Hands-On Tutorials: First-principles computation of quantum materials

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Contents

1. Linux常用命令及PBS系统简介

- ls　　列出文件
- cd　　转移目录(文件夹)
- mkdir　创建目录
- mv　　移动文件/目录/重命名
- pwd　当前目录的绝对路径
- cp　　复制
- rm　　删除 (注意不可逆，慎用)
- cat　　显示/合并文件

. .. ~

```
cd  ~;  cd ..; cd /home/dftcourse/Users/
```

```
mkdir test
```

```
mv  test/  test1/
```

```
cp   ./INCAR  ../INCAR_bak
cp  –r test1/ test2/
```

```
rm –r test1/
```

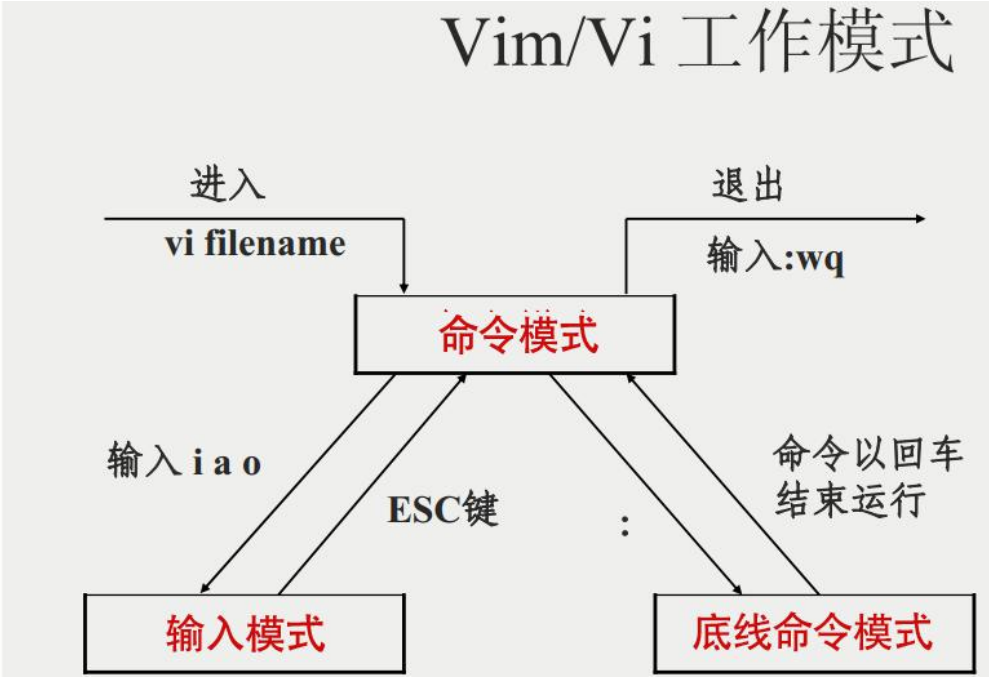
```
cat A B > C
cat A B >> C
```

常用快捷操作

- **Ctrl + c : 终止当前命令**
- **Tab键: 命令补齐**

https://www.runoob.com/linux/linux-command-manual.html

- vi/vim　　文本编辑



- grep　文本搜索
- more, less　分页查看文件
- head, tail　显示文件开头/结尾
- diff　　比较文件不同
- sz, rz　　Linux系统与本机间的文件传输

在直接复制粘贴PDF或word文档中的命令或字符使用时，请加以小心

PBS作业管理系统

- PBS脚本run.sh

```
$ cat run.sh
#PBS -N example
#PBS -l nodes=1:ppn=24
#PBS -l walltime=24:00:00
```

作业名称
节点数:核数
作业最长运行时间

- qsub 交作业

qsub run.sh

- qstat 查询作业状态 进阶版命令 j

```
$ j

w003:

                                                                  Req'd  Req'd   Elap
Job ID          Username Queue    Jobname    SessID NDS TSK Memory Time  S Time
--------------- -------- -------- ---------- ------ --- --- ------ ----- - -----
859509.w003     dftcours cmt      example     16550   1  24    90gb 24:00 R 00:00 node28/0*24
```

- qdel 杀作业(作业号)

qdel 859509

2. Introduction to *ab initio* electronic structure calculation

$$(H^{\sigma}_{\mathrm{KS}} - \varepsilon^{\sigma}_{i})\psi^{\sigma}_{i}(\mathbf{r}) = 0, \qquad H^{\sigma}_{\mathrm{KS}}(\mathbf{r}) = -\frac{1}{2}\nabla^{2} + V^{\sigma}_{\mathrm{KS}}(\mathbf{r}),$$

$$V^{\sigma}_{\mathrm{KS}}(\mathbf{r}) = V_{\mathrm{ext}}(\mathbf{r}) + V_{\mathrm{Hartree}}(\mathbf{r}) + V^{\sigma}_{\mathrm{xc}}(\mathbf{r}).$$

