11月6日上机实习安排

使用MS软件CASTEP模块完成：

Graphene的DFT计算

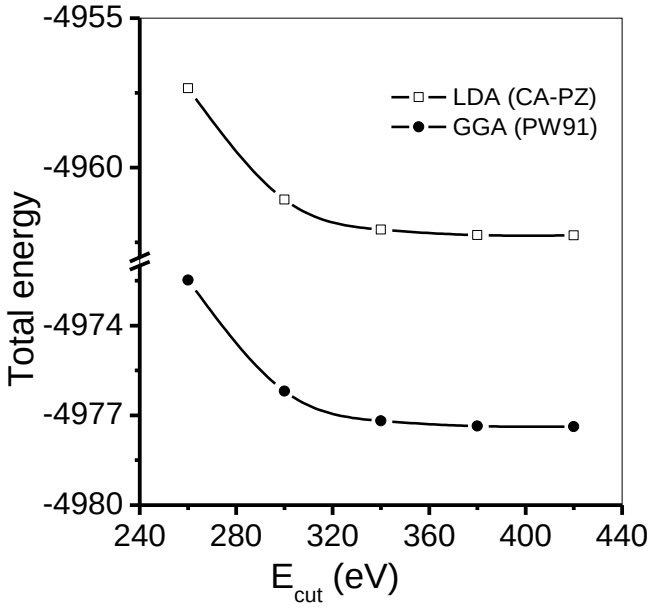
1. 结构优化→
2. 电荷密度计算（高精度单点能）→
3. 能带结构计算（FBZ高对称*K*点）→
4. 态密度计算(DOS & PDOS)

PPT展示：

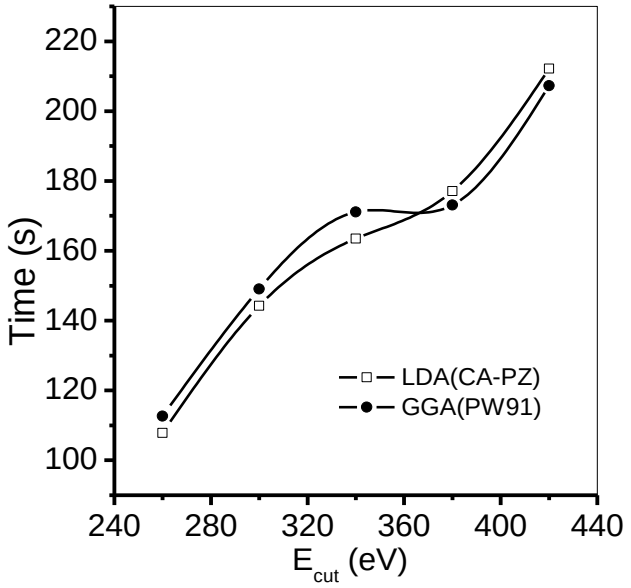
董家豪(+10)：Graphene DFT计算的结果可靠性测试

Graphene DFT计算的结果可靠性测试

1. 截断能(cutoff energy)



