10月28日上机实习安排

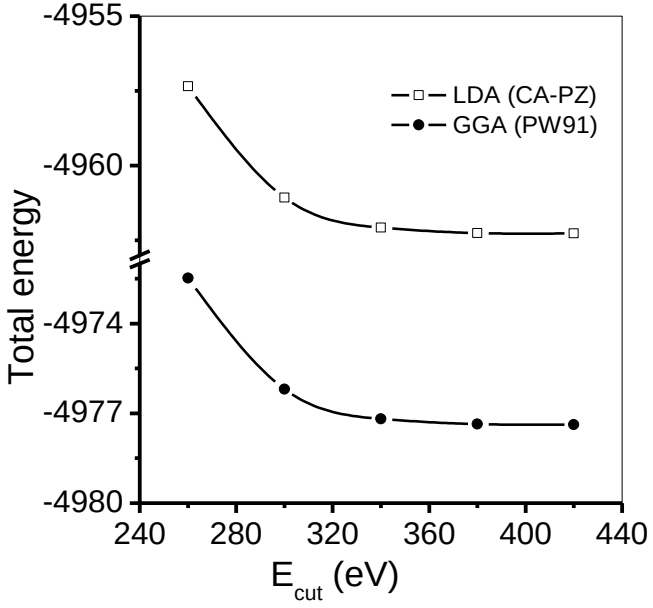
使用MS软件CASTEP模块完成：

Graphene的第一性原理(DFT)计算

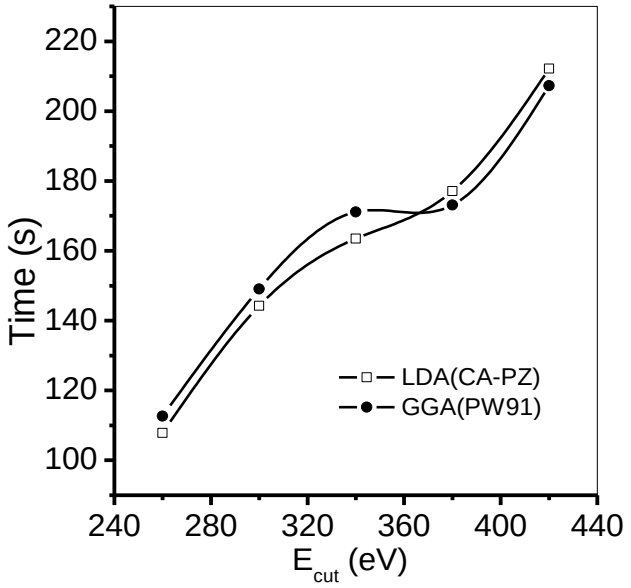
1. 建模→
2. 结构优化→
3. 电荷密度计算（高精度单点能）→
4. 能带结构计算（FBZ高对称*K*点）→
5. 态密度计算(DOS & PDOS)

Graphene DFT计算的结果可靠性测试

1. 截断能(cutoff energy)



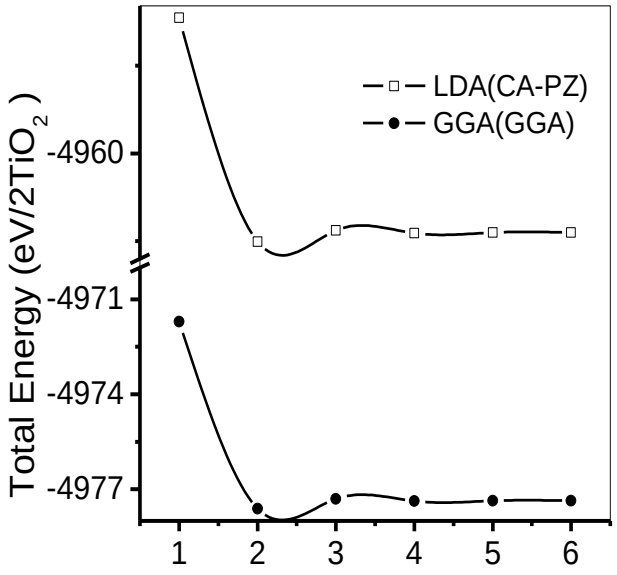
截断能与总能量的关系



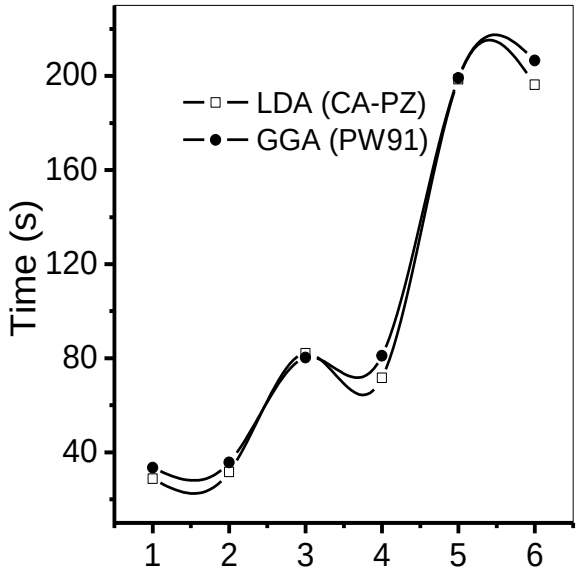
截断能与计算时间的关系

Graphene DFT计算的结果可靠性测试

2. *K* points



*K*点设置与总能量的关系



*K*点设置与计算时间的关系

Graphene DFT计算的参考文献

1. A. G. Marinopoulos et al. Ab Initio Study of the Optical Absorption and Wave-Vector-Dependent Dielectric Response of Graphite. *Phys. Rev. B* **2004**, 69, 245419.
2. N. Ooi, A. Rairkar, and J. B. Adams. Density Functional Study of Graphite Bulk and Surface Properties. *Carbon* **2006**, 44, 231-242.

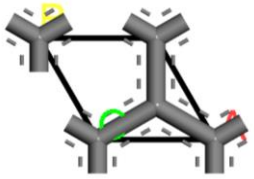
1. Slab Model Building

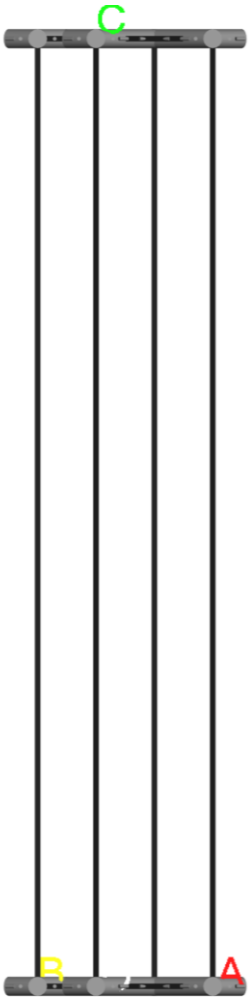
(1) Import crystal structure of graphite in MS

(2) Make “P1” to delete a layer graphene

(3) “Rebuild Crystal” to change the lattice parameter ***c*** into **20 Å**

Top View





Side View

$a = b = 2.460$ Å

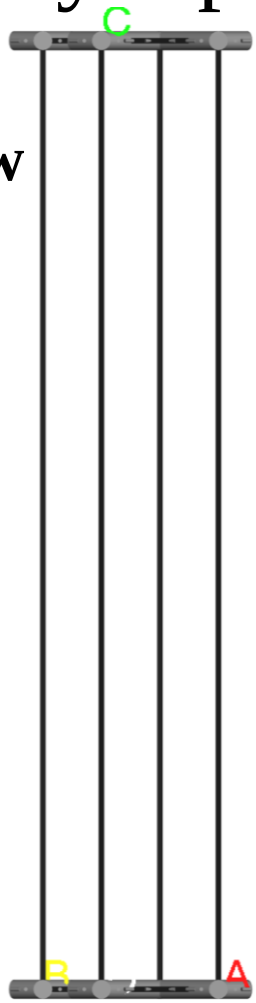
$c = 20.0$ Å

$\alpha = \beta = 90.0°$

$\gamma = 120.0°$

2. Geometry Optimization

Top View



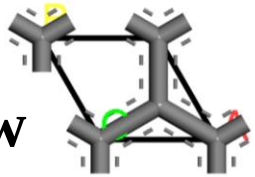
Before

$a = b = 2.460$ Å
$c = 20.0$ Å
$\alpha = \beta = 90.0^\circ$
$\gamma = 120.0^\circ$

After

$a = b = 2.460$ Å
$c = 20.0$ Å
$\alpha = \beta = 90.0^\circ$
$\gamma = 120.0^\circ$