✓ Choice of basis sets

- Plane waves and related basis functions

  Plane waves + pseudopotentials — eg. VASP, Quantum espresso, abinit, CASTEP, …

  (Linearized) augmented plane waves - (L)APW's — eg. Wien2K, Elk, …

  (Linearized) muffin-tin orbitals - (L)MTO's

  Projector augmented waves -PAW's

- Localized orbitals — eg. FHI-aims, Gaussian, ABACUS… OpenMX, …

  Atomic orbitals - LCAO's

  Gaussian orbitals

- …

✓ Choice of XC functionals

Deficiencies of Kohn-Sham DFT

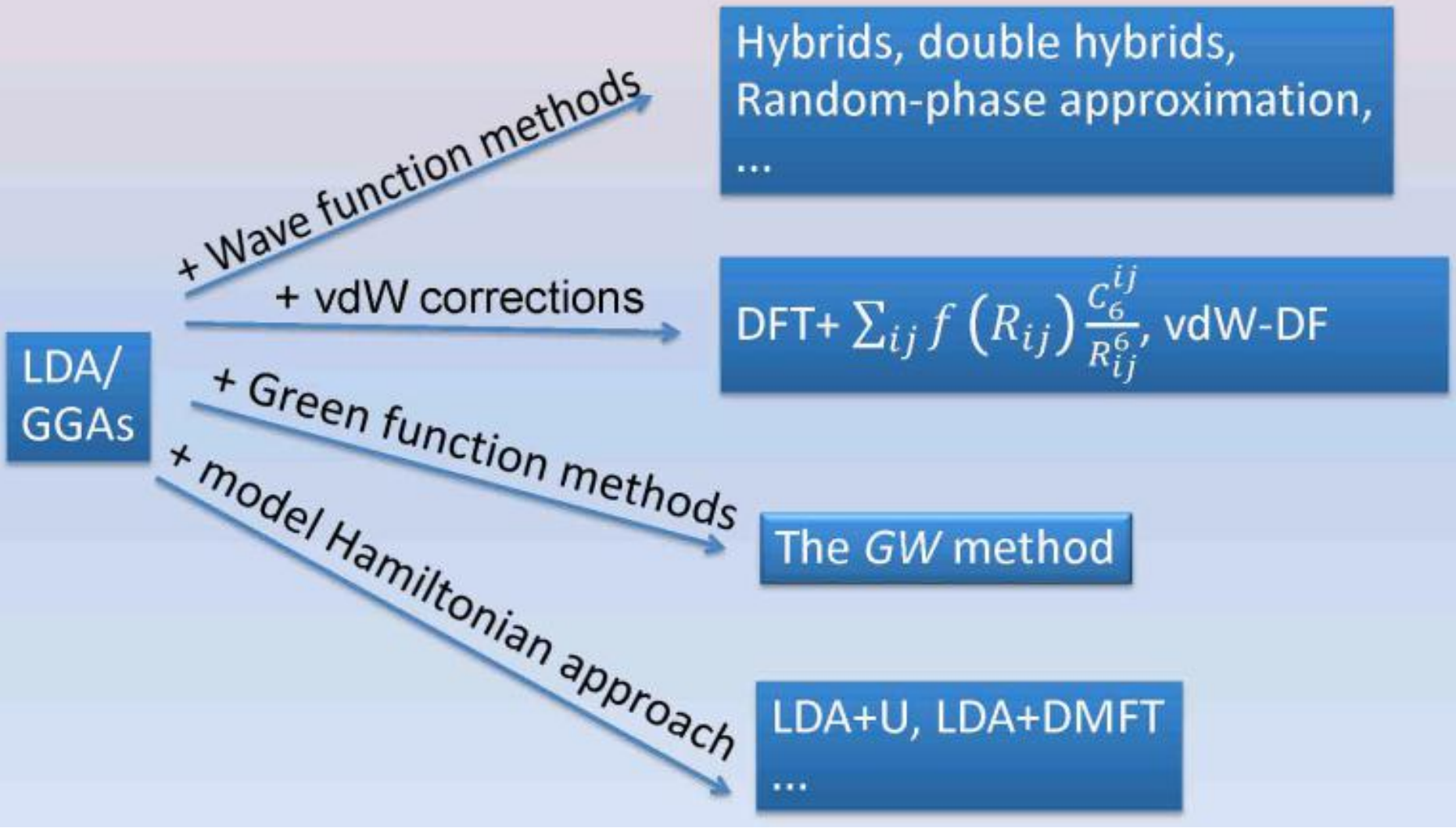
- ✓ exact DFT
- ✓ exact Kohn-Sham theory
- ✓ exchange-correlation approximations (LDA, GGA, …)

- Self-interaction error (delocalization error)
  - Too small band gaps
  - Underestimated reaction barrier heights
  - Unable to describe localized electronic states
  - Overestimated polarizability
  - The XC potential decays too fast (no negative ions, no Rydberg states)

  *Cohen, Mori-Sánchez, and Yang, Science **321**, 792 (2008).*

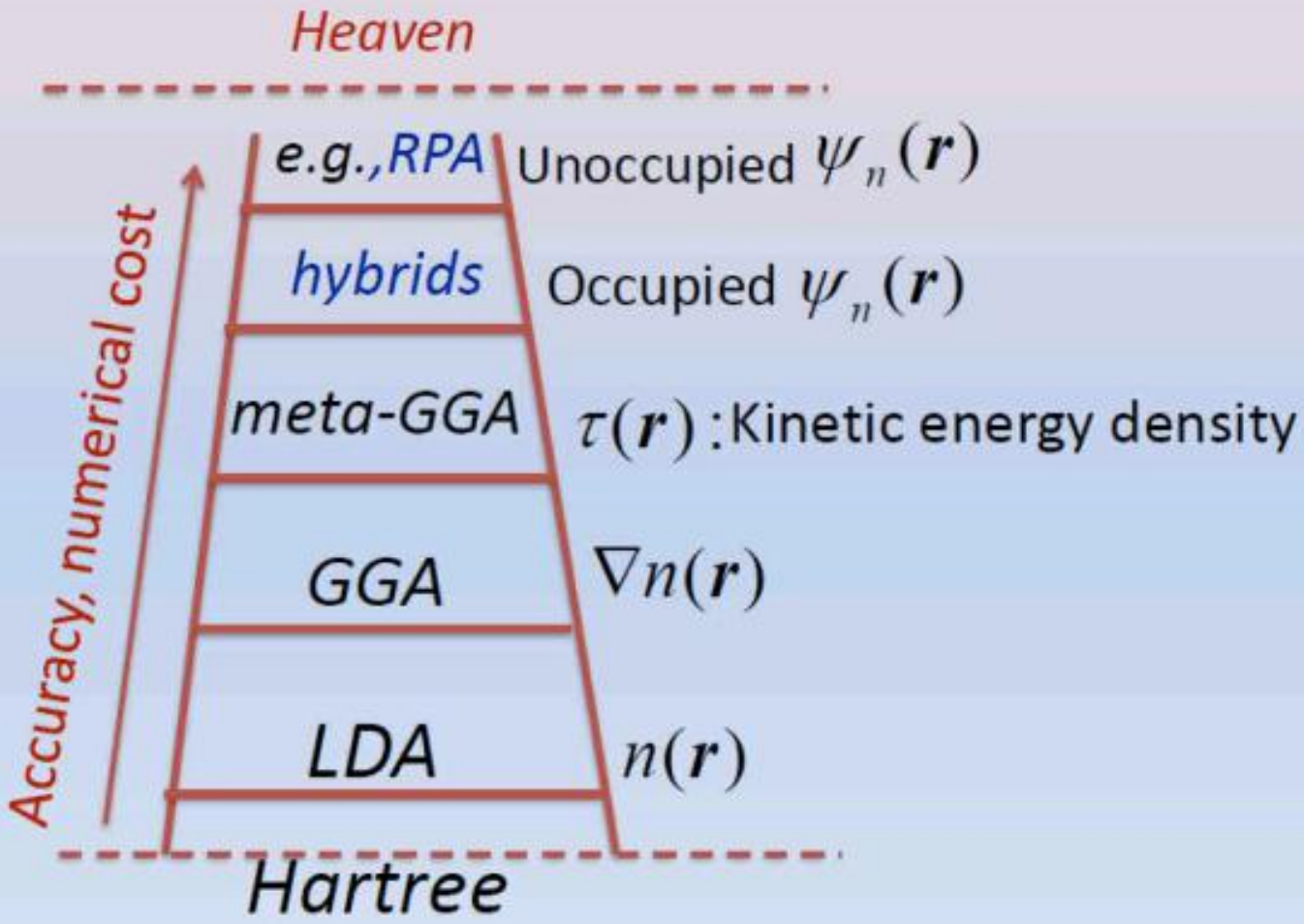
- Unable to describe "strong correlation" (open-shell *d* and *f* electron systems)
- Absence of van der Waals interactions
- No access to excited states in general

Computational schemes beyond LDA and GGAs



Ref: 蒋鸿, 张旻烨, 《中国科学:化学》 **50**, 1344 (2020)

Jacob's ladder of DFT



J. Perdew & K. Schmidt, *Density functional theory and its application to materials*, edited by V. Van Doren et al. (2001)

VASP = Vienna Ab-initio Simulation Package

VASP is a complex package for performing ab-initio quantum-mechanical molecular dynamics (MD) simulations using pseudopotentials (如超软赝势 US-PP) or the projector-augmented wave (PAW) method and a plane wave basis set.