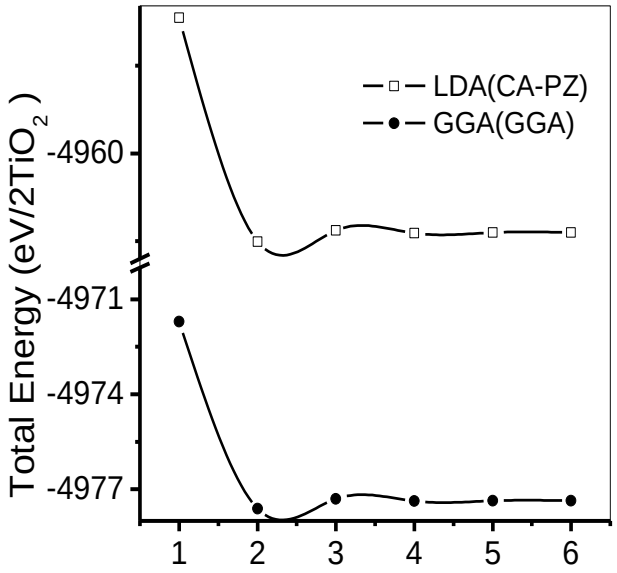
截断能与总能量的关系



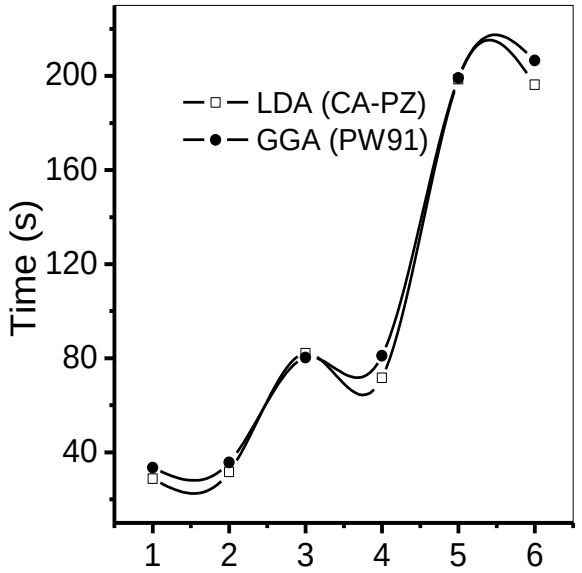
截断能与计算时间的关系

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

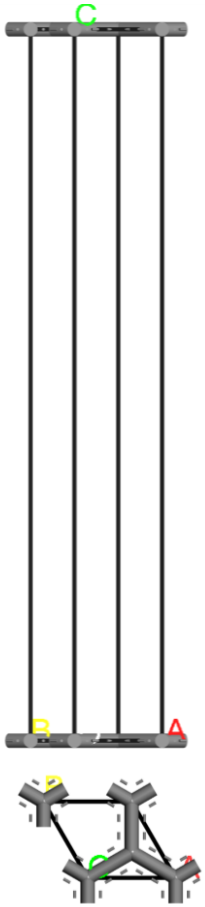
Graphene DFT计算的参考文献

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. Geometry Optimization of Graphene

Setting:

- Quality: fine (for optimization)
- Mark “Optimize cell”
- Method: BFGS
- Cutoff energy: 400 eV
- *K* points: 6×6×1
- Pseudopotential: ultrasoft



Before

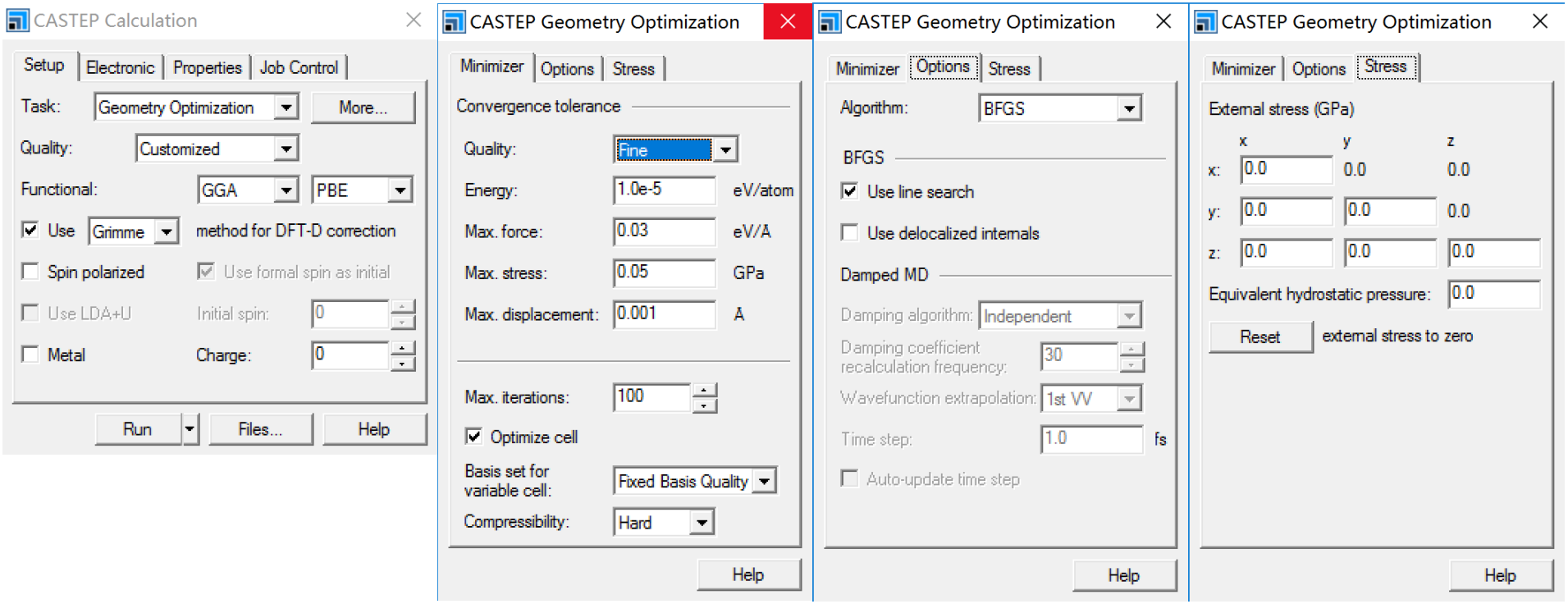
$a = b = 2.460$ Å
$c = 20.0$ Å
$\alpha = \beta = 90.0°$
$\gamma = 120.0°$