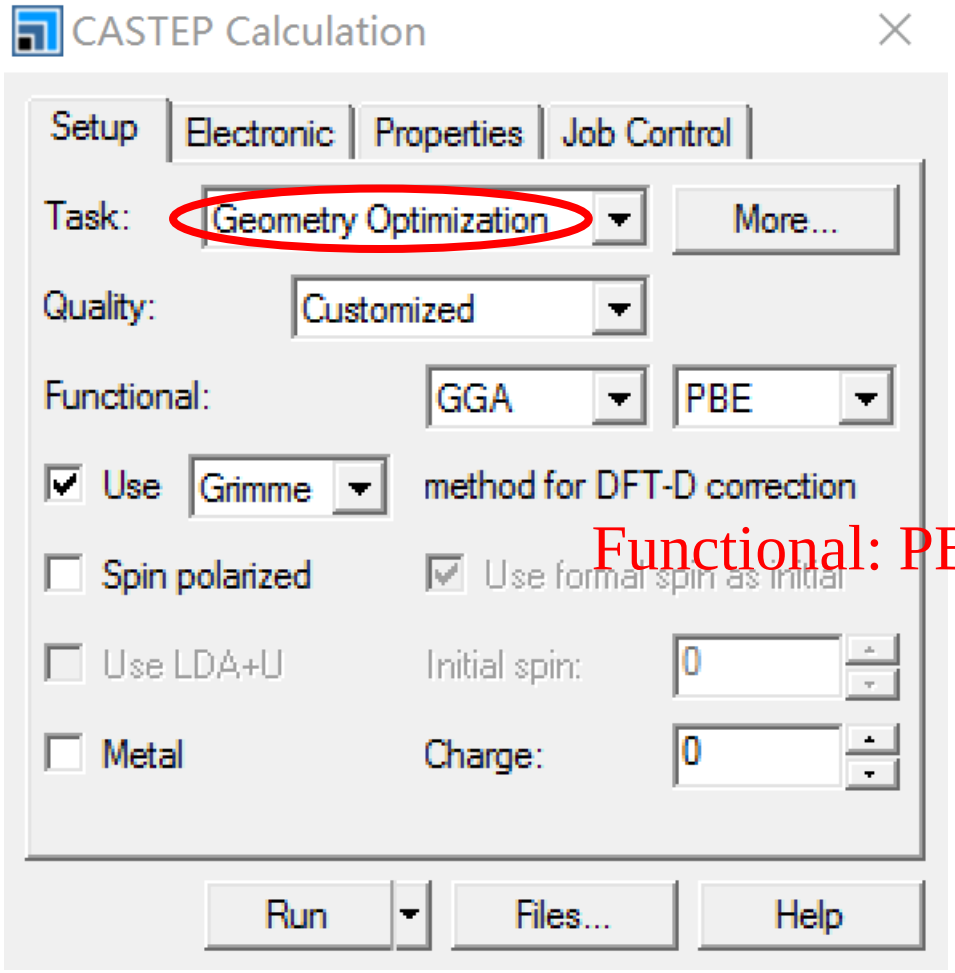
Side View



2. Geometry Optimization

CASTEP Calculation

Setup



Functional: PBE-D2

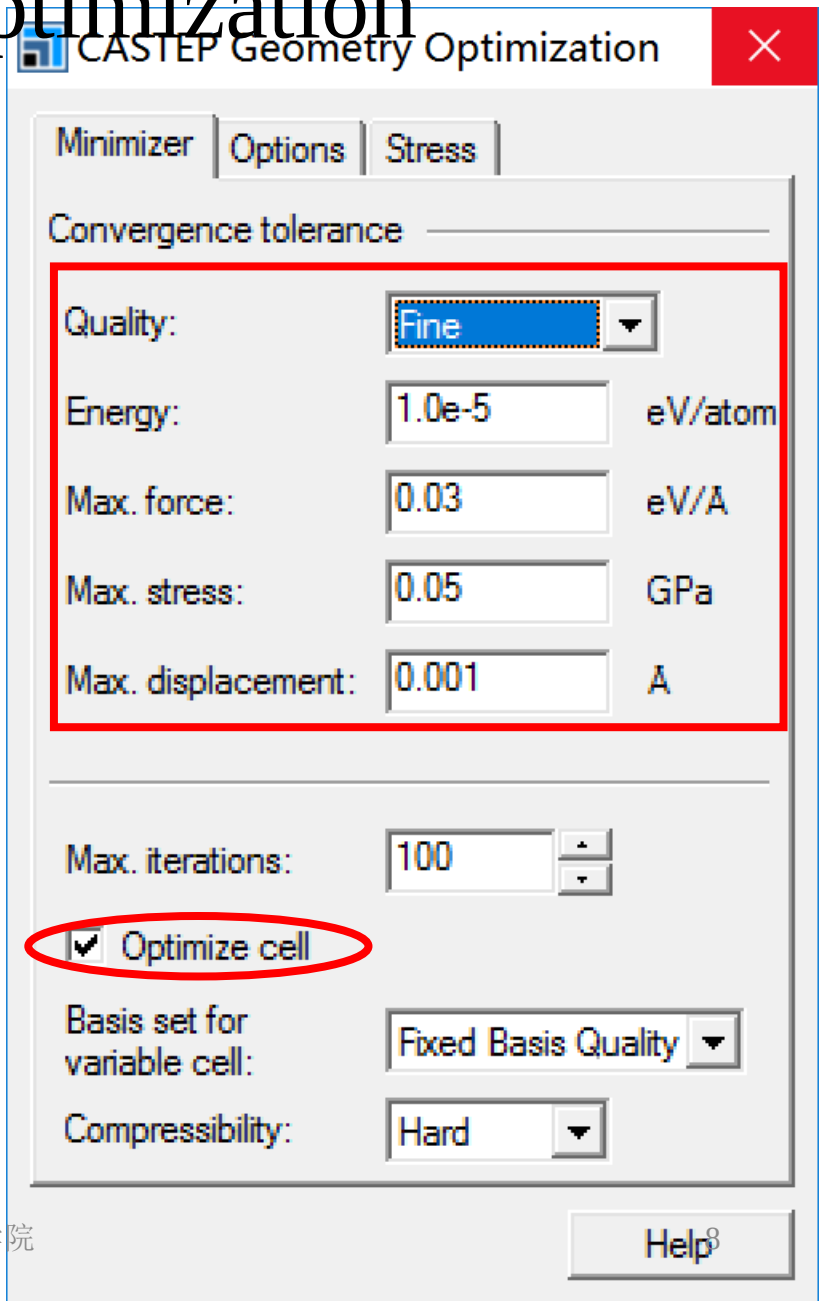
2. Geometry Optimization

CASTEP Calculation

Setup → More… for **Minimizer**

优化结束的判据:

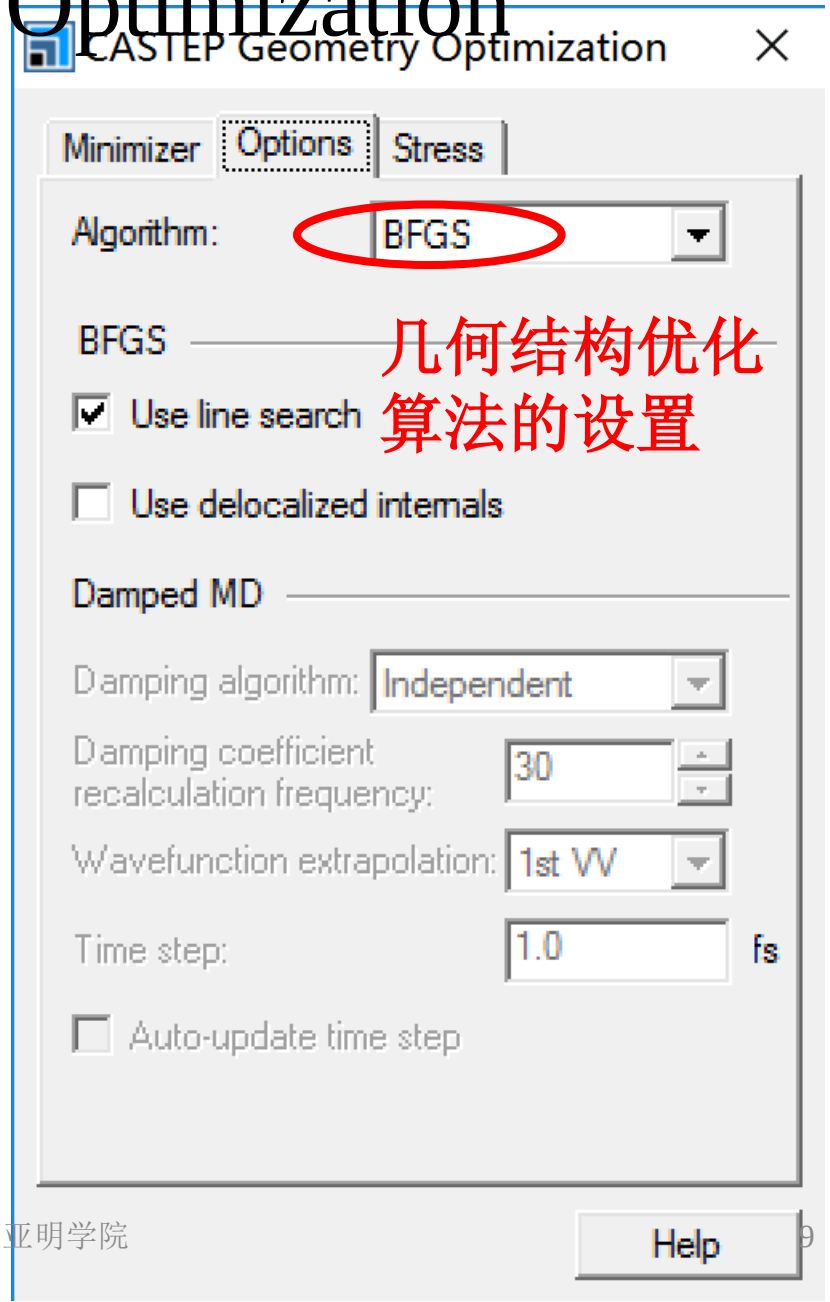
- 能量判据：相继两次结构对应能量差足够小
- 力判据：单个原子受力小于设定的最大值
- 应力判据：保证结构模型单元中的应力足够小
- 位移判据：相继两次结构变化引起的原子位移足够小



