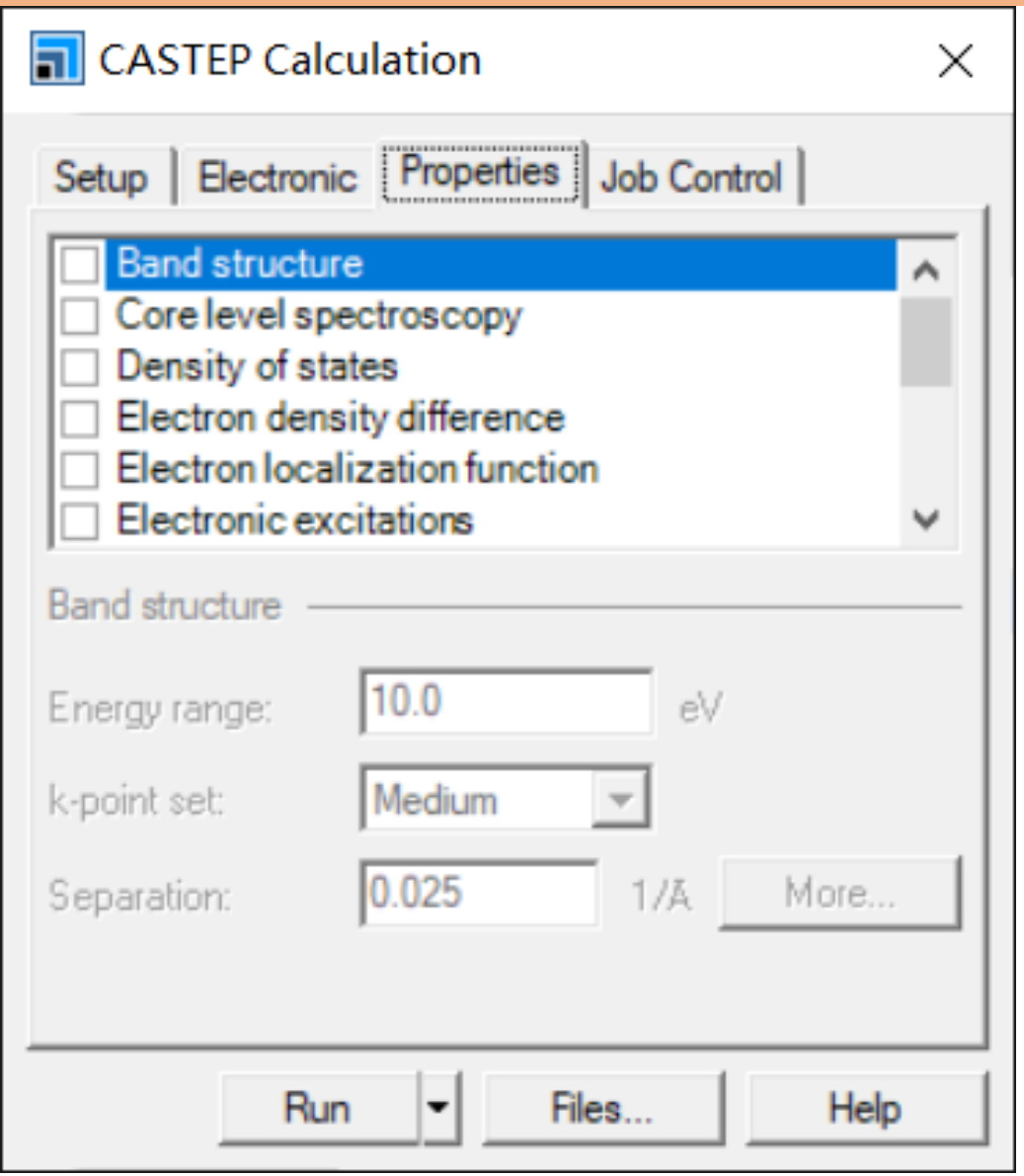
- ✓ **Task**
  - ➢ Energy
  - ➢ Geometry Optimization
  - ➢ Dynamics
- ✓ **Quality**
  - ➢ Coarse
  - ➢ Medium
  - ➢ Fine
  - ➢ Ultra-fine
- ✓ **Functional**
  - ➢ GGA-PBE
  - ➢ LDA-CA-PZ
- ✓ **Metal options**