https://www.vasp.at/

3. 第一性原理软件基本流程: 以VASP为例

晶格结构来源:
数据库(ICSD, Materials project, …)
文献,
自己构造

CHGCAR
OUTCAR
……

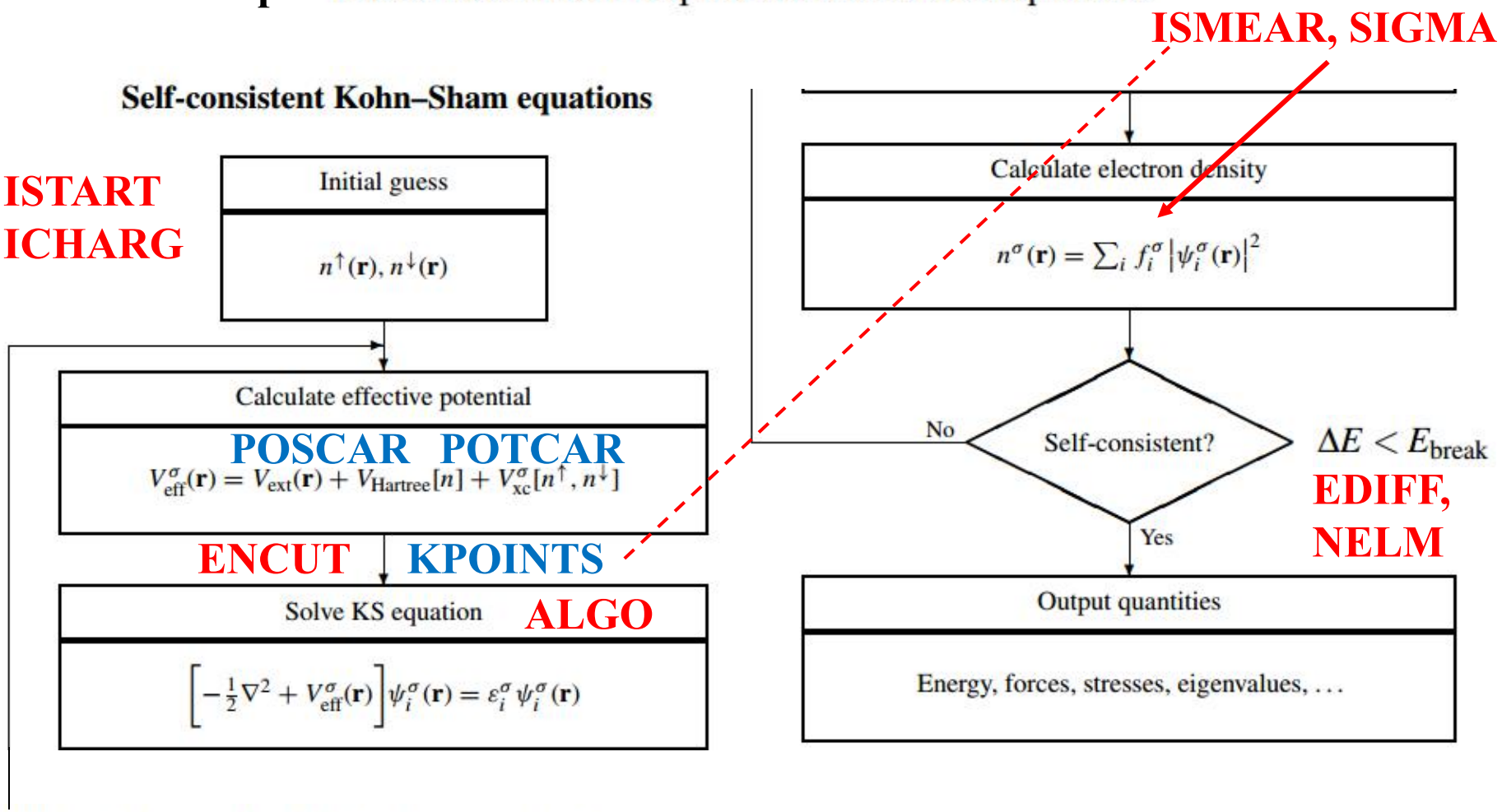
后处理: 能带结构, 态密度, 物理性质(弹性, 光学性质, 稳定性, 迁移率 …)

https://mp.weixin.qq.com/s/gJJhMYKrRqHfbYyJI4mwhg

Input files:

- **INCAR** steering the calculations
- **POSCAR** structural data basis vectors and positions
- **POTCAR** pseudopotential file
- **KPOINTS** Brillouin zone sampling

Electronic step: The self-consistent loop for solution of KS equations



mixing of charge density $\rho_{\text{in}}, \rho_{\text{out}} \Rightarrow$ new ρ_{in}

AMIX,
AMIX_MAG,
BMIX,
BMIX_MAG …

Ionic step: IBRION, ISIF
EDIFFG,
NSW

4. VASP基本输入、输出文件及后处理

4.1 POSCAR　　POTCAR

POSCAR

```
Zr2 Si2 Te2  #header
   1.000   #scaling
     3.6986    0.0000    0.0000
     0.0000    3.6986    0.0000
     0.0000    0.0000   24.8871  #a1,a2,a3
   Zr   Si   Te          #atom type
    2    2    2         #atom number
Direct      # Cartesian
  0.25  0.75  0.4140696
  0.75  0.25  0.5859304
  0.75  0.75  0.5000000
  0.25  0.25  0.5000000
  0.75  0.25  0.3597371
  0.25  0.75  0.6402629
```

Direct: $\vec{R} = x_1\vec{a}_1 + x_2\vec{a}_2 + x_3\vec{a}_3$

Cartesian: $\vec{R} = s\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$

VESTA: other formats (eg. cif) -> VASP POSCAR

4. VASP基本输入、输出文件及后处理

4.1 POSCAR　　POTCAR

POSCAR

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    Zr   Si   Te          #atom type
     2    2    2         #atom number
Direct      # Cartesian
  0.25  0.75  0.4140696
  0.75  0.25  0.5859304
  0.75  0.75  0.5000000
  0.25  0.25  0.5000000
  0.75  0.25  0.3597371
  0.25  0.75  0.6402629
```

POTCAR

/home/dftcourse/Users/Tutorial/POTCARs目录下

```
cat Zr/POTCAR
    Si/POTCAR
    Te/POTCAR >>
POTCAR
```

与POSCAR中元素类型一一对应

VESTA: other formats (eg. cif) -> VASP POSCAR

POTCAR

- 根据方法不同有Ultra-soft赝势(USPP)和投影缀加波的赝势(PAW)
- 根据交换关联函数的不同有LDA和GGA
- 根据处理了半芯态有A, A_sv和A_pv的不同
- 根据ENMAX的大小有A, A_s和A_h的不同

```
PAW W 19Jan2001
6.00000000000000000
parameters from PSCTR are:
  VRHFIN =W: 5p6s5d
  LEXCH  = CA
  EATOM  =   206.5370 eV,   15.1800 Ry

  TITEL  = PAW W 19Jan2001
  LULTRA =       F    use ultrasoft PP ?
  IUNSCR =       1    unscreen: 0-lin 1-nonlin 2-no
  RPACOR =    2.330    partial core radius
  POMASS =  183.850; ZVAL   =    6.000    mass and valenz
  RCORE  =    2.750    outmost cutoff radius
  RWIGS  =    2.750; RWIGS  =    1.455    wigner-seitz radius (au A)
  ENMAX  =  223.126; ENMIN  =  167.344 eV
  RCLOC  =    2.147    cutoff for local pot
  ..................