2. Geometry Optimization

CASTEP Calculation

Setup → More… for **Options**

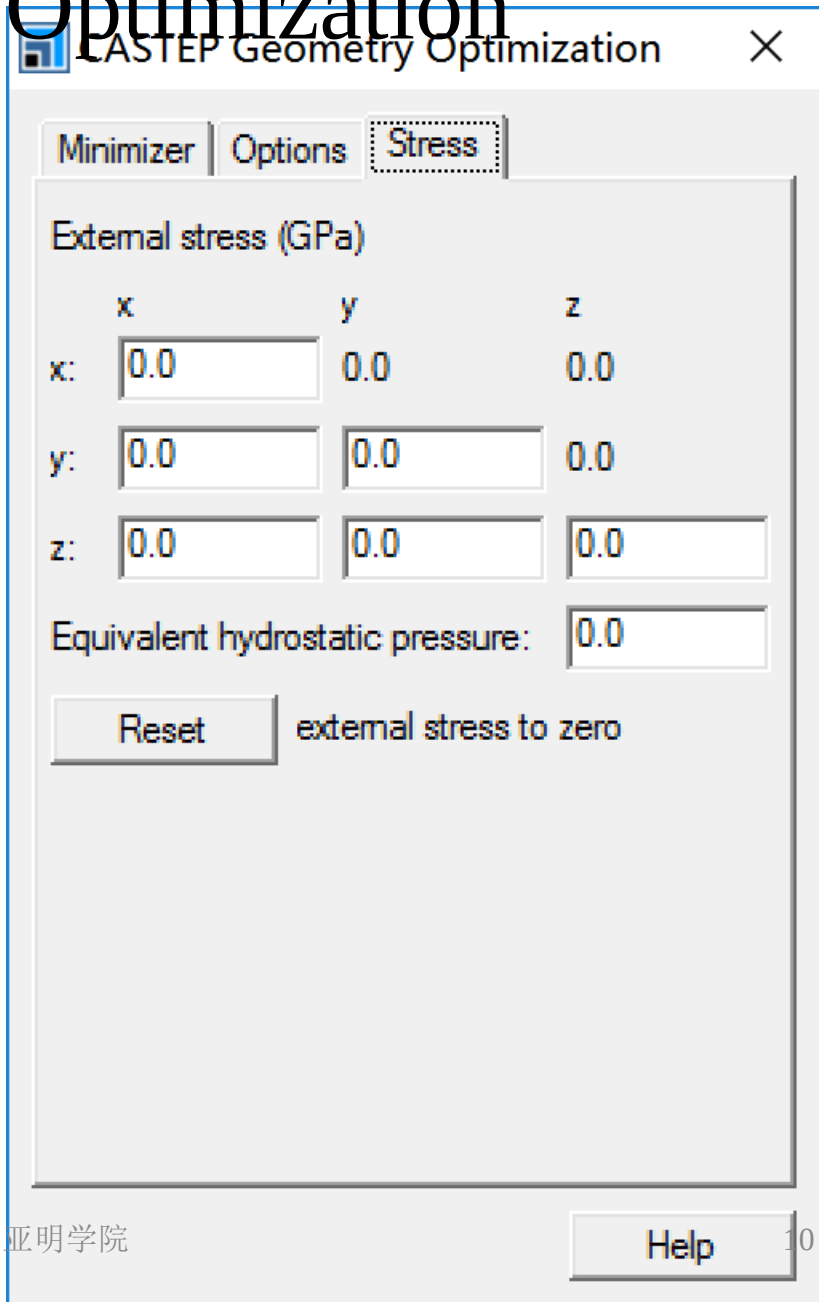


2. Geometry Optimization

CASTEP Calculation

Setup → More… for **Stress**

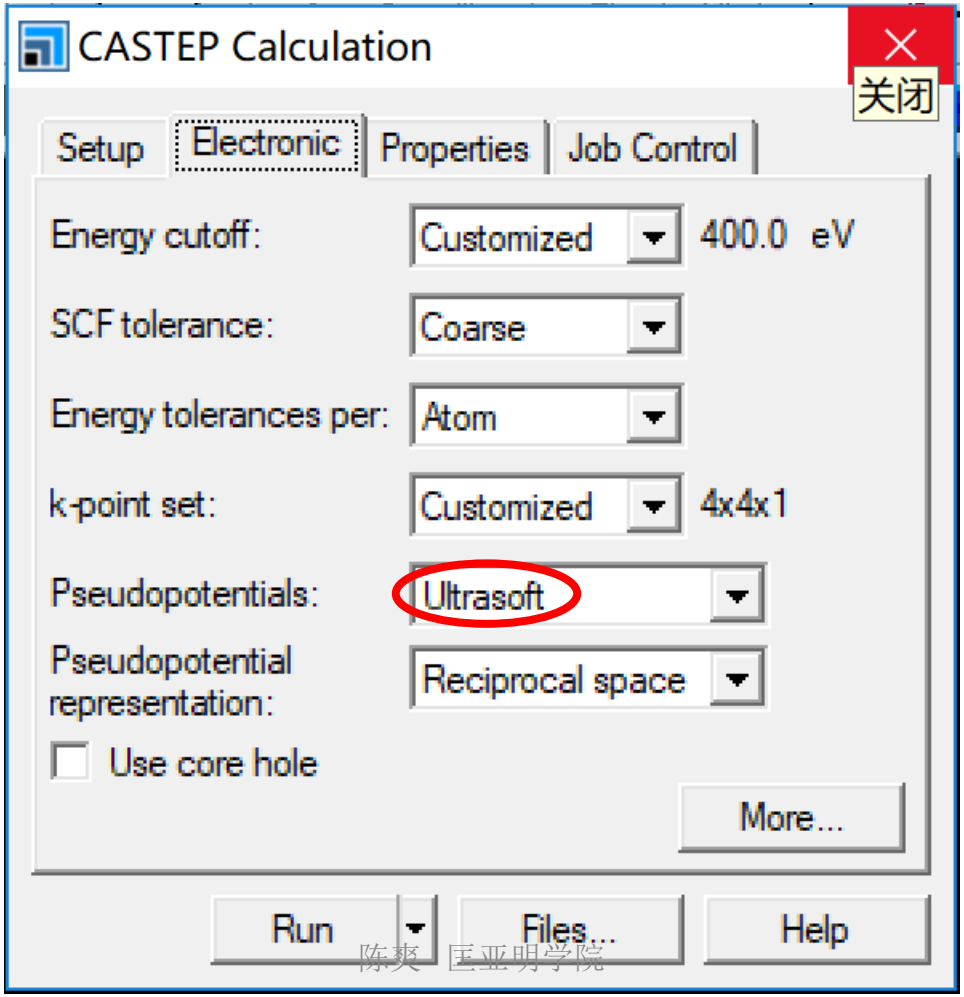
(默认设置没有更改)