After

$a = b = 2.463$ Å
$c = 20.0$ Å
$\alpha = \beta = 90.0°$
$\gamma = 120.0°$

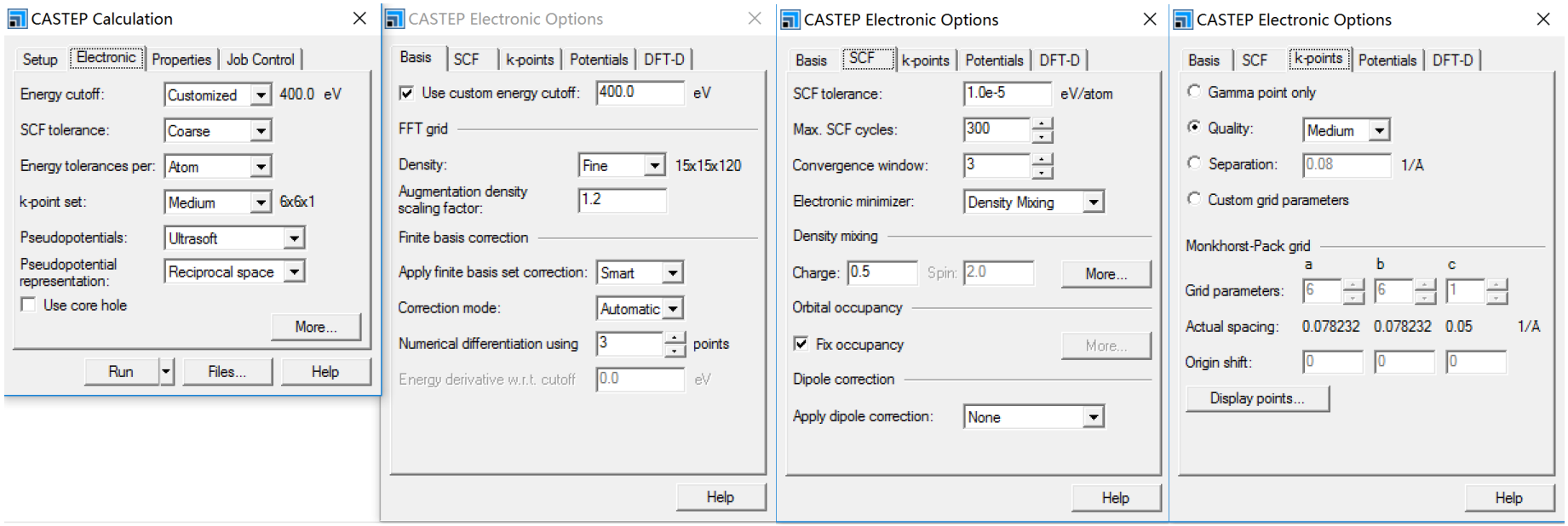
1. Geometry Optimization of Graphene

Task: Geometry Optimization → More·····



1. Geometry Optimization of Graphene

Task: Electronic → More·····



Geometry Optimization: No properties!!!