  Description
   l    E      TYP  RCUT    TYP  RCUT
   2   .000     23  2.500
  ..................
```

ENCUT

POTCAR

- 根据方法不同有Ultra-soft赝势(USPP)和投影缀加波的赝势(PAW)
- 根据交换关联函数的不同有LDA和GGA
- 根据处理了半芯态有A, A_sv和A_pv的不同
- 根据ENMAX的大小有A, A_s和A_h的不同

```
 PAW_PBE W 08Apr2002
  6.00000000000000
parameters from PSCTR are:
  VRHFIN =W : 6s5d
  LEXCH  = PE
  EATOM  =   204.6103 eV,   15.0384 Ry

  TITEL  = PAW_PBE W 08Apr2002
  LULTRA =        F    use ultrasoft PP ?
  IUNSCR =        1    unscreen: 0-lin 1-nonlin 2-no
  RPACOR =    2.330    partial core radius
  POMASS =  183.850; ZVAL   =    6.000    mass and valenz
  RCORE  =    2.750    outmost cutoff radius
  RWIGS  =    2.750; RWIGS  =    1.455    wigner-seitz radius (au A)
  ENMAX  =  223.057; ENMIN  =  167.293 eV
  RCLOC  =    2.147    cutoff for local pot
  LCOR   =        T    correct aug charges
  LPAW   =        T    paw PP
  EAUG   =  373.438
  DEXC   =    0.000
  RMAX   =    2.801    core radius for proj-oper
  RAUG   =    1.300    factor for augmentation sphere
  RDEP   =    2.886    radius for radial grids
  RDEPT  =    2.230    core radius for aug-charge
```

ENCUT

grep ENMAX POTCAR

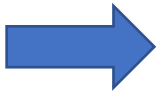
https://www.vasp.at/wiki/index.php/Available_PAW_potentials

4.2 INCAR

注意不同流程中的参数变化！

结构弛豫

```
ICHARG = 2    # 2-atom 11-nsc
ENCUT = 400  # from POTCAR
ISMEAR = 0    # smearing method
SIGMA = 0.05   #  broadening in eV
IBRION= 2      # CG
ISIF = 2       #晶格弛豫参数 2,3,4
NSW = 50    #最大弛豫次数
EDIFFG = -0.01  #弛豫精度
NELM   = 50       #最大电子步次数
EDIFF   = 1E-5    #电子步精度
LCHARG = .FALSE.  #不输出电荷密度
LWAVE = .FALSE.     #不输出波函数
```



静态自洽（晶格固定）

```
ICHARG = 2
ENCUT = 400
ISMEAR = 0
SIGMA = 0.05
IBRION= -1   #不再弛豫
ISIF = 2
NSW = 0      #不再弛豫
EDIFFG = -0.01
NELM   = 50
EDIFF   = 1E-5
LCHARG = .TRUE. #输出电荷密度
LWAVE = .FALSE.
```

4.2 INCAR

注意不同流程中的参数变化！

静态自洽（晶格固定）

```
ICHARG = 2
ENCUT = 400
ISMEAR = 0
SIGMA = 0.05
IBRION= -1   #不再弛豫
ISIF = 2
NSW = 0      #不再弛豫
EDIFFG = -0.01
NELM   = 50
EDIFF   = 1E-5
LCHARG = .TRUE. #输出电荷密度
LWAVE = .FALSE.
```

能带（非自洽计算）

```
ICHARG=11   #  11-nsc 2-atom
ENCUT = 400
ISMEAR = 0
SIGMA = 0.05
IBRION = -1
ISIF = 2
NSW = 0
EDIFFG = -0.01
NELM   = 50
EDIFF   = 1E-5
LCHARG = .FALSE.
LWAVE = .FALSE.
```

不懂的参数先去看**vasp wiki**

https://www.vasp.at/wiki/index.php/The_VASP_Manual

◆ The most important parameters, source of errors

A compromise between speed and accuracy

VASP GUIDE Chapter 8

✓ ENCUT

$$\psi_{n\mathbf{k}}(\mathbf{r}) = u_{n\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\mathbf{r}} \qquad \text{with } u_{n\mathbf{k}}(\mathbf{r}+\mathbf{R}) = u_{n\mathbf{k}}(\mathbf{r}).$$

$$u_{n\mathbf{k}}(\mathbf{r}) = \frac{1}{\Omega^{1/2}}\sum_{\mathbf{G}} C_{\mathbf{G}n\mathbf{k}}e^{i\mathbf{G}\mathbf{r}} \qquad \psi_{n\mathbf{k}}(\mathbf{r}) = \frac{1}{\Omega^{1/2}}\sum_{\mathbf{G}} C_{\mathbf{G}n\mathbf{k}}e^{i(\mathbf{G}+\mathbf{k})\mathbf{r}}$$

$$E_{cut} = \frac{\hbar^2 G^2_{\max}}{2m}$$

$$\left|\vec{G}+\vec{k}\right| \le G_{\max}$$

grep ENMAX POTCAR

* Pulay stress: cell shape and volume relaxations
(increase ENMAX by 30%)

https://www.vasp.at/wiki/index.php/Energy_vs_volume_Volume_relaxations_and_Pulay_stress

◆ The most important parameters, source of errors

✓ Number of k-points, and method for smearing: ISMEAR, SIGMA

$$\sum_n \frac{1}{\Omega_{BZ}} \int_{\Omega_{BZ}} \varepsilon_{n\mathbf{k}}\,\Theta(\varepsilon_{n\mathbf{k}}-\mu)\,\mathrm{d}\mathbf{k}, \;\rightarrow\; \sum_n \sum_{\mathbf{k}} w_{\mathbf{k}}\varepsilon_{n\mathbf{k}}\,\Theta(\varepsilon_{n\mathbf{k}}-\mu)$$

partial occupation: replace the step function $\Theta(\varepsilon_{n\mathbf{k}}-\mu)$ by a (smooth) function $f(\{\varepsilon_{n\mathbf{k}}\})$

- ISMEAR: −5 tetrahedron method with Blöchl corrections # Γ-center k-mesh
  0 Gaussian smearing
  1..*N* method of Methfessel-Paxton order *N*.
- SIGMA: width of smear $f(\frac{\varepsilon-\mu}{\sigma}) = \frac{1}{2}\left(1-\mathrm{erf}\left[\frac{\varepsilon-\mu}{\sigma}\right]\right)$

- For semiconductors or insulators use the tetrahedron method (`ISMEAR=-5`), if the cell is too large (or if you use only a single or two k-points) use `ISMEAR=0` in combination with a small `SIGMA=0.05`.
- For relaxations *in metals* always use `ISMEAR=1` or `ISMEAR=2` and an appropriate `SIGMA` value (the entropy term should be less than 1 meV per atom). *Mind:* Avoid to use `ISMEAR>0` for semiconductors and insulators, since it might cause problems.

  For metals a sensible value is usually `SIGMA= 0.2` (which is the default).
- For the calculations of the DOS and very accurate *total energy* calculations (no relaxation in metals) use the tetrahedron method (`ISMEAR=-5`).

`entropy T*S` in the OUTCAR file) must be small (i.e. < 1-2 meV/per atom).

https://www.vasp.at/wiki/index.php/ISMEAR

✓ INCAR 结构弛豫相关

- IBRION = 2 # IBRION=1
- NSW
- EDIFFG
- ISIF

ISIF	calculate force	calculate stress tensor	relax ions	change cell shape	change cell volume
0	yes	no	yes	no	no
1	yes	trace only *	yes	no	no
2	yes	yes	yes	no	no
3	yes	yes	yes	yes	yes
4	yes	yes	yes	yes	no
5	yes	yes	no	yes	no
6	yes	yes	no	yes	yes
7	yes	yes	no	no	yes

Summary

- Calculation of the equilibrium volume:
  - FIt the energy over a certain volume range to an equation of state.
  - When internal degrees of freedom exist (e.g. c/a), the structure must be optimized. Use a conjugate-gradient algorithm (IBRION=2) and at each volume do e.g. 10 ionic steps (NSW=10) and allow change of internal parameters and shape (ISIF=4).
- Simpler but less reliable: relaxing all degrees of freedom including volume.
  - To relax all degrees of freedom use ISIF=3 (internal coordinates, shape and volume).
  - Mind pulay stress problem. Increase plane wave cutoff by 25-30% when the volume is allowed to change.

cp CONTCAR POSCAR

✓ INCAR 控制输出

LCHARG = .TRUE. #自洽步一定要存!

LWAVE = .FALSE.

LORBIT = 11 $P_{Nlmn\mathbf{k}} \equiv \langle Y_{lm}^{N} | \phi_{n\mathbf{k}} \rangle$

4.3 KPOINTS

设置布里渊区 k 点网格取样大小或能带结构计算时沿高对称方向的 k 点：

a) 手动输入即自定义各个 k 点的坐标和权重：