2. Geometry Optimization

CASTEP Calculation

Electronic

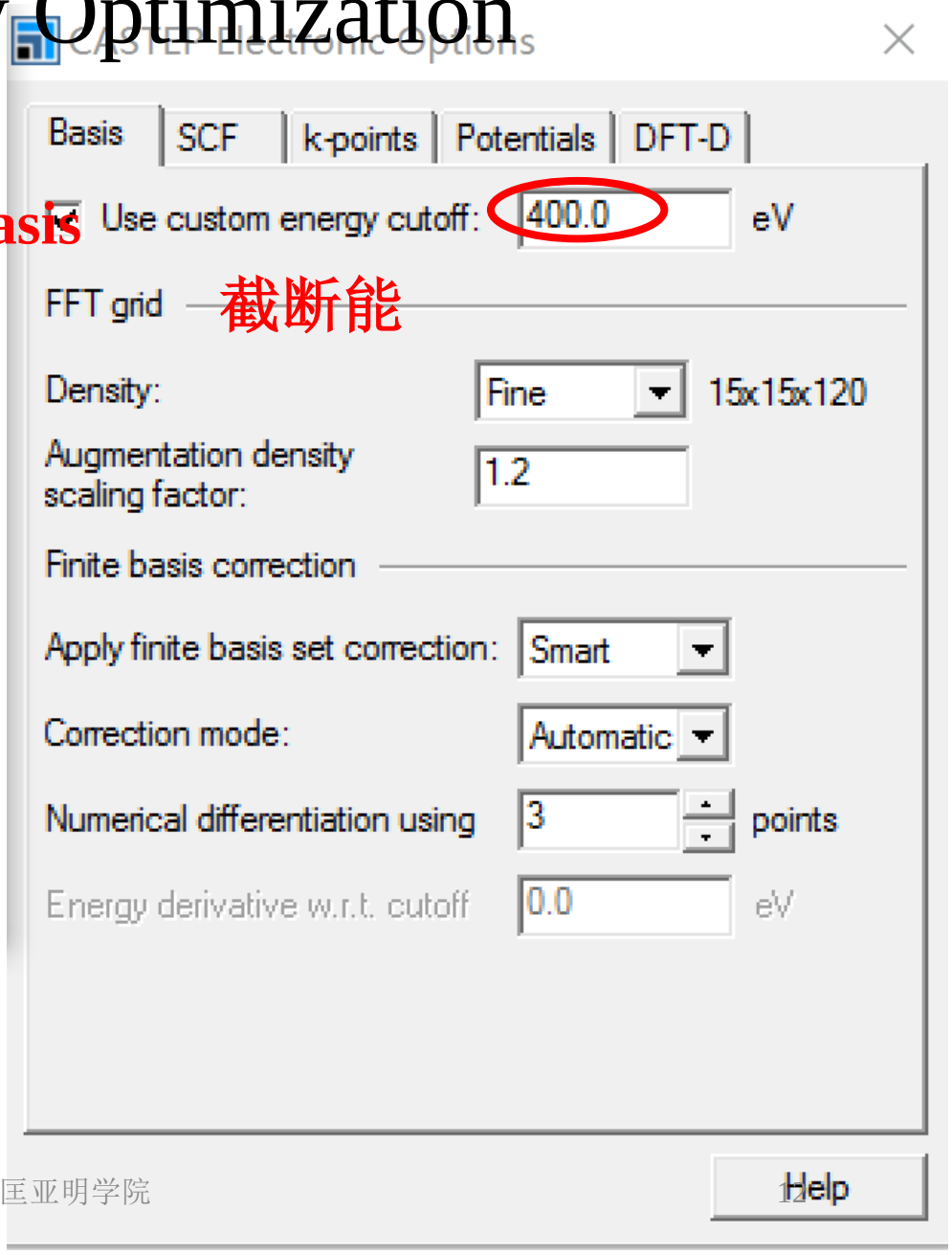


超软赝势

2. Geometry Optimization

CASTEP Calculation

Electronic → More… for **Basis**

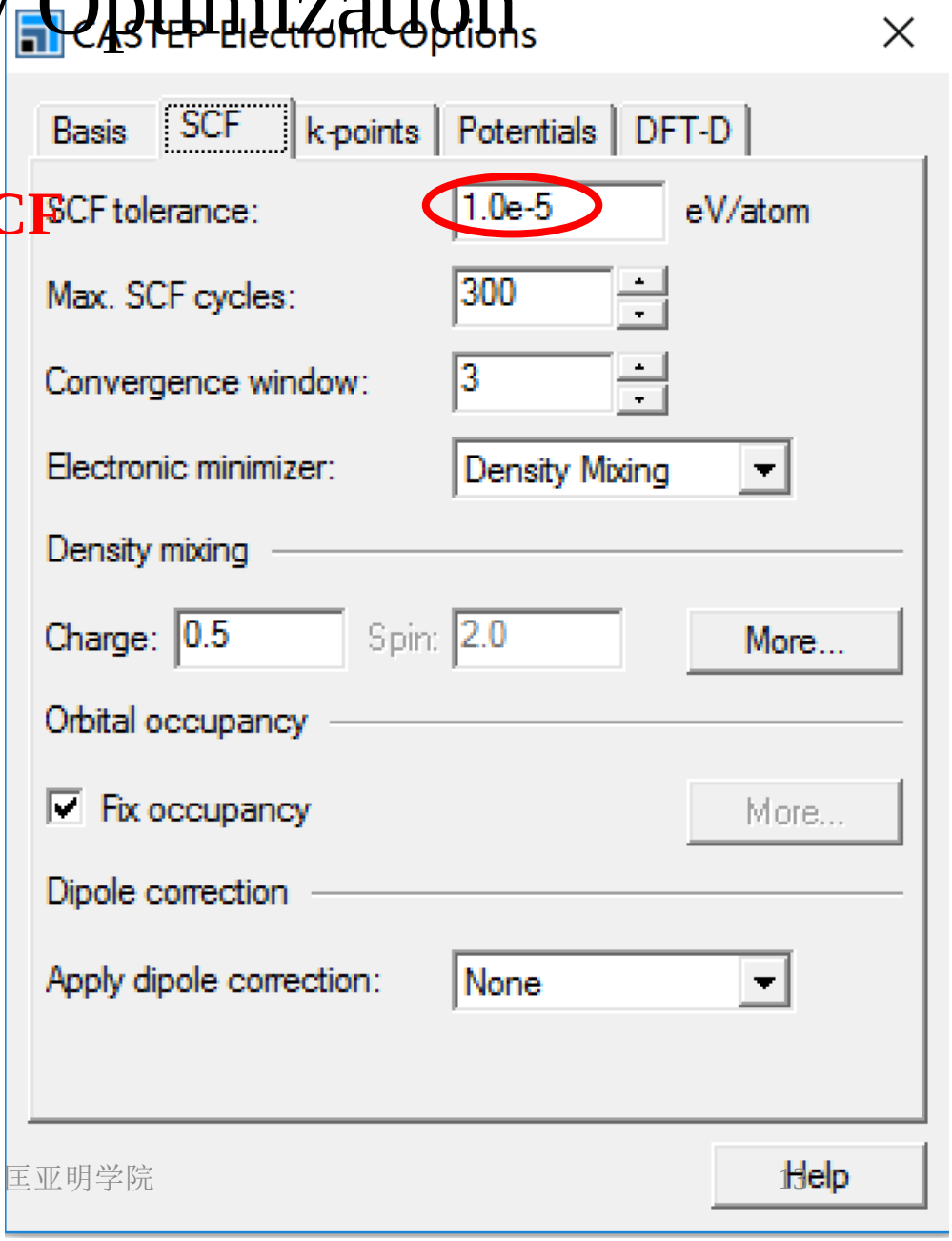


2. Geometry Optimization

CASTEP Calculation

Electronic → More… for **SCF**

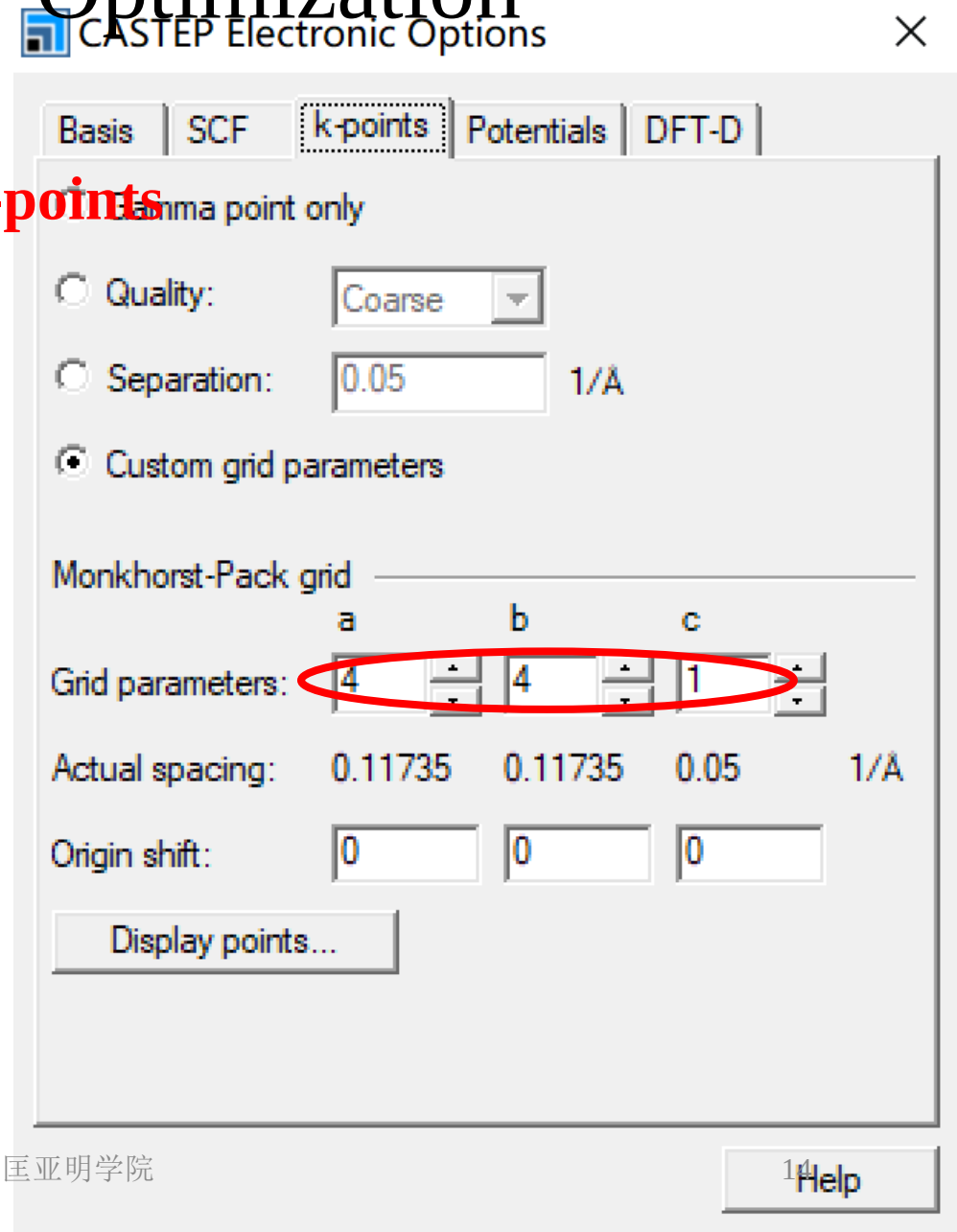
自洽收敛标准：
两次波函数更新能量差



2. Geometry Optimization

CASTEP Calculation

Electronic → More… for **k-points**

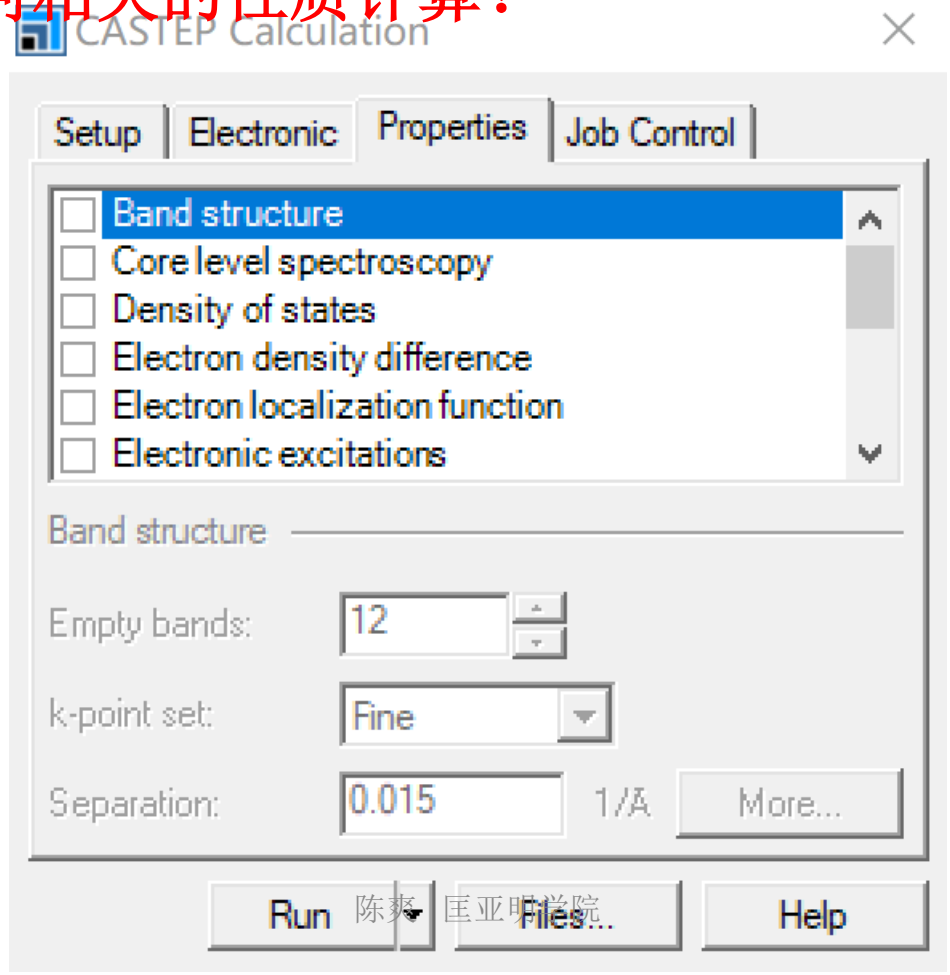


2. Geometry Optimization

CASTEP Calculation

Properties