Castep package ~ Calculation quality control



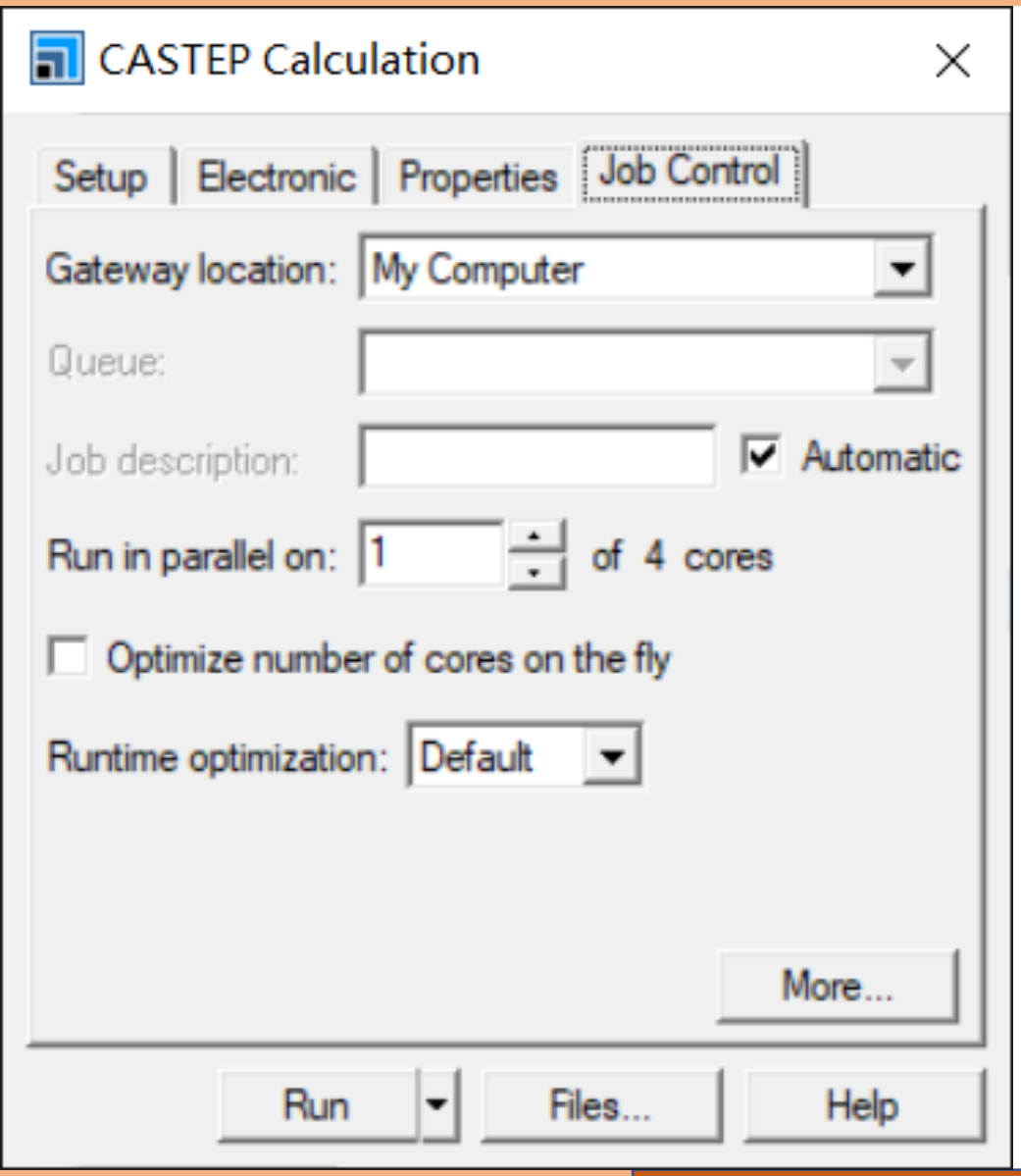
- ✓ **Energy cutoff**
  - ➢ Coarse
  - ➢ Medium
  - ➢ Fine
  - ➢ Ultra-fine
- ✓ **SCF tolerance**
  - ➢ Medium
- ✓ **k-points**
  - ➢ Gamma
  - ➢ Coarse
  - ➢ Medium
  - ➢ Fine
- ✓ **Pseudopotentials**

Castep package ~ Calculation results control



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

Castep package ~ Job Control



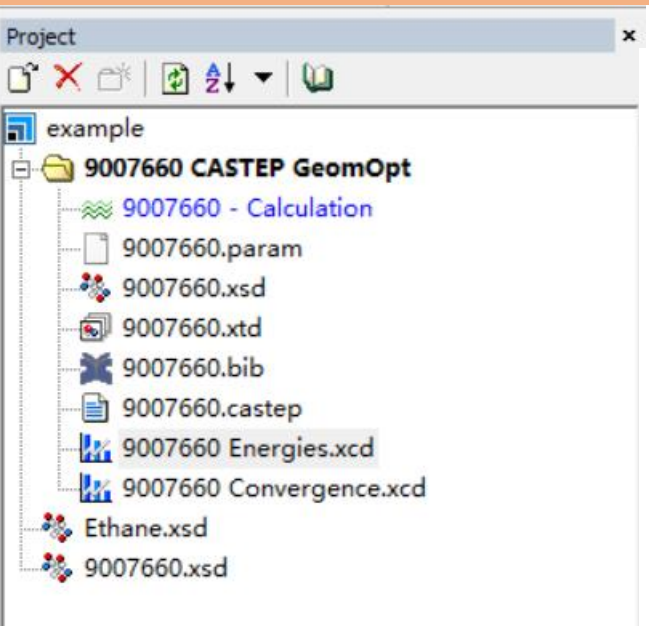
- ✓ **Parallel Setting**
  - ➢ Maximum: 4 (for most personal computer)
- ✓ **Runtime optimization**

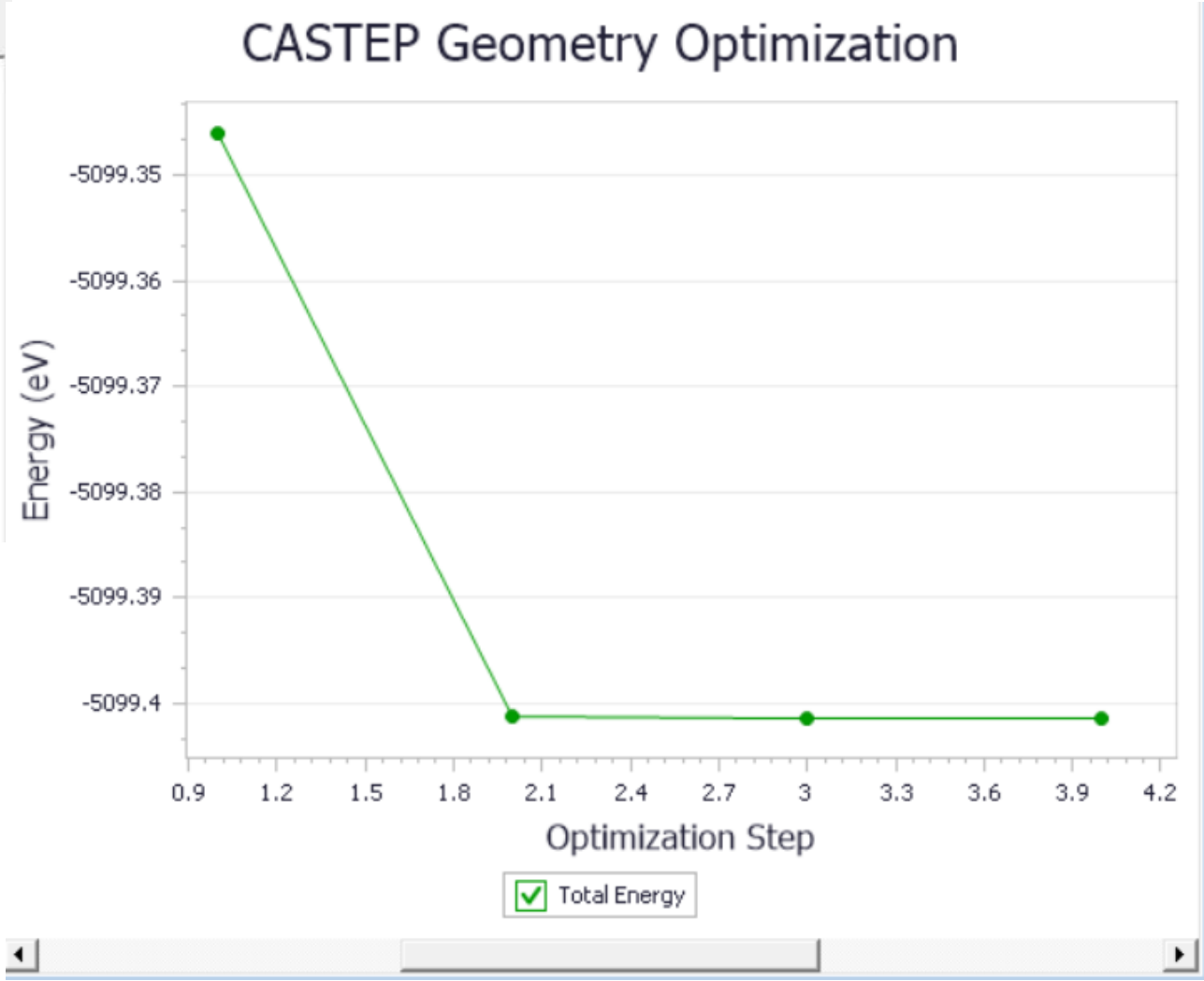
Example 1: Predict MoS_2 lattice parameter using castep