```
Example file
4
Cartesian
0.0   0.0   0.0    1.
0.0   0.0   0.5    1.
0.0   0.5   0.5    2.
0.5   0.5   0.5    4.
```

b) Line-mode：在计算能带时用 https://mp.weixin.qq.com/s/Ptnj_oDZl-_foaAPcp6imA

例子:

```
k-points along high symmetry lines   !注释行，无特别的意义
10                                    !沿 G-X 特殊点之间产生 10 个 k 点
Line-mode                             !程序自动产生特殊 k 点间的 k 点
Reciprocal                            !各 k 点相对于倒格子基矢来写的
0.00    0.00    0.00                  !Gamma
0.50    0.00    0.50                  !X
```

vaspkit -task 303

c) 程序自动产生 k 点：最常用的，定义网格取样大小

例子：

```
Automatic generation          !注释行
0                             !自动产生 k 点，这一行必须设为 0
Monhkorst-Pack                !Monhkorst-Pack 方法产生 k 点
9       9       9             !在各个基矢方向上分割各基矢的点数
0.0     0.0     0.0           !是否移动网格点以及移动多少(这里不移动)
```

```
(echo 102;echo 2;echo 0.03) | vaspkit
```

例子:

```
Automatic generation          !注释行
0                             !自动产生 k 点，这一行必须设为 0
Gamma                         !明确定义以 Gamma 点为中心,根据 M-P 方法产生 k 点
9   9   7
0.0   0.0   0.0
```

- Symmetry is used (for ISYM≥0) to reduce the number of k-points to the irreducible subset of symmetry inequivalent k-points (IBZKPT)

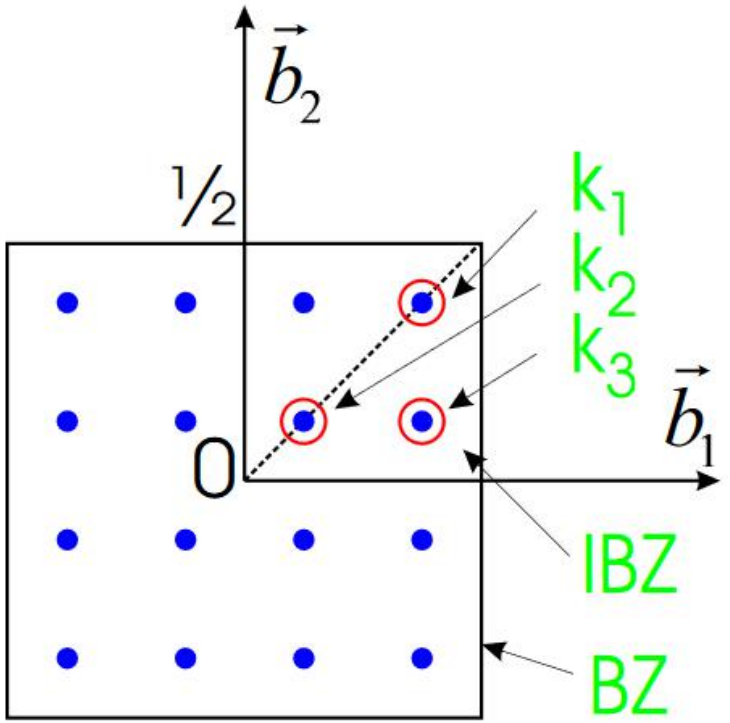
M-P方法

$$\mathbf{k}_{prs} = u_p\mathbf{b}_1 + u_r\mathbf{b}_2 + u_s\mathbf{b}_3$$

$$u_r = \frac{2r - q_r - 1}{2q_r} \qquad r = 1, 2, \ldots, q_r$$

$\mathbf{b}_i$ reciprocal lattice-vectors

q_r determines number of k-points in r-direction



IBZKPT（不可约k点）