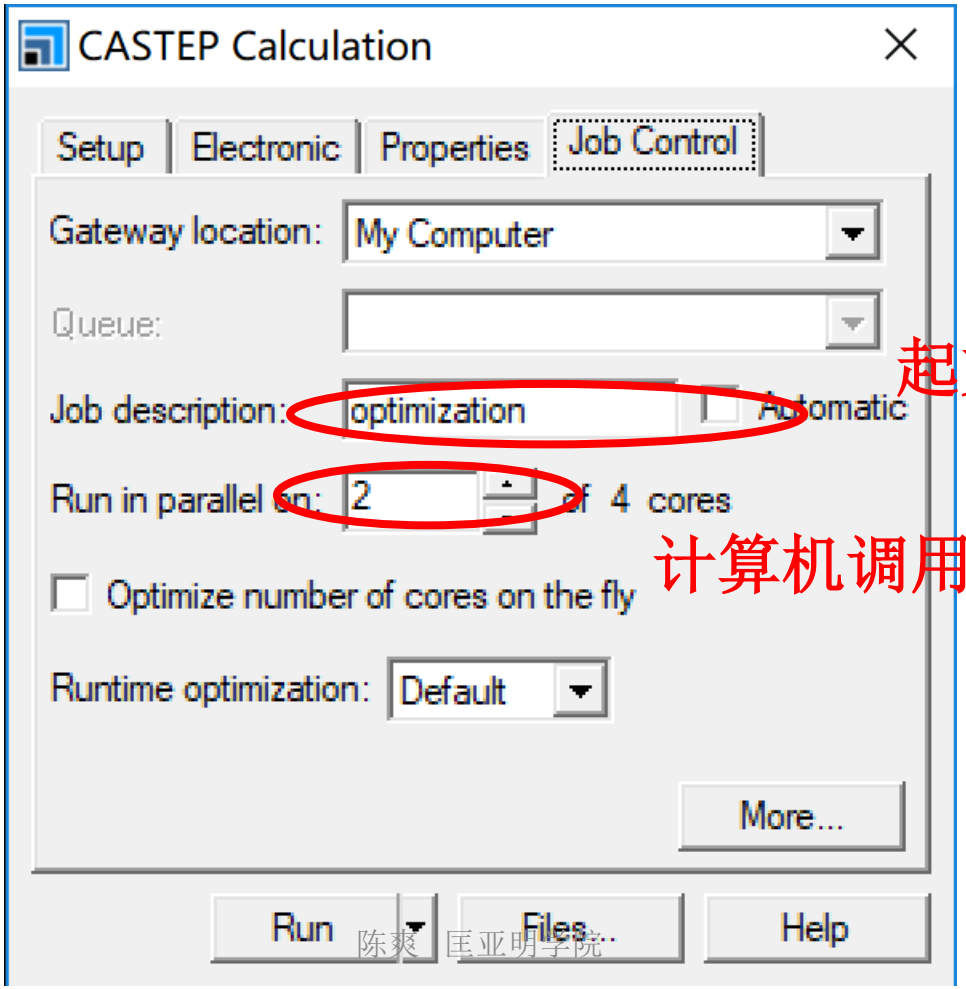
不要勾选任何相关的性质计算！



2. Geometry Optimization

CASTEP Calculation

Job Control



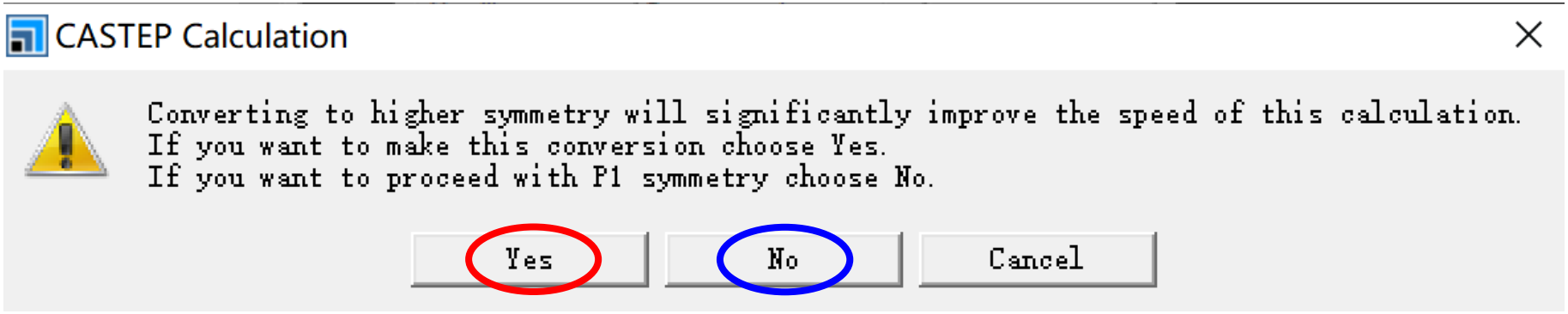
起文件名

计算机调用核数

2. Geometry Optimization

CASTEP Calculation

After submitting this job:



回到2个原子的六方单胞

还是4个原子的正交单胞

3. Charge Density

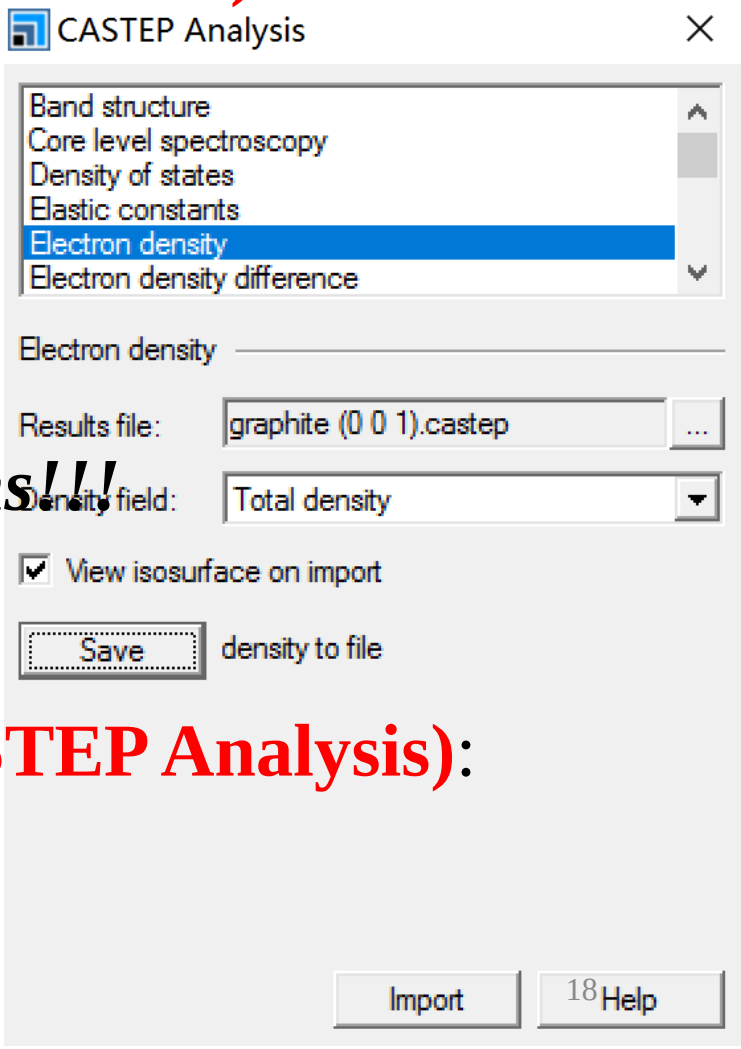
(1) Setting for higher-computational-accuracy single-point calculations **(CASTEP Calculation)**:

① Task: Energy

② *K*-point set: 8×8×1

③ SCF tolerance: 10e-6 eV/atom

Taking the optimal structure* (*.xsd) *for the following property calculations!!!