2. Single-Point Energy Calculation for Charge Density

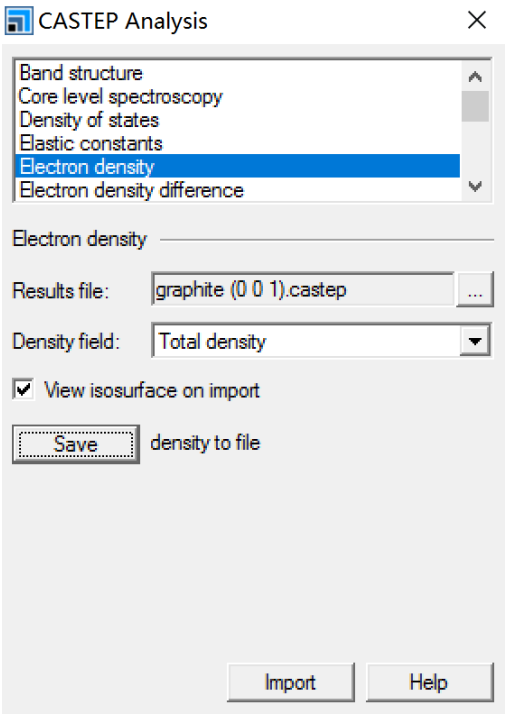
Setting for **changed (higher computational accuracy)**:

- Task: Energy
- *K*-point set: 8×8×1
- SCF tolerance: 10e-6 eV/atom

No properties!!!

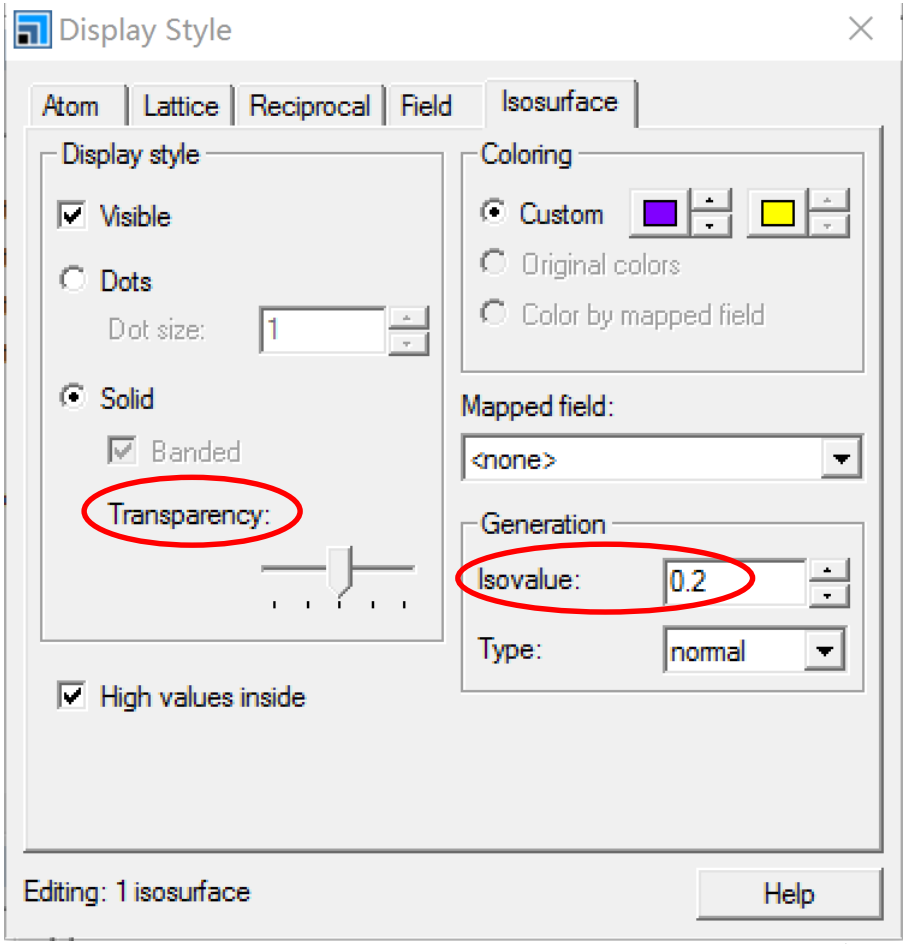
Visualize charge density (Analysis):