```
Kpoints for relax
0   #automatic
M-P    # Gamma
10 8 4  #b1,b2,b3
```

全奇数包含Γ点

Symmetry reduction of the mesh

Bravais lattice	variant	mesh choices	subsection choices
triclinic	primitive	Γ-centered, Monkhorst Pack	$\|\mathbf{a}_1\|^{-1} : \|\mathbf{a}_2\|^{-1} : \|\mathbf{a}_3\|^{-1}, \|\mathbf{b}_1\| : \|\mathbf{b}_2\| : \|\mathbf{b}_3\|$
monoclinic	primitive	Γ-centered, Monkhorst Pack	$\|\mathbf{a}_1\|^{-1} : \|\mathbf{a}_2\|^{-1} : \|\mathbf{a}_3\|^{-1}, \|\mathbf{b}_1\| : \|\mathbf{b}_2\| : \|\mathbf{b}_3\|$
	base-centered	Γ-centered, Monkhorst Pack	$\|\mathbf{a}_1\|^{-1} : \|\mathbf{a}_2\|^{-1} : \|\mathbf{a}_3\|^{-1}, \|\mathbf{b}_1\| : \|\mathbf{b}_2\| : \|\mathbf{b}_3\|$
orthorhombic	primitive	Γ-centered, Monkhorst Pack	$\|\mathbf{a}_1\|^{-1} : \|\mathbf{a}_2\|^{-1} : \|\mathbf{a}_3\|^{-1}, \|\mathbf{b}_1\| : \|\mathbf{b}_2\| : \|\mathbf{b}_3\|$
	base-centered	Γ-centered, Monkhorst Pack	$\|\mathbf{a}_1\|^{-1} : \|\mathbf{a}_2\|^{-1} : \|\mathbf{a}_3\|^{-1}, \|\mathbf{b}_1\| : \|\mathbf{b}_2\| : \|\mathbf{b}_3\|$
	body-centered	Γ-centered, Monkhorst Pack	$\|\mathbf{a}_1\|^{-1} : \|\mathbf{a}_2\|^{-1} : \|\mathbf{a}_3\|^{-1}$
	face-centered	Γ-centered	$\|\mathbf{b}_1\| : \|\mathbf{b}_2\| : \|\mathbf{b}_3\|$
tetragonal	primitive	Γ-centered, Monkhorst Pack	$\|\mathbf{a}_1\|^{-1} : \|\mathbf{a}_2\|^{-1} : \|\mathbf{a}_3\|^{-1}, \|\mathbf{b}_1\| : \|\mathbf{b}_2\| : \|\mathbf{b}_3\|$
	body-centered	Γ-centered, Monkhorst Pack	$\|\mathbf{a}_1\|^{-1} : \|\mathbf{a}_2\|^{-1} : \|\mathbf{a}_3\|^{-1}$
hexagonal	rhombohedral	Γ-centered	$\|\mathbf{a}_1\|^{-1} : \|\mathbf{a}_2\|^{-1} : \|\mathbf{a}_3\|^{-1}, \|\mathbf{b}_1\| : \|\mathbf{b}_2\| : \|\mathbf{b}_3\|$
	hexagonal	Γ-centered	$\|\mathbf{a}_1\|^{-1} : \|\mathbf{a}_2\|^{-1} : \|\mathbf{a}_3\|^{-1}, \|\mathbf{b}_1\| : \|\mathbf{b}_2\| : \|\mathbf{b}_3\|$
cubic	primitive	Γ-centered, Monkhorst Pack	$\|\mathbf{a}_1\|^{-1} : \|\mathbf{a}_2\|^{-1} : \|\mathbf{a}_3\|^{-1}, \|\mathbf{b}_1\| : \|\mathbf{b}_2\| : \|\mathbf{b}_3\|$
	body-centered	Γ-centered, Monkhorst Pack	$\|\mathbf{a}_1\|^{-1} : \|\mathbf{a}_2\|^{-1} : \|\mathbf{a}_3\|^{-1}, \|\mathbf{b}_1\| : \|\mathbf{b}_2\| : \|\mathbf{b}_3\|$
	face-centered	Γ-centered	$\|\mathbf{a}_1\|^{-1} : \|\mathbf{a}_2\|^{-1} : \|\mathbf{a}_3\|^{-1}, \|\mathbf{b}_1\| : \|\mathbf{b}_2\| : \|\mathbf{b}_3\|$

https://www.vasp.at/wiki/index.php/KPOINTS

4.4 输出文件及后处理

(*.o* *.e* # for PBS)
stdout (output.*)
OUTCAR
OSZICAR
CHGCAR
WAVECAR
DOSCAR
PROCAR
CONTCAR
vasprun.xml
…

Input parameter
Symmetry
TOTEN
LOOP TIME
……

```
grep * OUTCAR | tail
```

OUTCAR *file*

individual parts are separated by lines

- first part: reading INCAR, POTCAR, POSCAR
- nearest neighbor distances and analysis of symmetry
- information on what was parsed from INCAR
- verbose job information
- information on lattice, k-points and positions
- information on the basis set (number of plane waves)
- non local pseudopotential information
- information for each electronic step (one line in OSZICAR)

grep -A2 TOTEN OUTCAR

```
free  energy   TOTEN  =       -11.15933907 eV

energy  without entropy=      -11.15101726  energy(sigma->0) =      -11.15517817
```

tail -1 OSZICAR

```
1 F= -.11159339E+02 E0= -.11155178E+02  d E =-.832181E-02
```

Post-processing for VASP

vaspkit https://vaspkit.com/index.html

注意：
(1) 支持命令行模式
(2) band减掉的Fermi level自行解决