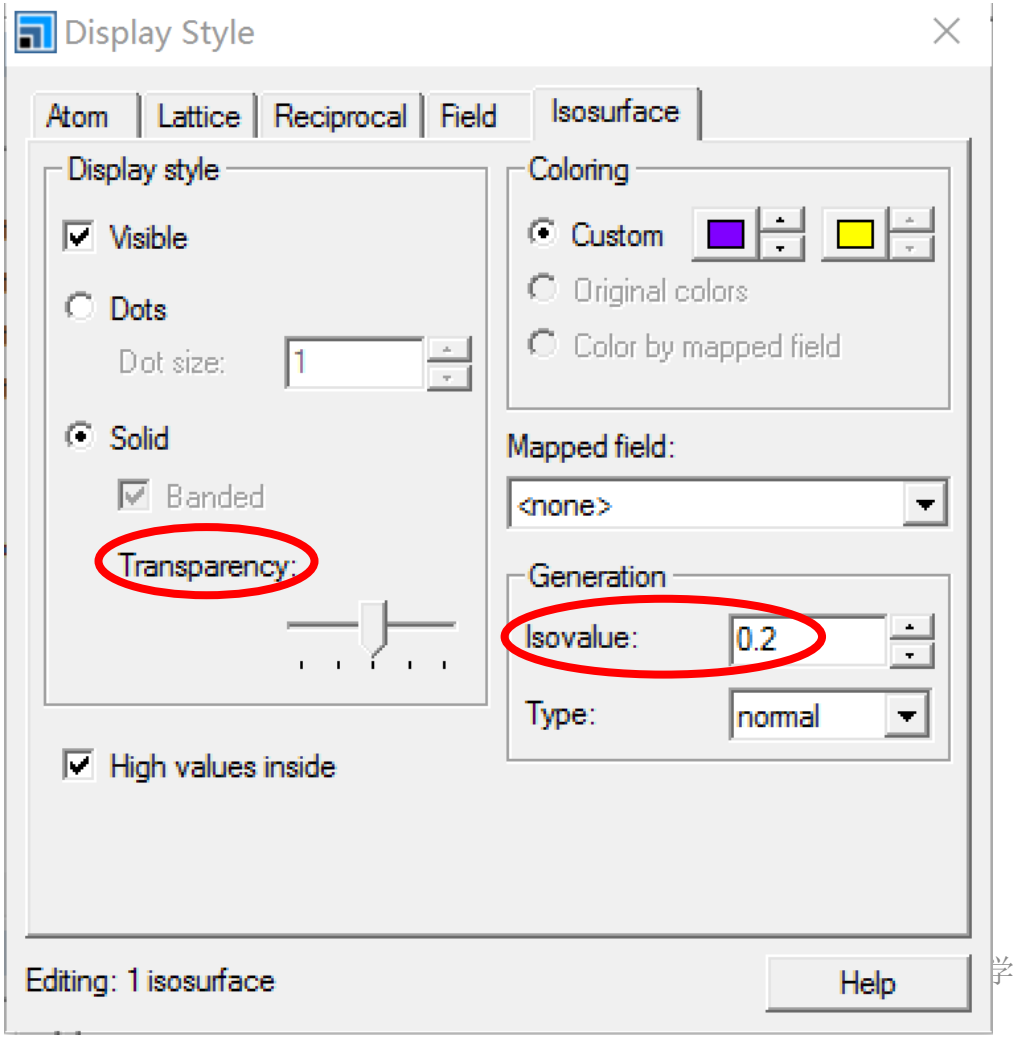
(2) Visualize charge density **(CASTEP Analysis)**:

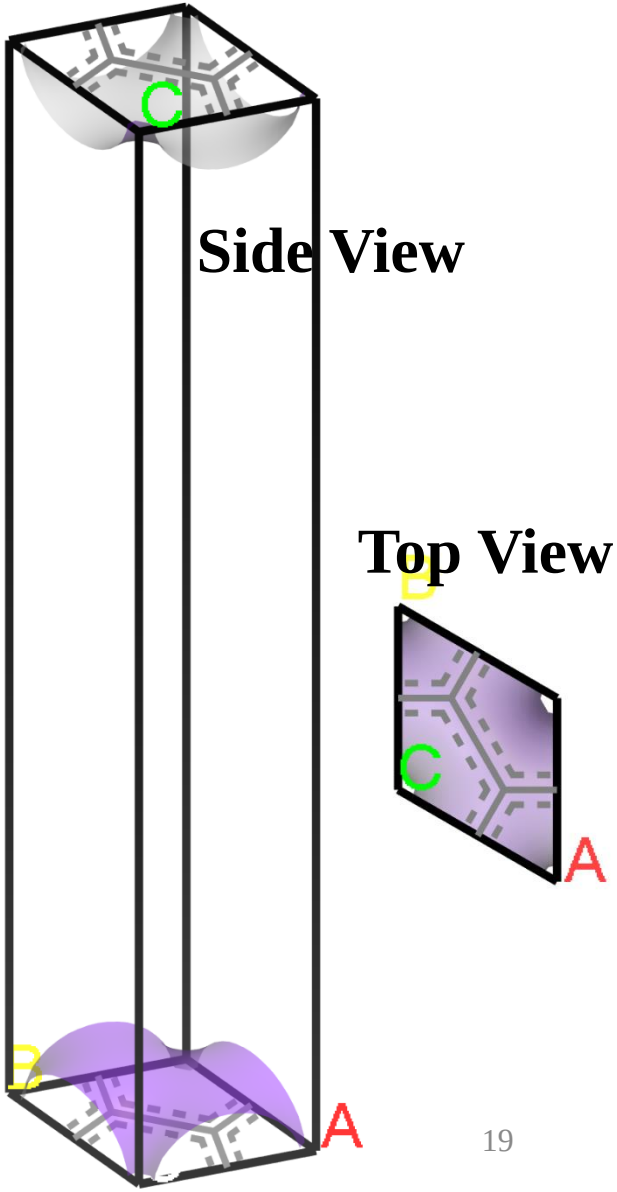
① Select “Electron density”

② Import

3. Charge Density

(3) Change “Display Style”



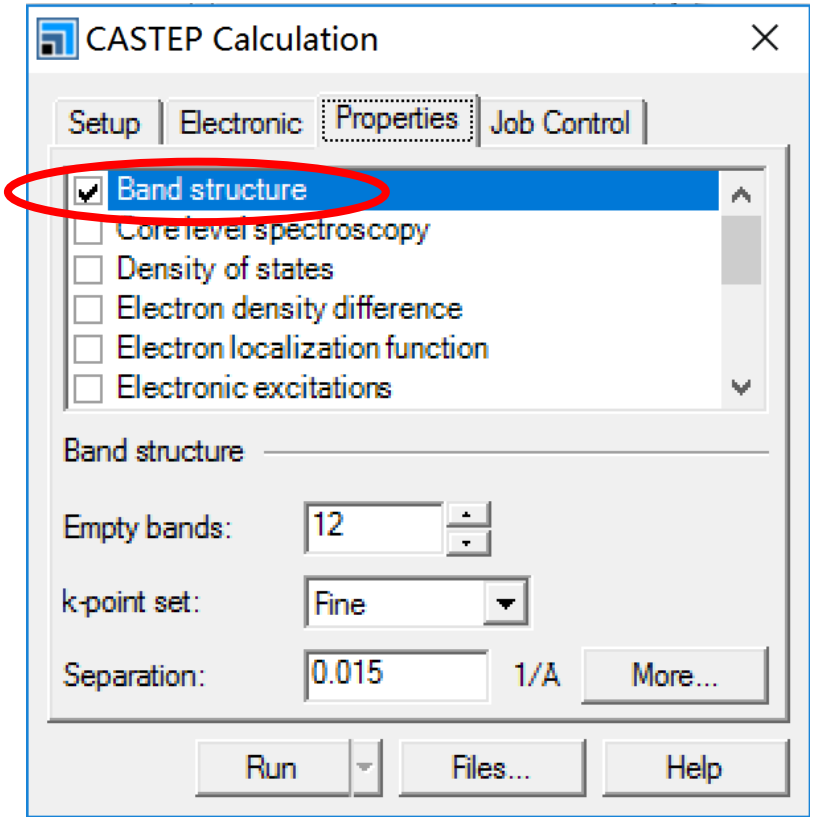


4. Band Structure

(1) Setting:

① Setup → Task: Properties

② Properties → Mark “Band structure”



4. Band Structure

(1) Setting:

③ Set high-symmetry *K* points: "**Tools → Brillouin Zone Path**"