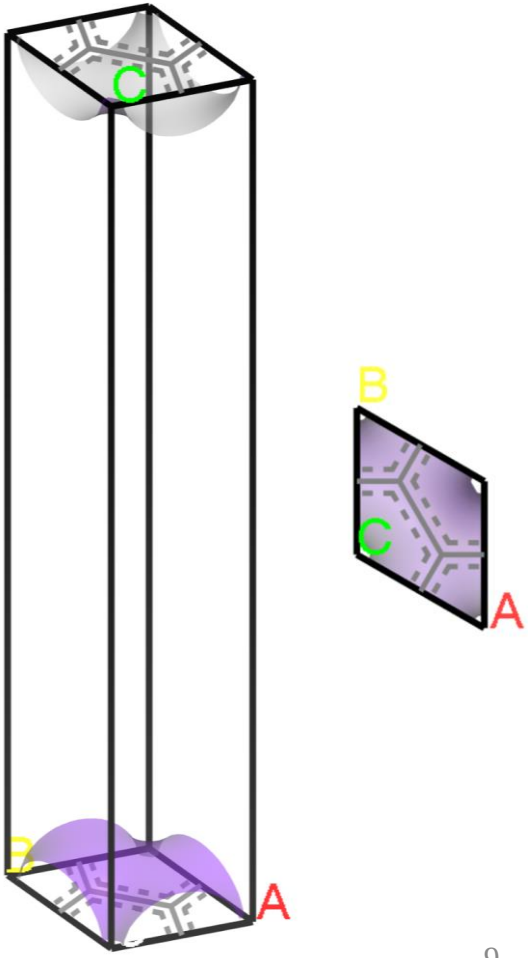
- Select “Electron density”
- Import



2. Single-Point Energy Calculation for Charge Density

Change “Display Style”

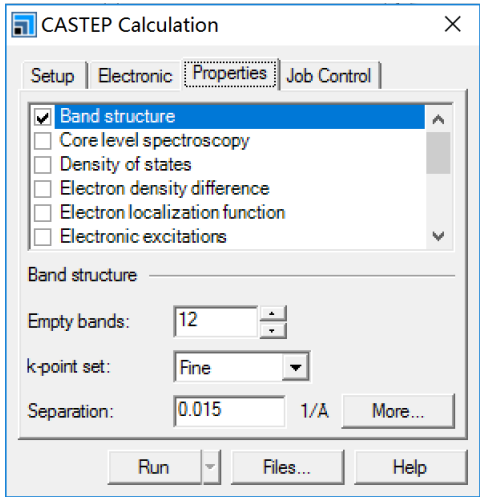


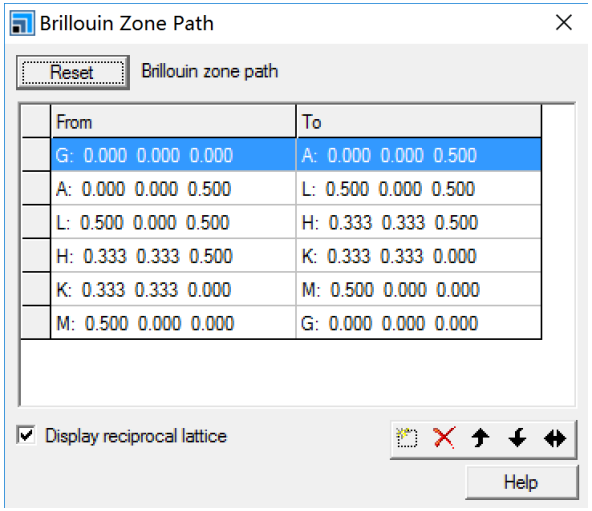


3. Band Structure

Setting:

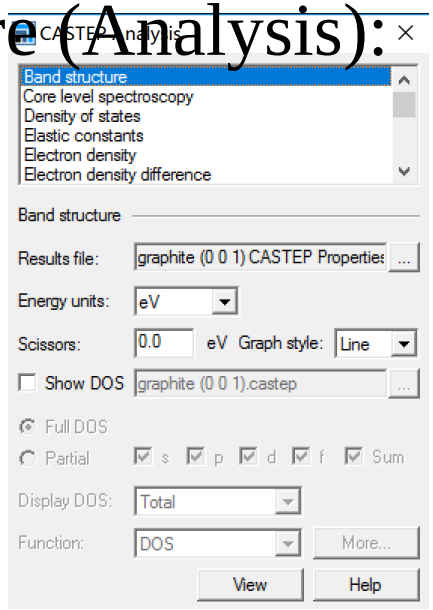
- Task: Properties
- Properties: Mark “Band structure”
- Set high-symmetry *K* points: “Tools→Brillouin Zone path”