Parameter Setting:

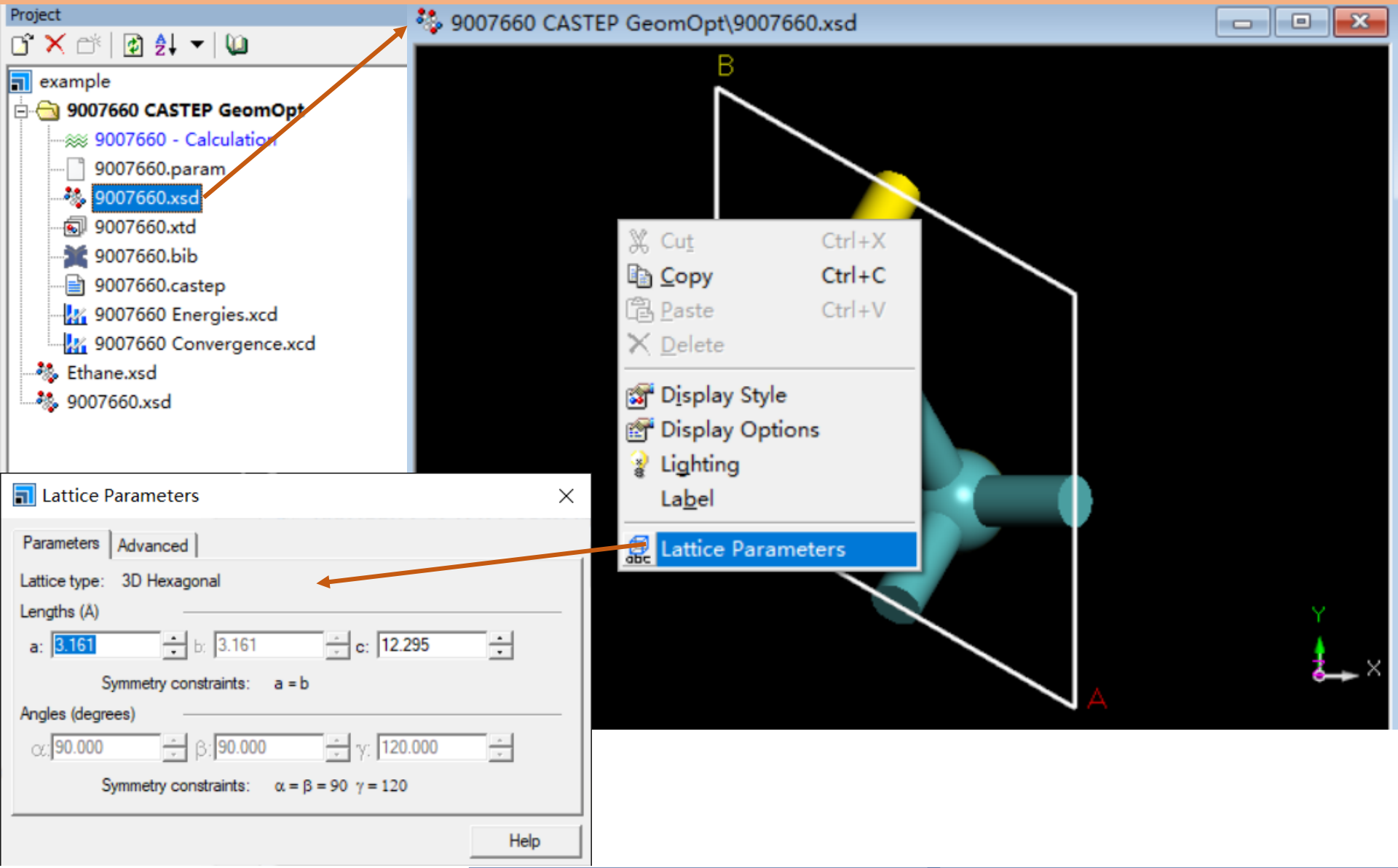
- ✓ **Task**
  - ➢ Geometry Optimization
- ✓ **Quality**
  - ➢ Medium
- ✓ **Functional**
  - ➢ GGA-PBE
- ✓ **Metal options**
  - ➢ Selected
- ✓ **Parallel Setting**
  - ➢ Maximum: 4 (for most personal computer)
- ✓ **Runtime optimization**
  - ➢ **default**
- ✓ **Energy cutoff**
  - ➢ Medium
- ✓ **SCF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