高对称点信息的获取：

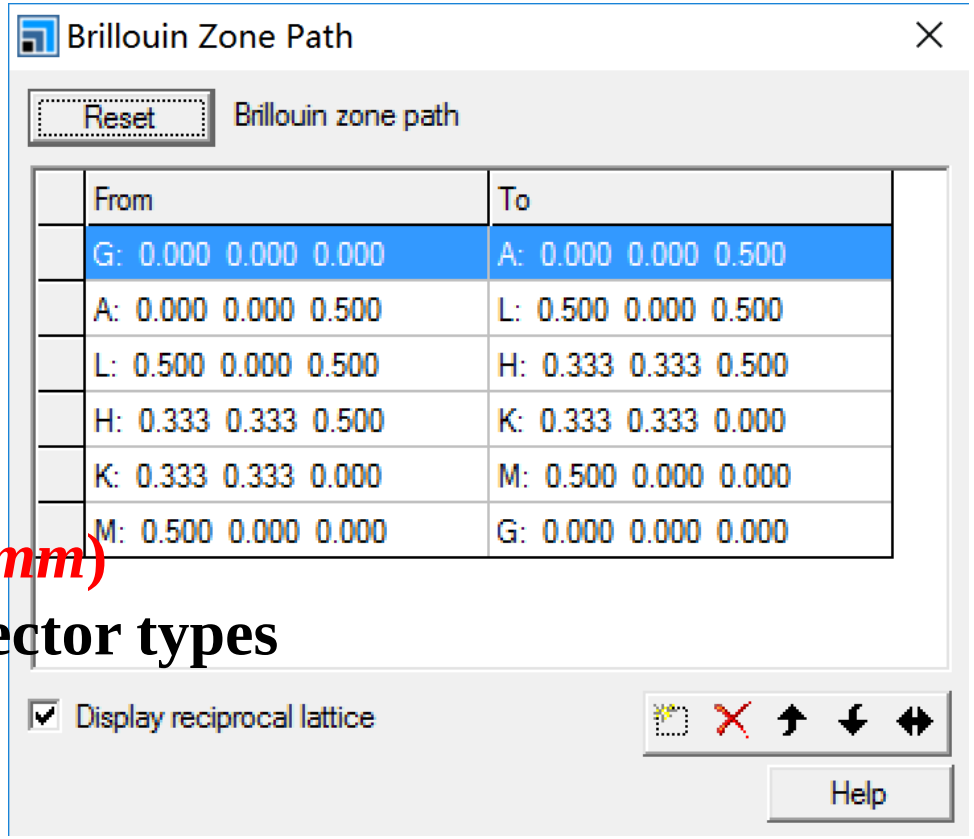
借助网站**http://cryst.ehu.es/**

→ Space-group symmetry

→ KVEC for k vectors

→ Choose space group (*P6/mmm*)

→ Comparative listing of k-vector types



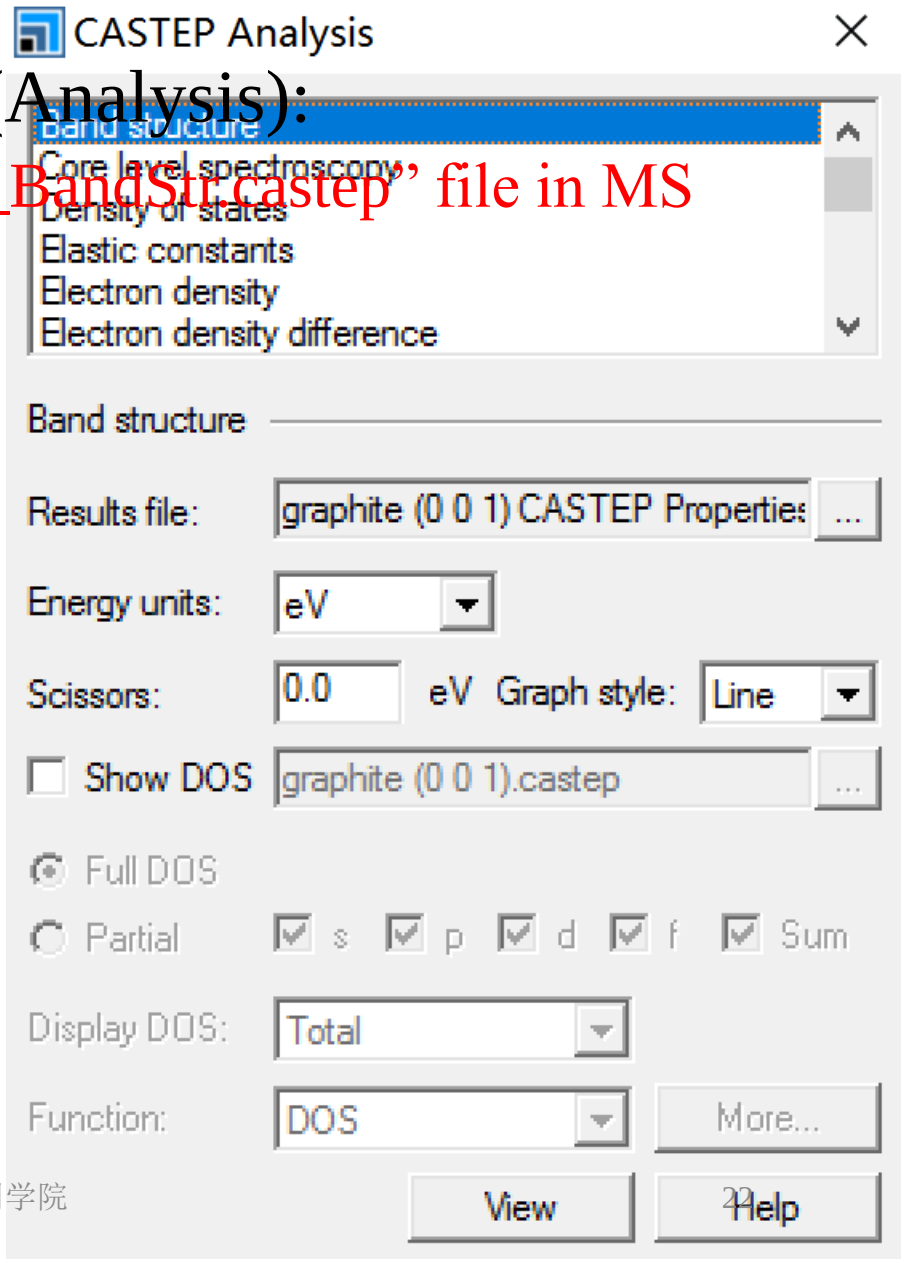
4. Band Structure

(2) Visualize band structure (Analysis):

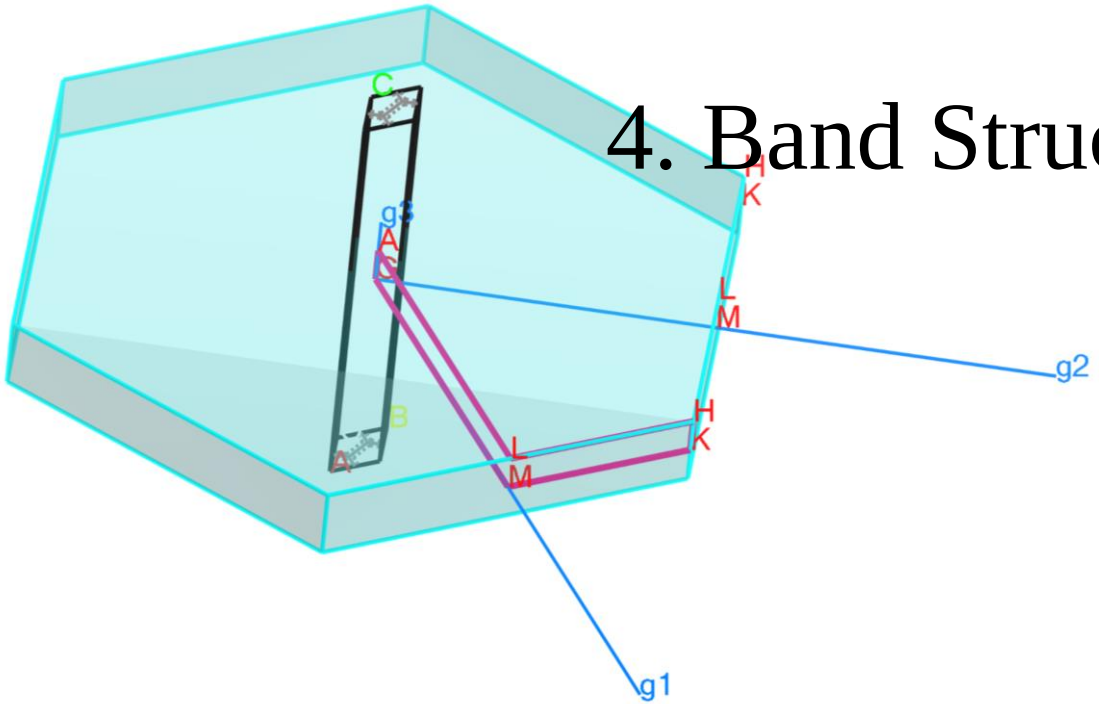
① Open file “band structure_BandStr.castep” file in MS window

② Select “Band structure”

③ View



4. Band Structure

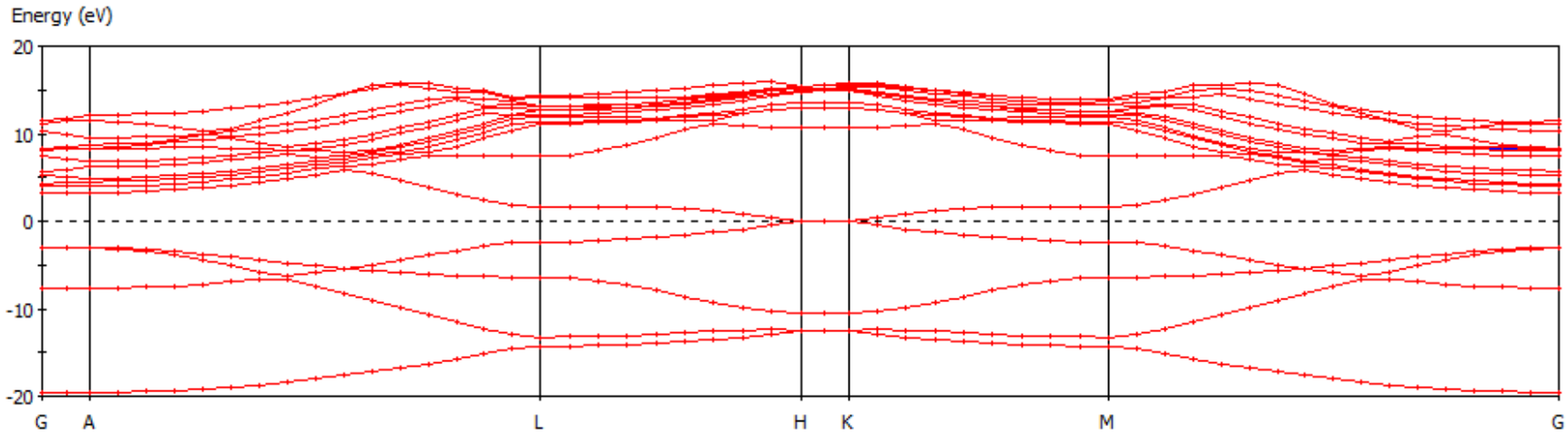


Brillouin Zone Path

Reset Brillouin zone path

From	To
G: 0.000 0.000 0.000	A: 0.000 0.000 0.500
A: 0.000 0.000 0.500	L: 0.500 0.000 0.500
L: 0.500 0.000 0.500	H: 0.333 0.333 0.500
H: 0.333 0.333 0.500	K: 0.333 0.333 0.000
K: 0.333 0.333 0.000	M: 0.500 0.000 0.000
M: 0.500 0.000 0.000	G: 0.000 0.000 0.000