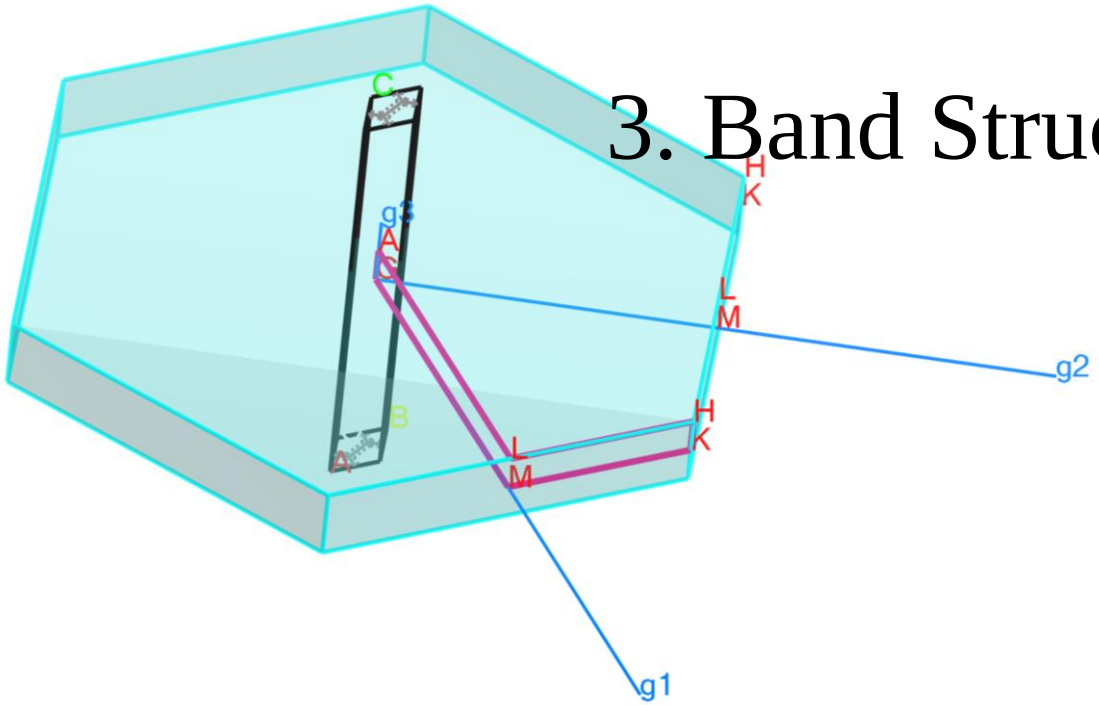


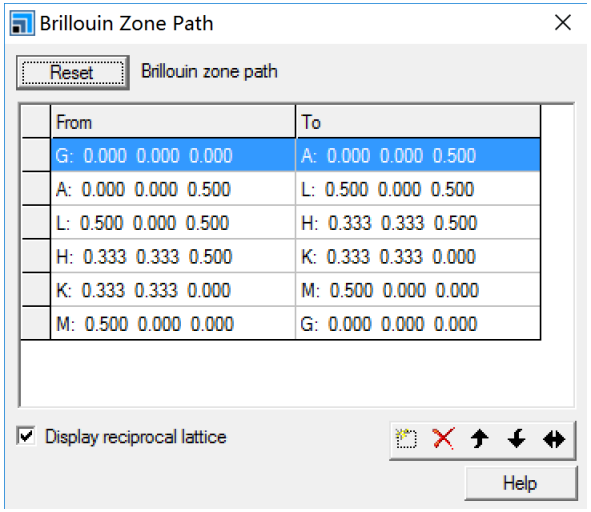
Visualize band structure (Analysis):