```
echo -e "\n" $(sed -n 6p DOSCAR | awk '{print $4}') > FERMI_ENERGY.in
```

5. Examples

(1) diamond & fcc Si

(2) Xene (graphene, silicene, germanene, stanene)

(3) Bi_2Se_3 family

(4) $MnBi_2Te_4$ family

(1) diamond & fcc Si

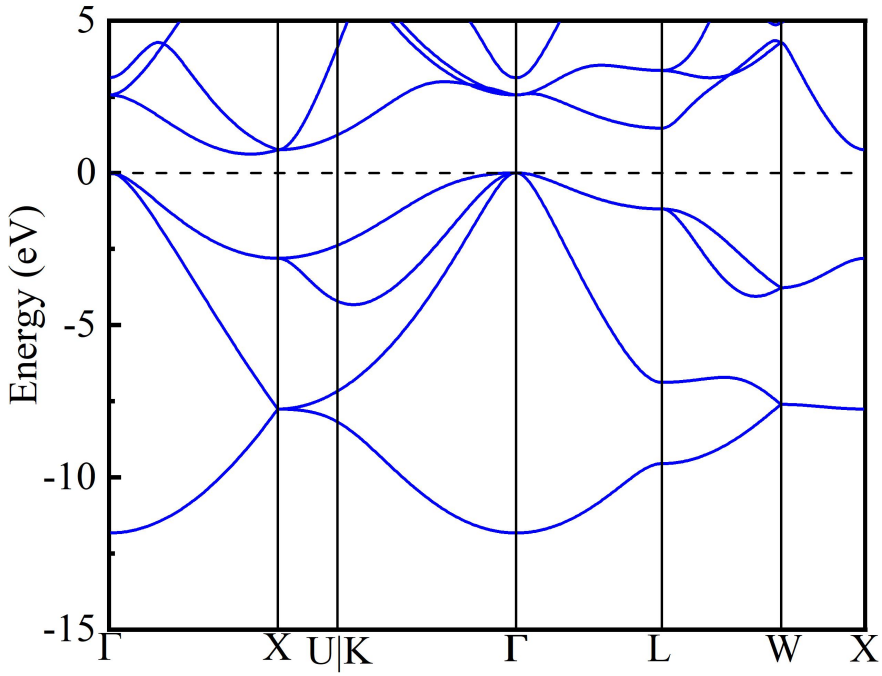
1. relax: ① relax all degrees of freedom;
② *E*-*V* curve & EOS fitting.

http://vaspkit.cn/index.php/48.html

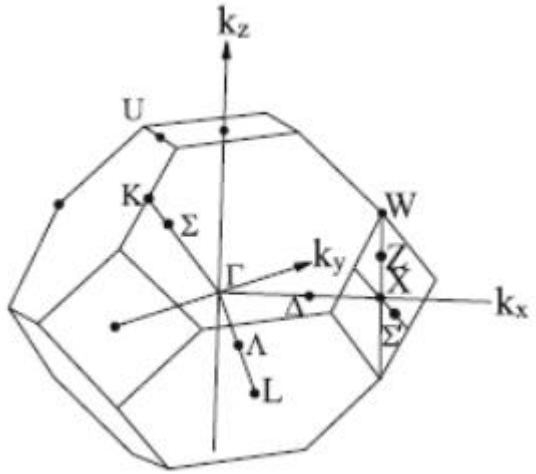
2. self-consistency (sc):
check settings of ENCUT & KPOINTS (smearing methods)

3. band:

diamond Si



band degeneracy & symmetry

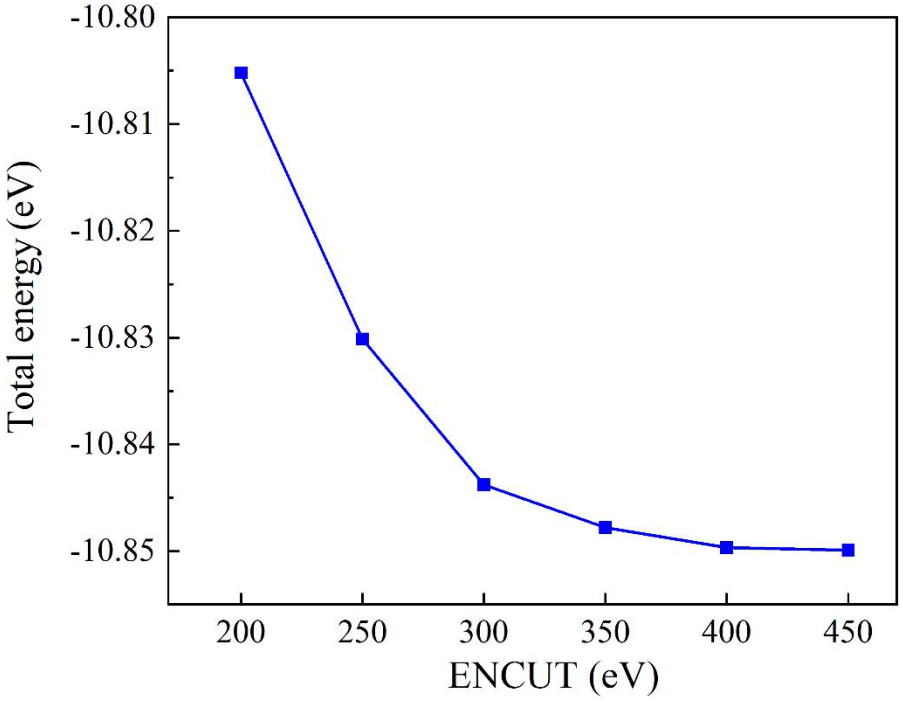


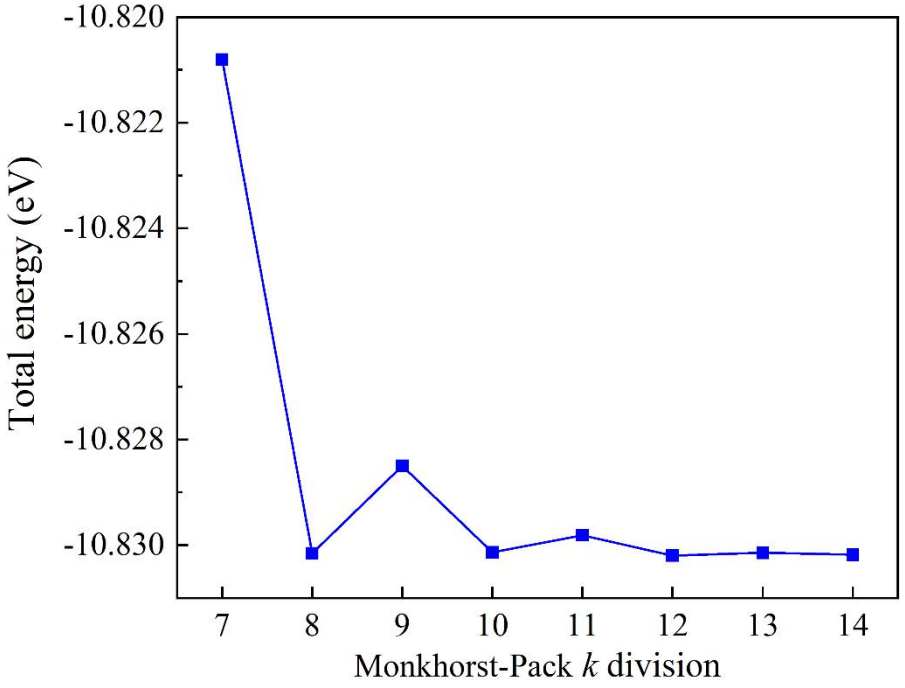
https://www.vasp.at/wiki/index.php/Cd_Si
https://www.vasp.at/wiki/index.php/Fcc_Si

(1) diamond & fcc Si

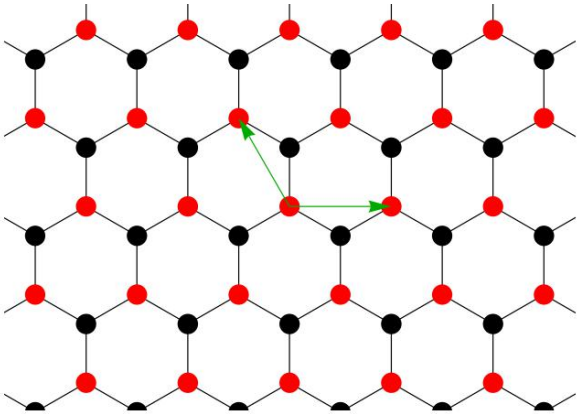
4. test: check settings of
   ① ENCUT
   ② KPOINTS & smearing methods (ISMEAR & SIGMA)

diamond Si (ISMEAR = 0 ; SIGMA = 0.05)

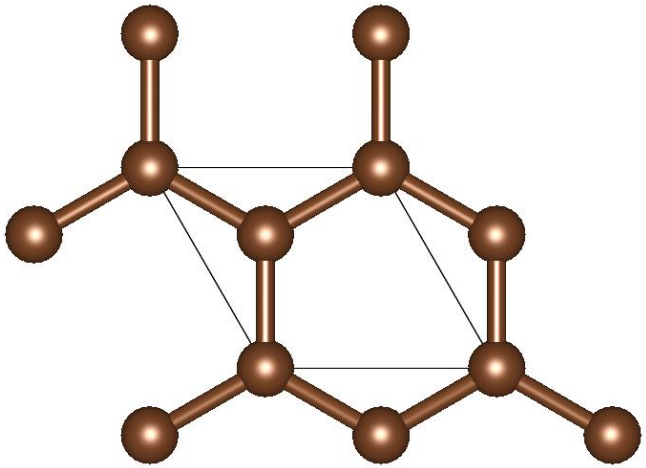




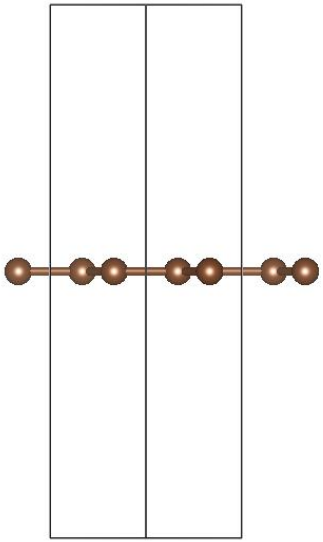
(2) Xene (graphene, …, stanene)