CASTEP Band Structure
Band gap is 0.019 eV



5. Density of States (DOS & PDOS)

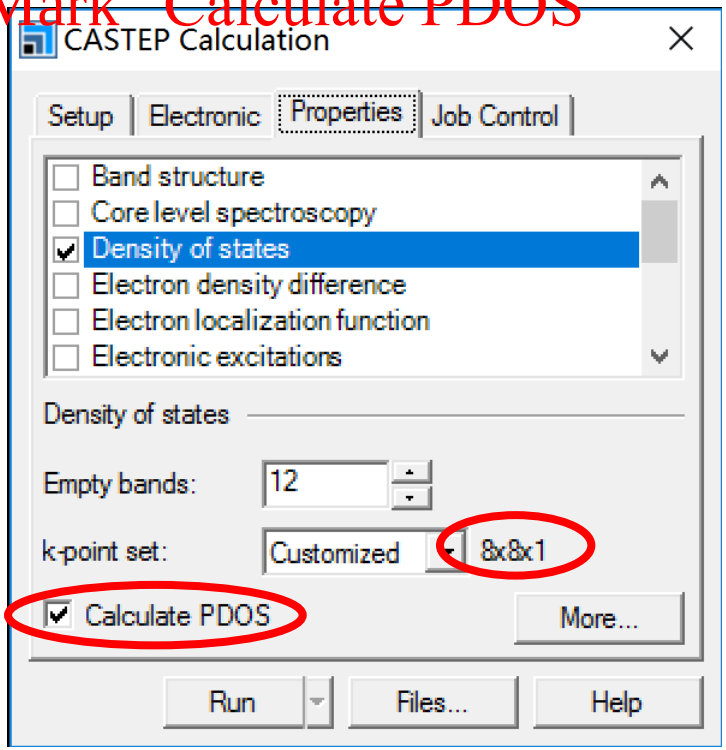
(1) Setting **(Calculation)**:

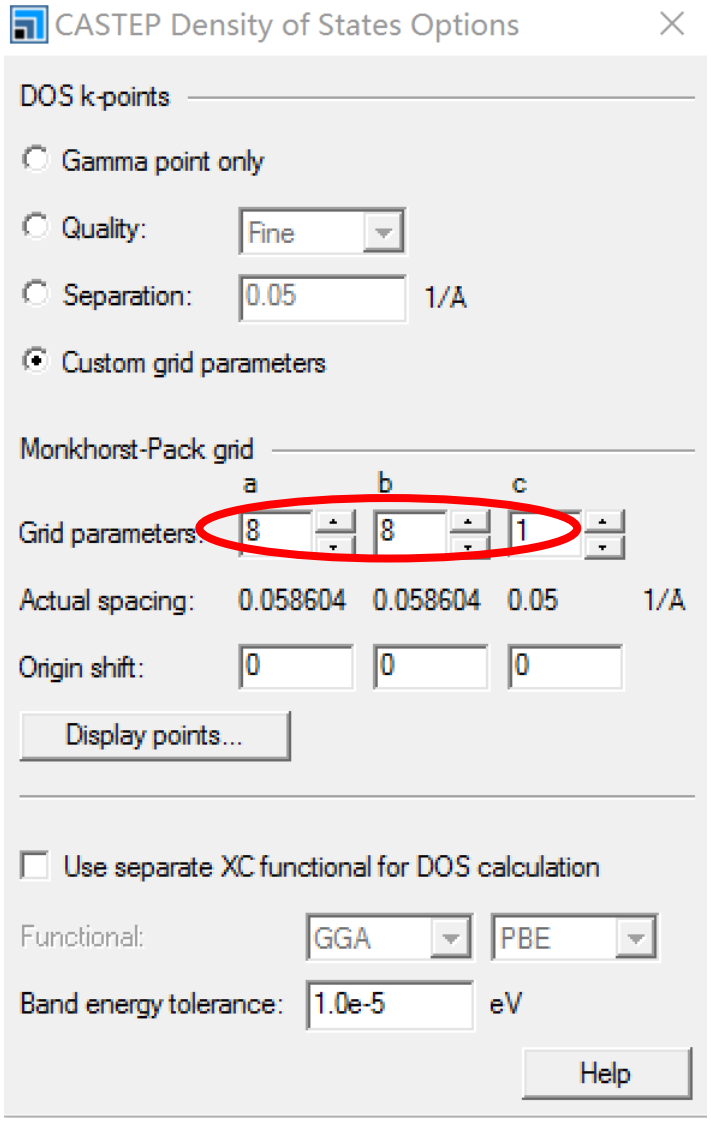
① Task: Properties

② Properties: Mark “Density of states”

③ More… for k-point set

④ Mark “Calculate PDOS”





5. Density of States (DOS & PDOS)

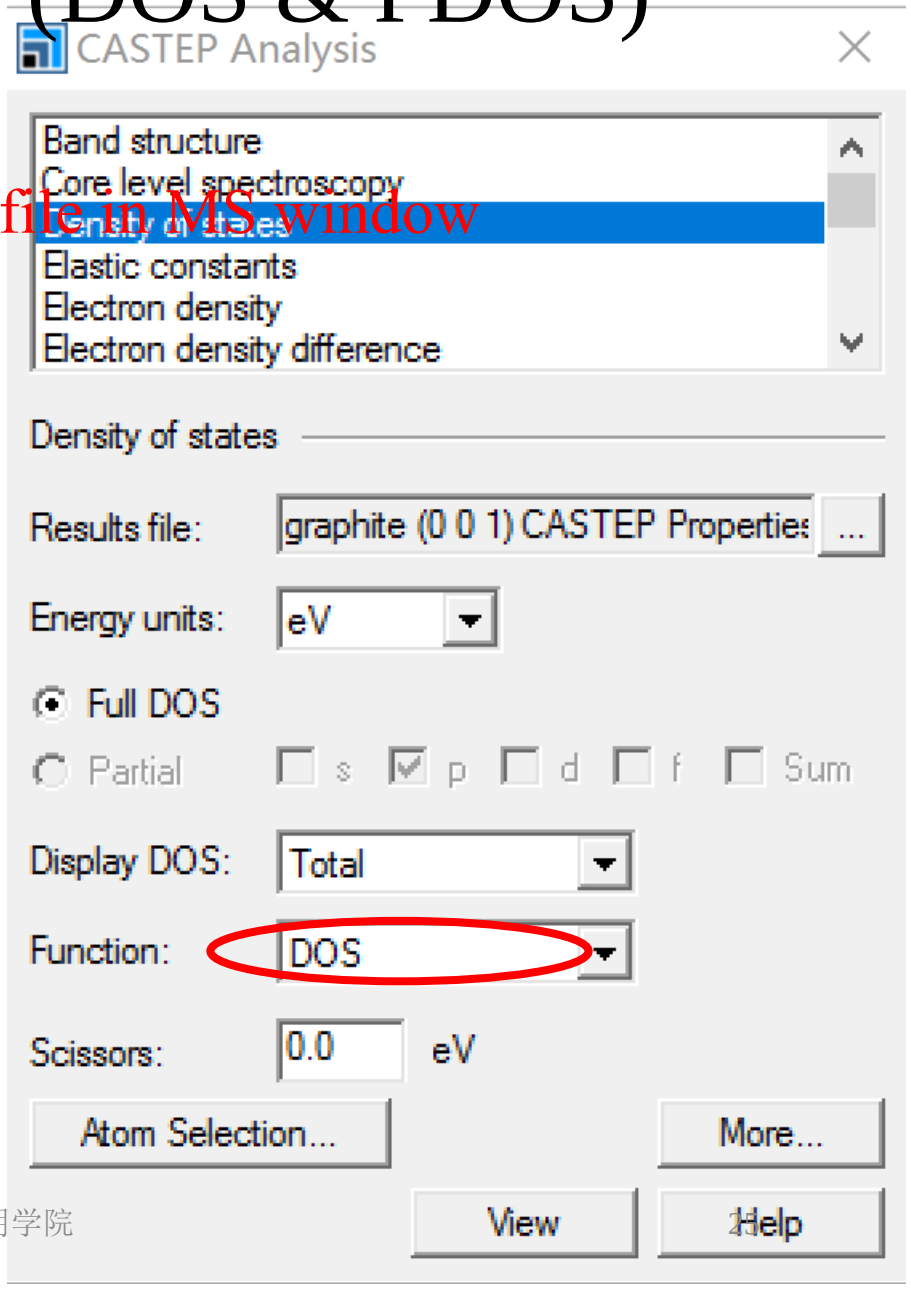
(2) Visualize DOS **(Analysis)**:

① Open file "DOS_DOS.castep" file in MS window

② Select "Density of states"

③ Select "Full DOS" or "Partial"

④ View



5. Density of States (DOS & PDOS)