Example 1: Predict MoS_2 lattice parameter using castep

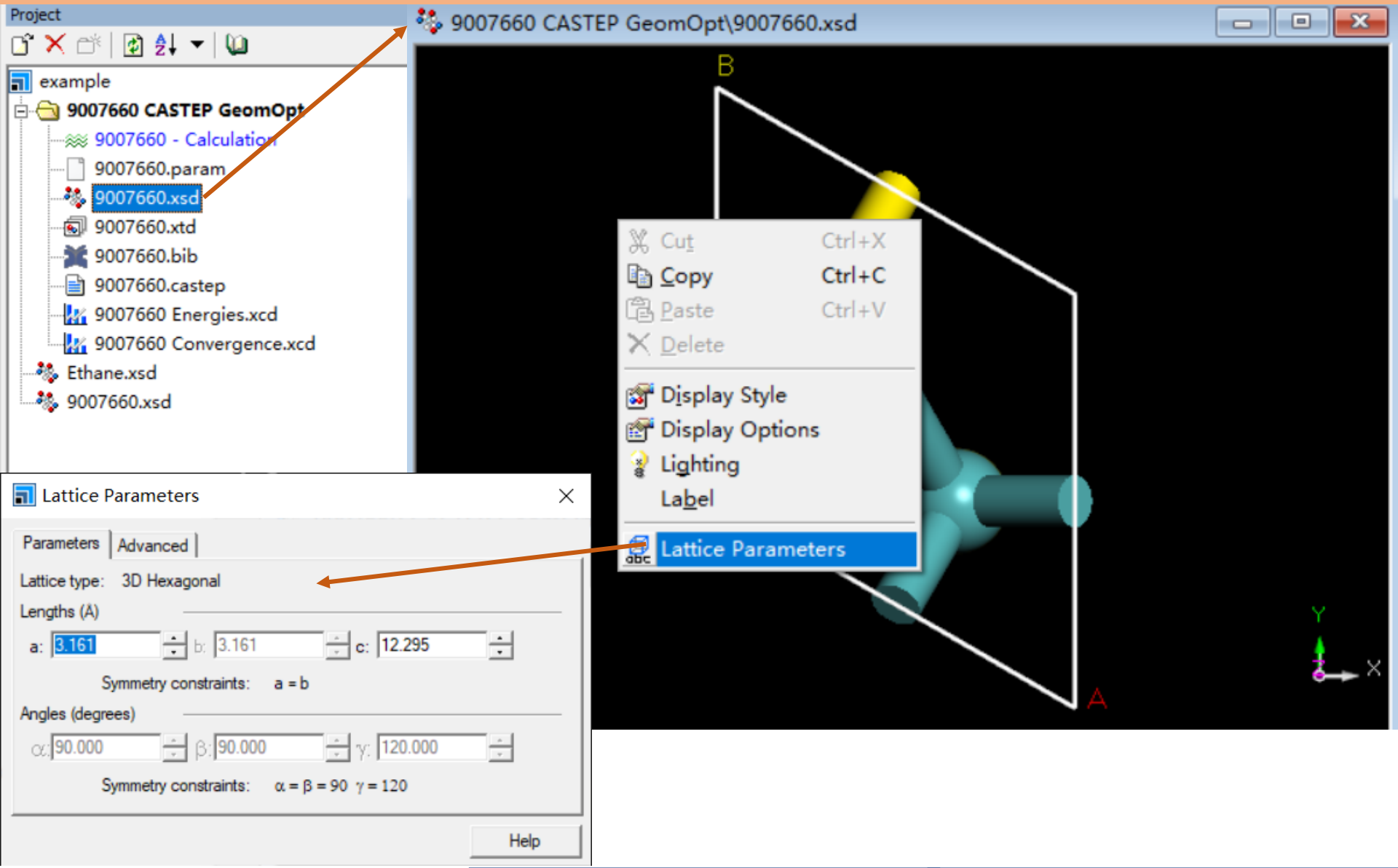




Example 1: Predict MoS_2 lattice parameter using castep

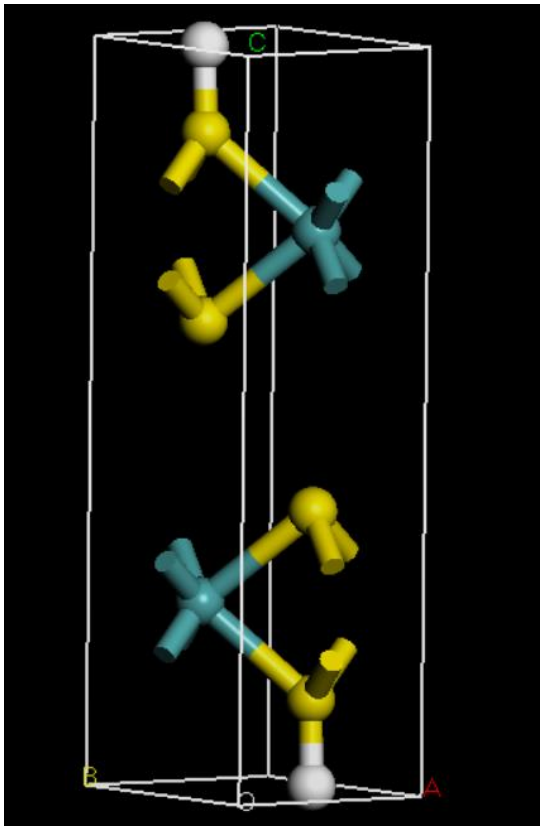


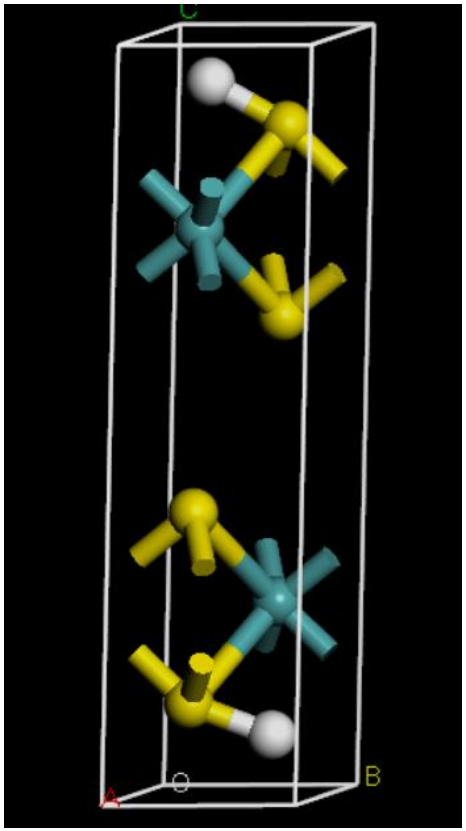
Example 2: Predict MoS_2 lattice parameter using castep



Test 1: Predict H@MoS_2 structure

- ✓ Use **drawer tools** add H atoms
- ✓ Use **optimized** MoS_2 structure as template
- ✓ Try **top and bridge** adsorption site