- Select “Band structure”
- View

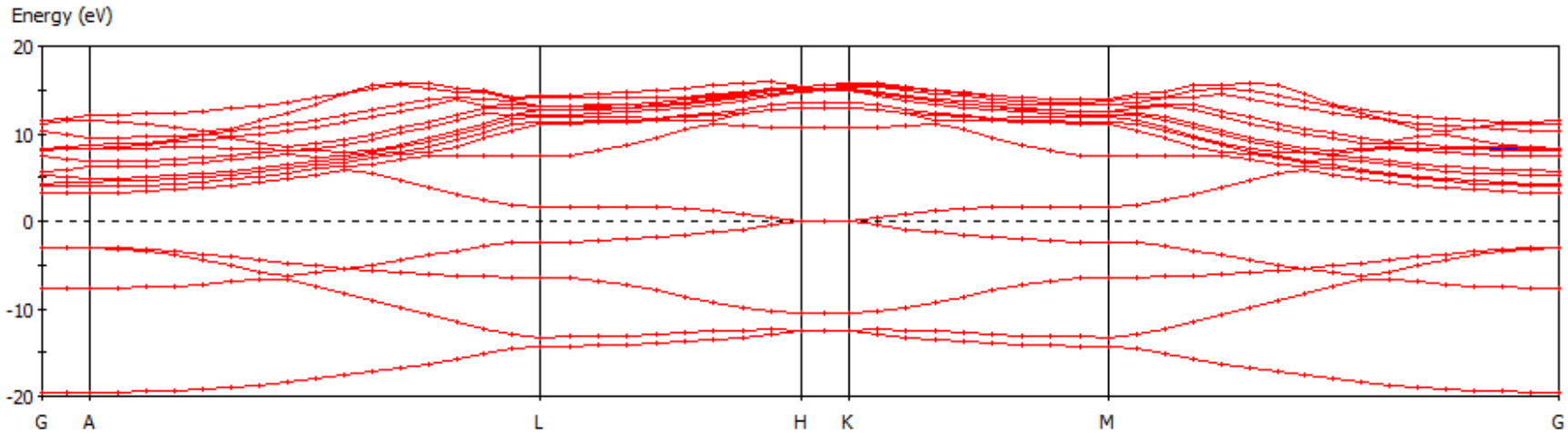


3. Band Structure





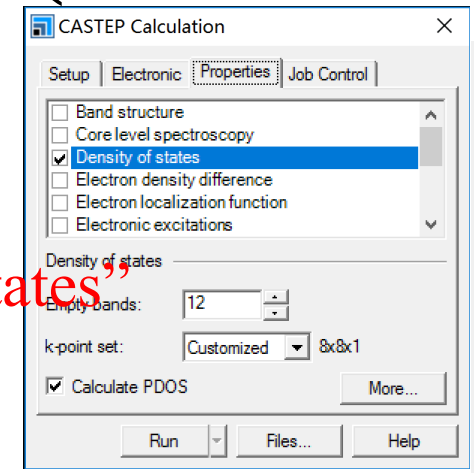
Band gap is 0.019 eV

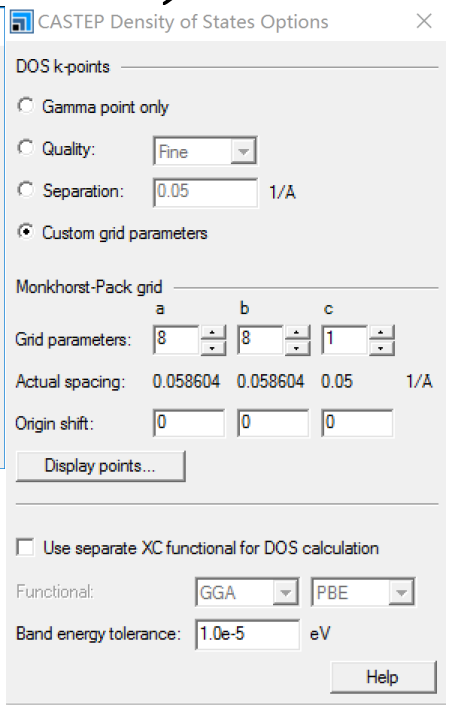


4. Density of States (DOS & PDOS)

Setting:

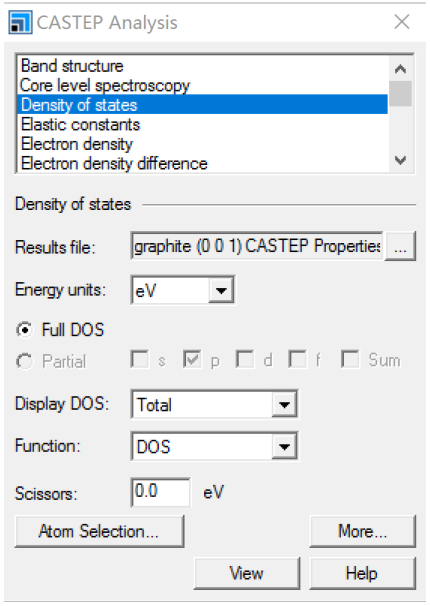
- Task: Properties
- Properties: Mark “Density of states”
- Mark “Calculate PDOS”



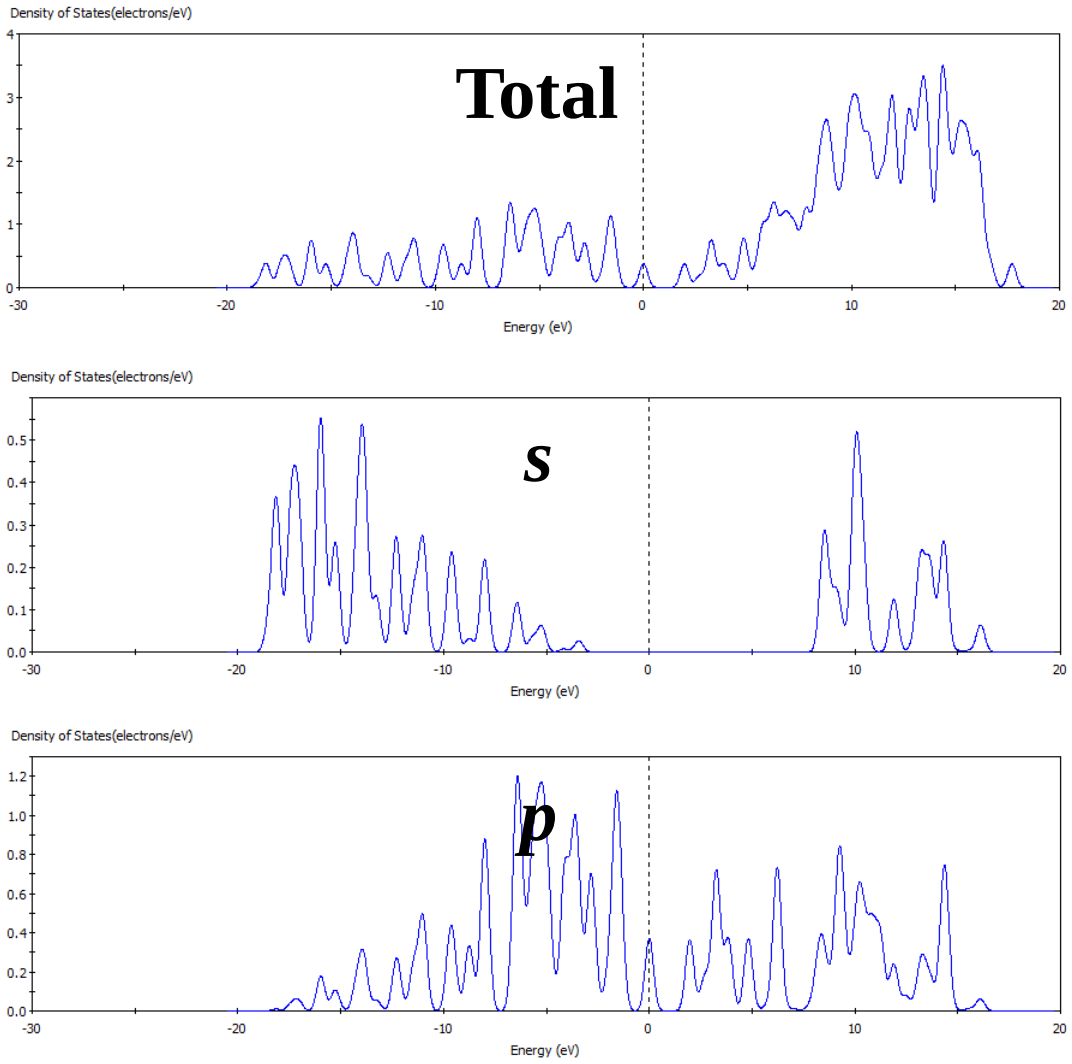


Visualize DOS (Analysis):

- Select “Density of states”
- Select “Full DOS” or “Partial”
- View



4. Density of States (DOS & PDOS)

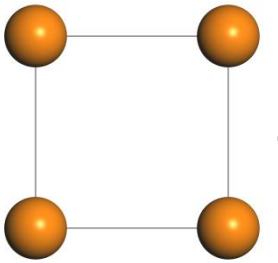


11月9日上机实习安排

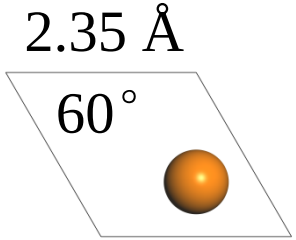
使用MS软件CASTEP模块完成：

Spin-polarized calculation for magnetic Fe membranes:

1. 建模(triangular vs square membranes)
2. Geometry optimizations for 2 model systems
3. Spin-polarized calculations for different magnetic states



FCC(100)_Square Membrane



HCP(001)_Rhombic Membrane

PPT展示：

?(+10)：Graphene DFT计算的VASP设置