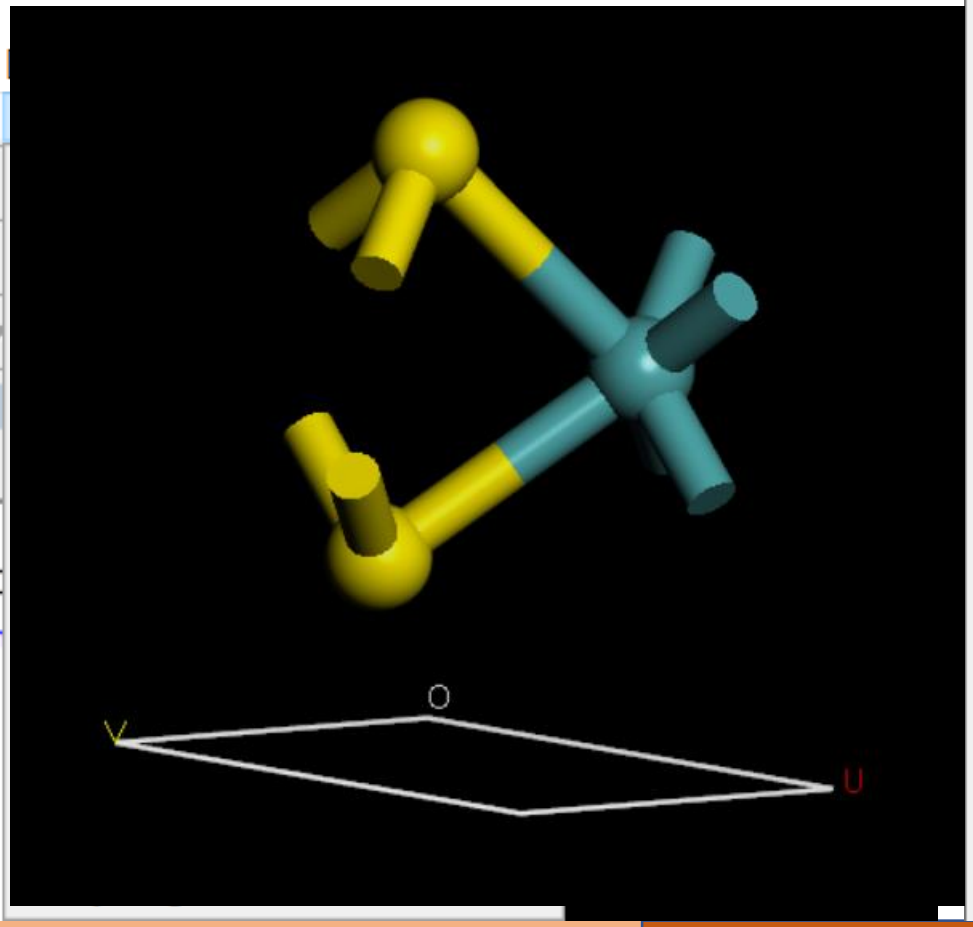


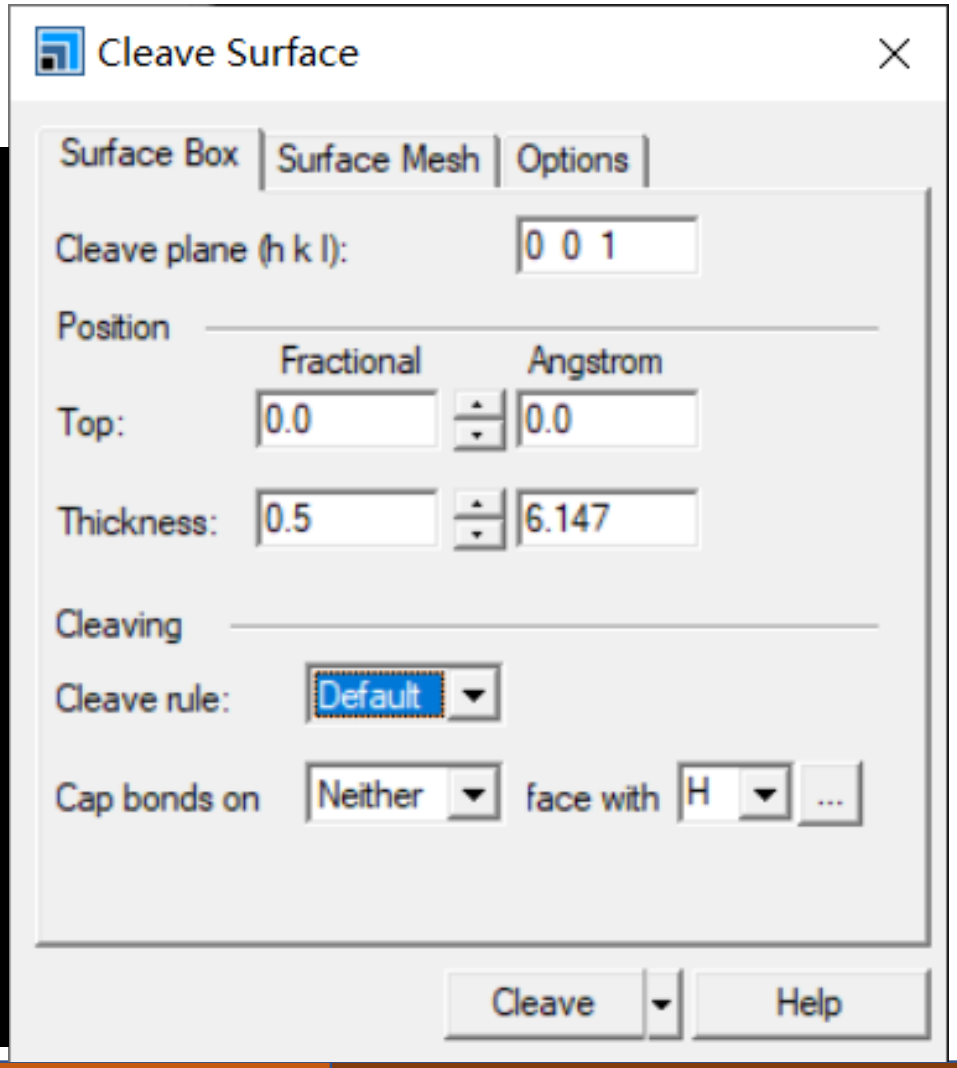


Example 2: Predict H@monolayer-MoS_2 structure

Slab Model

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

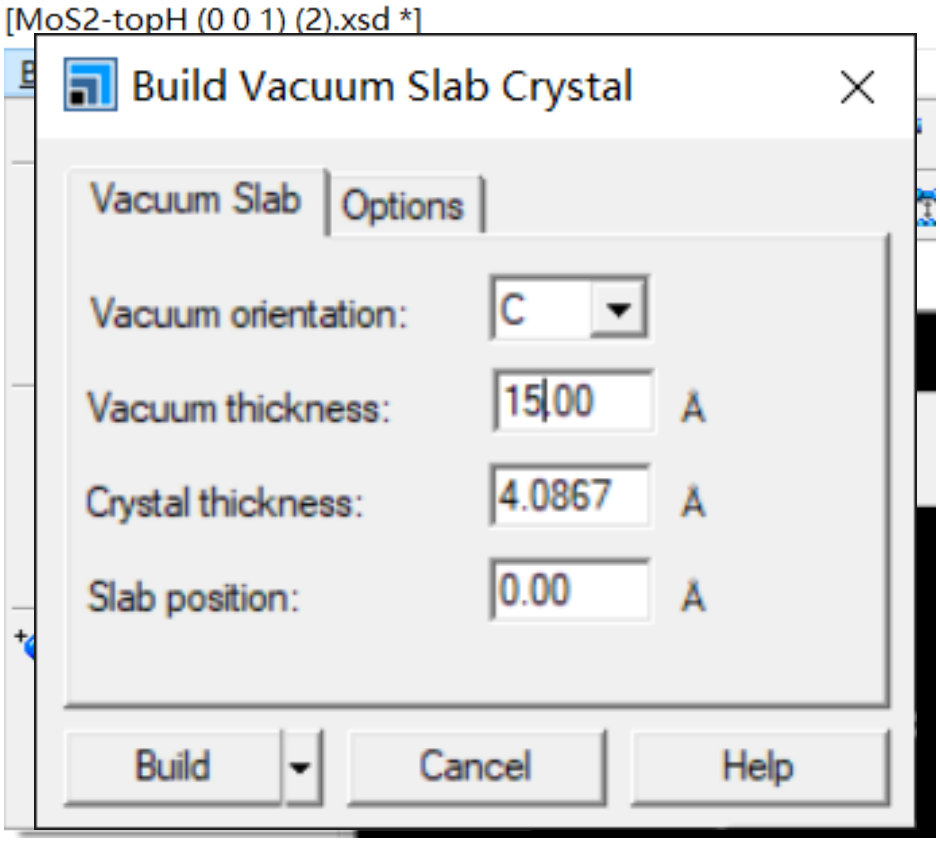


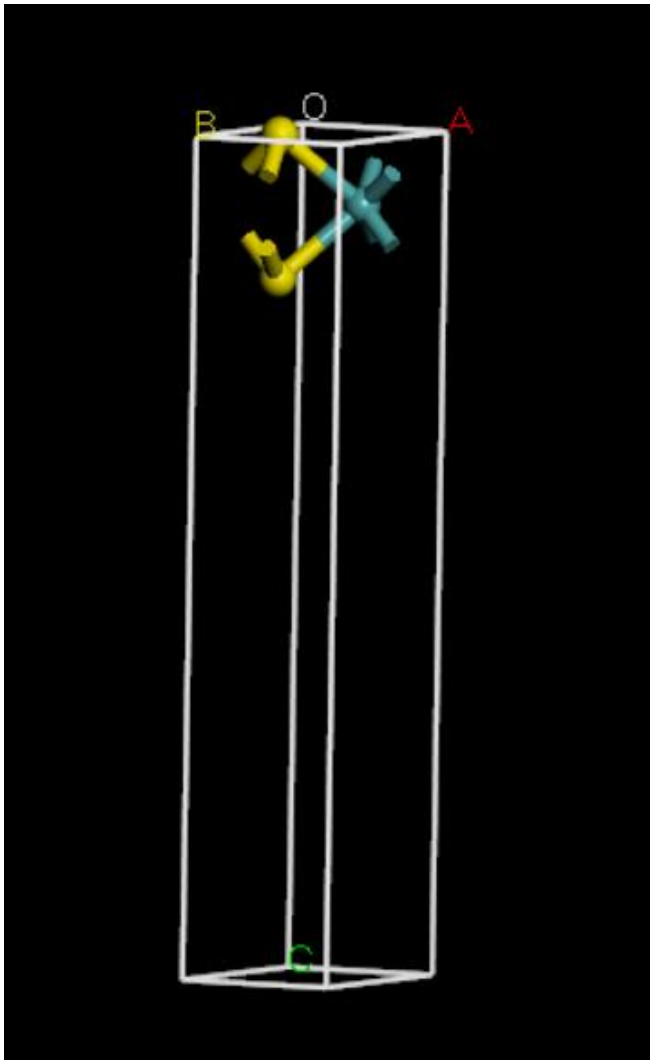


Example 2: Predict H@monolayer-MoS_2 structure

Slab Model

✓ Build vacuum layer

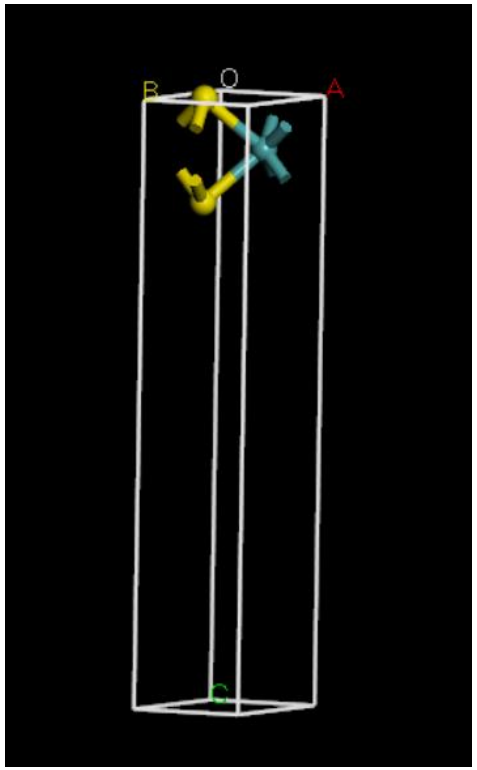


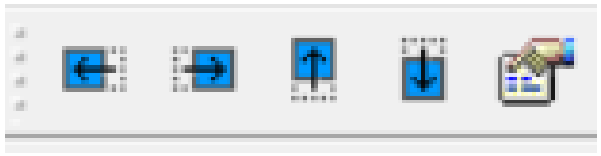


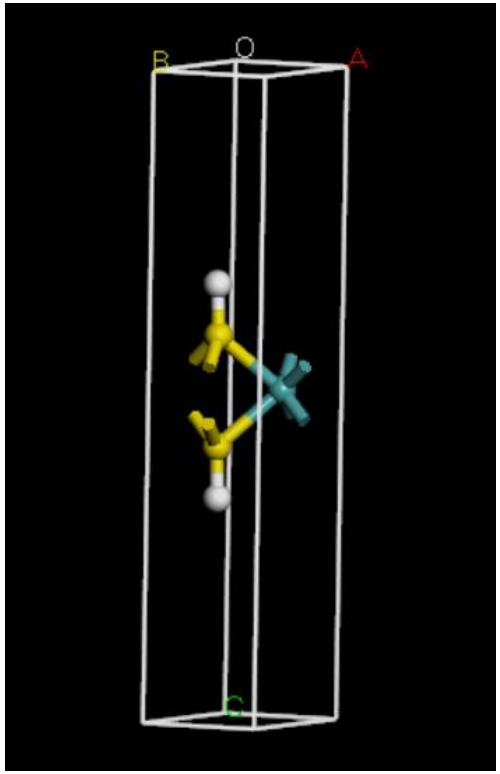
Example 2: Predict H@monolayer-MoS_2 structure

Slab Model

- ✓ Move MoS_2
- ✓ Add H atom







Example 2: Predict H@monolayer-MoS_2 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**

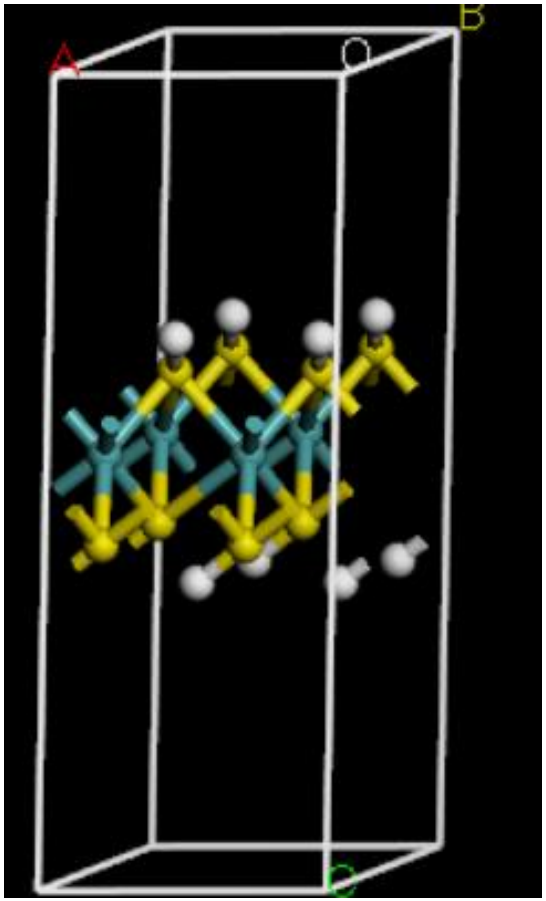
Same Parameters

Example 2: Predict H@monolayer-MoS_2 structure

Results

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_2 structure

Adsorption energy

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

$E(surf + n\mathrm{H})$ **MoS_2 energy**

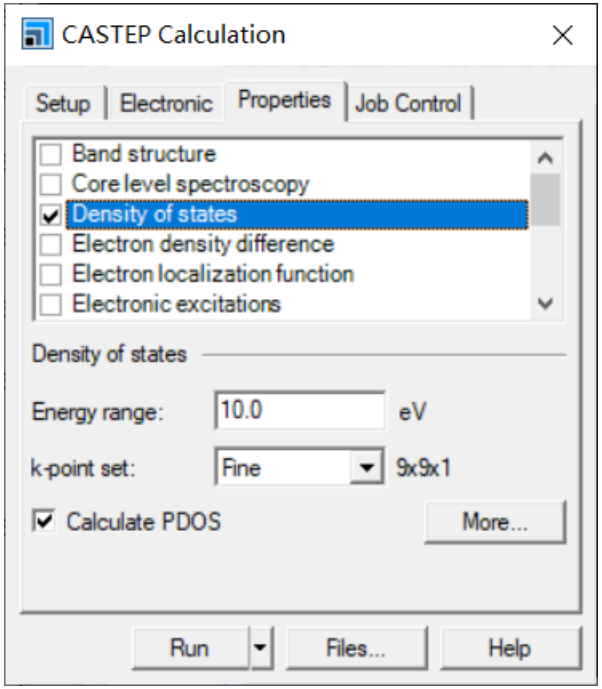
$E(surf)$ **H@MoS_2 energy**

$E(\mathrm{H}_2)$ **H energy**

Example 3: MoS_2 Density of State

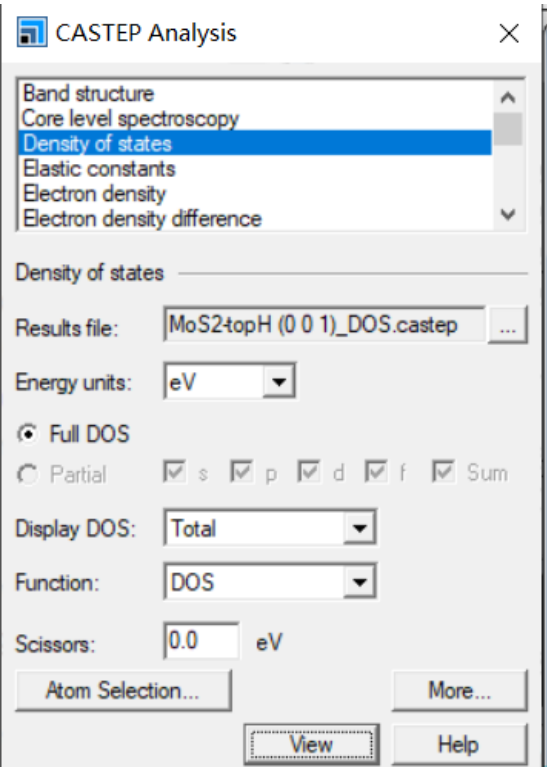
Castep module

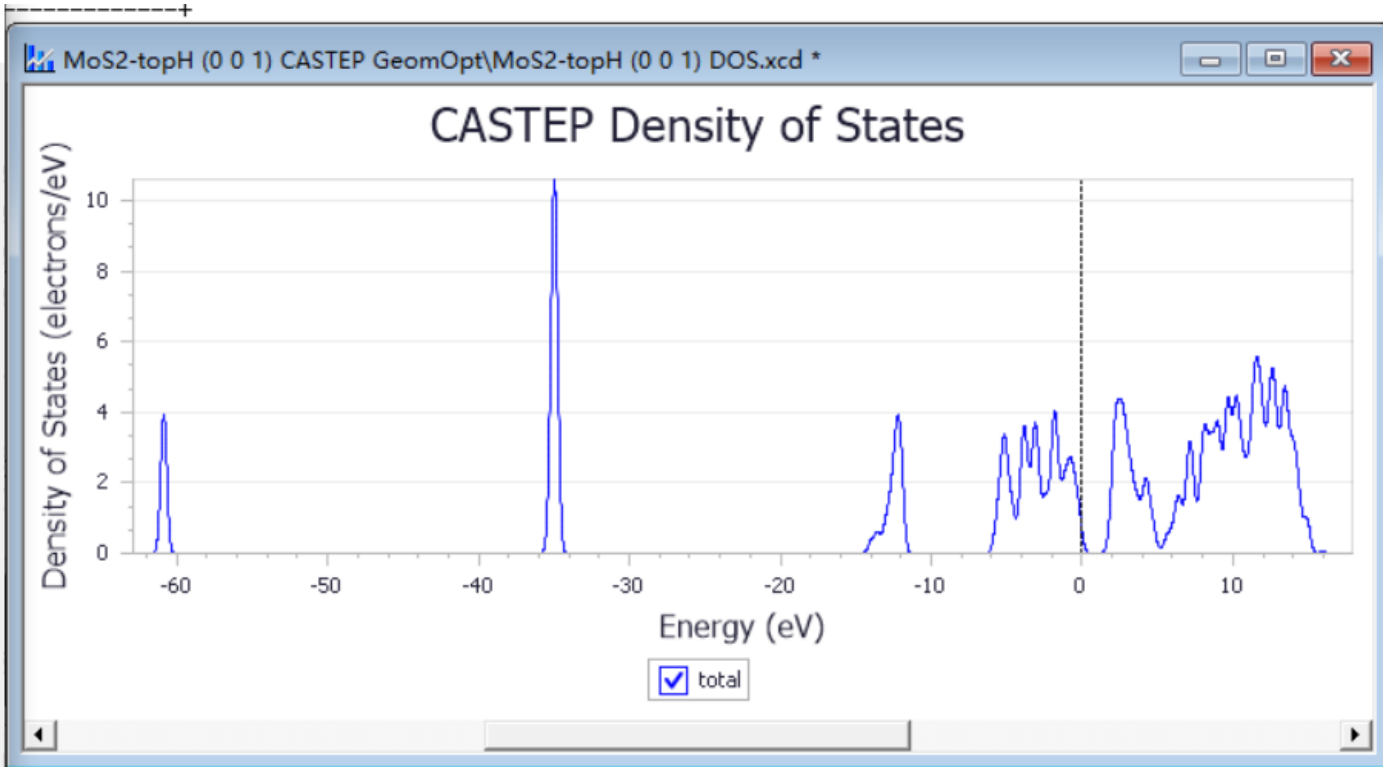
- ✓ **Task**
  - ➢ Geometry Optimization
- ✓ **Quality**
  - ➢ High
- ✓ **Functional**
  - ➢ GGA-PBE
- ✓ **Metal options**
  - ➢ Selected
- ✓ **Parallel Setting**
  - ➢ Maximum: 4 (for most personal computer)
- ✓ **Runtime optimization**
  - ➢ **default**
- ✓ **Energy cutoff**
  - ➢ High
- ✓ **SCF tolerance**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



Example 3: MoS_2 Density of State

Results



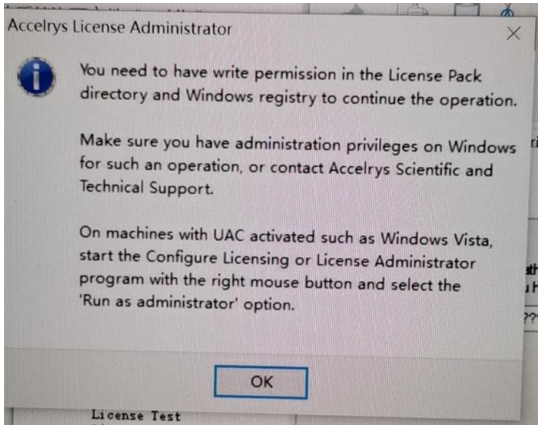


Installation Question Collection

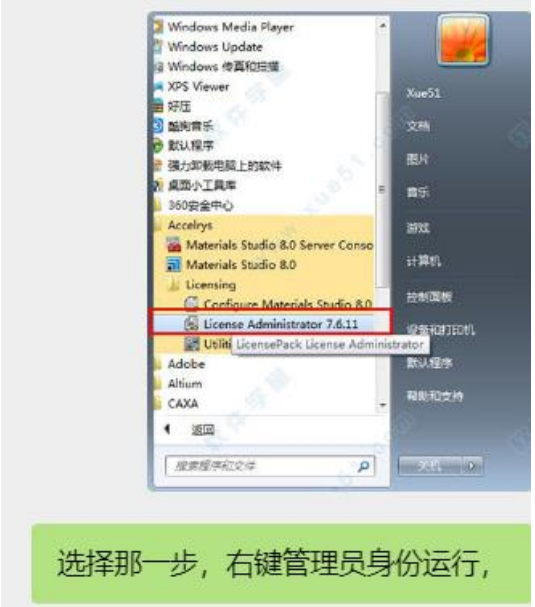
Q: Lic文件在哪里?

msi.lic 2020-02-20 12:37 74KB

Q:



A:



Thanks for your attention!