2D honeycomb lattice



ab-plane

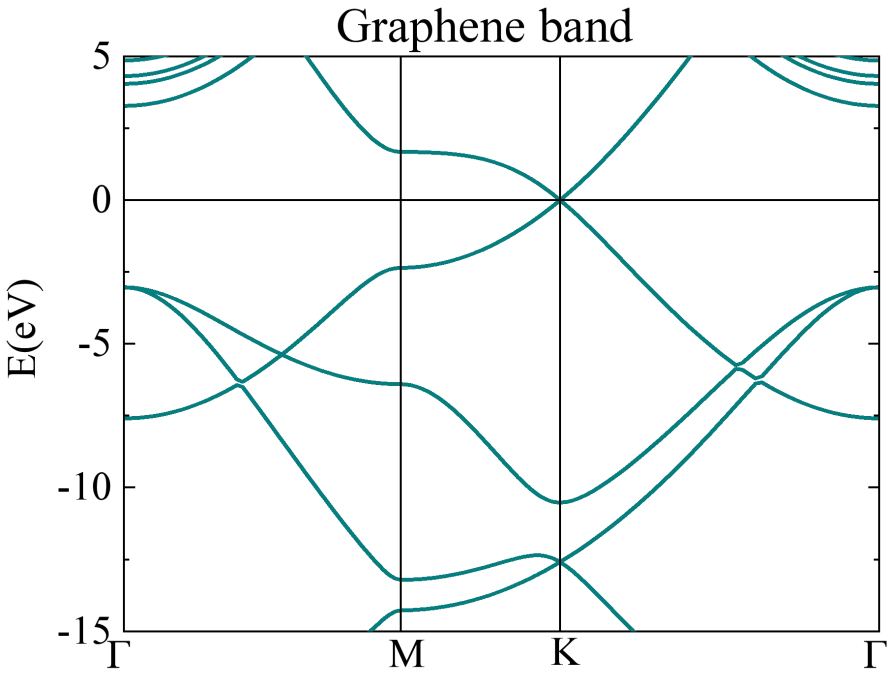


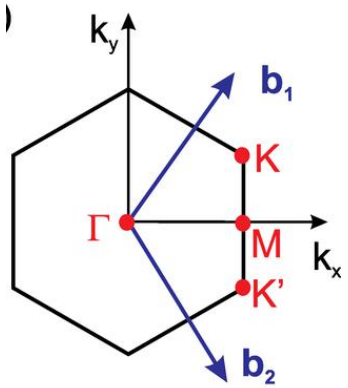
ac-plane

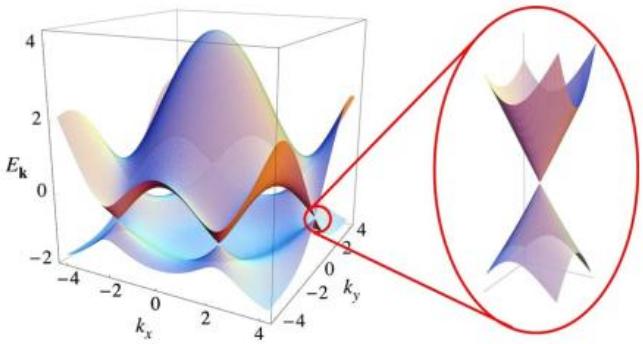
- Graphene

- check the setting of the thickness of the vacuum layer
- relax the lattice constant: ISIF = 4
- band projection LORBIT = 11

vaspkit -task 302







- Dirac point at K
- saddle point at M

Rev. Mod. Phys. **81**, 109 (2009)

✓ Strain engineering of Dirac points

- biaxial strain: keep all symmetries
- uniaxial strain: break C_{3z} symmetry

✓ multilayer graphene

- van der Waals interactions

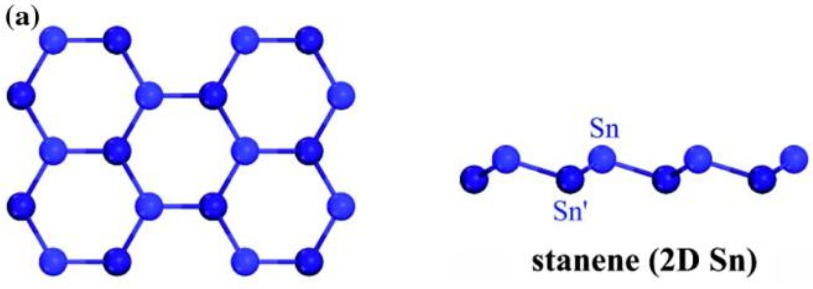
https://www.vasp.at/wiki/index.php/IVDW
https://www.vasp.at/wiki/index.php/Nonlocal_vdW-DF_functionals

- Interlayer stacking and effect of interlayer coupling

➢ Stanene

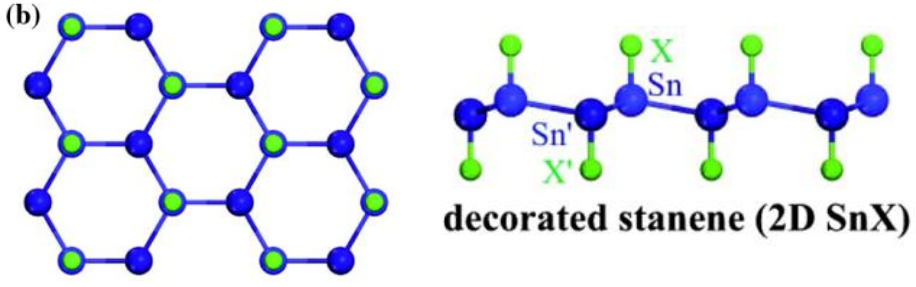
✓ 2D Sn

- structural buckling
- spin-orbit coupling (SOC) effect



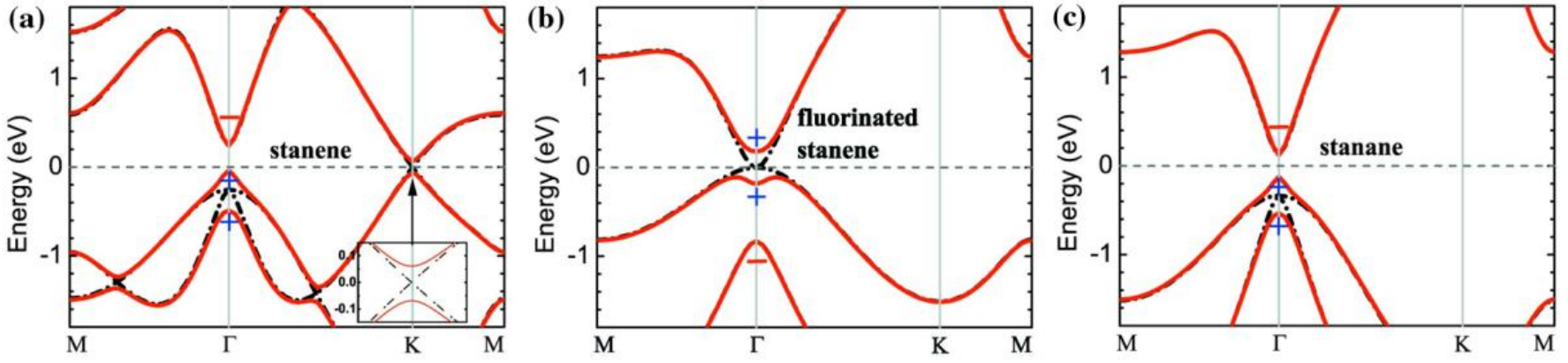

```
LSORBIT = .TRUE.
MAGMOM = 6*0
```

✓ Decorated stanene (SnX)

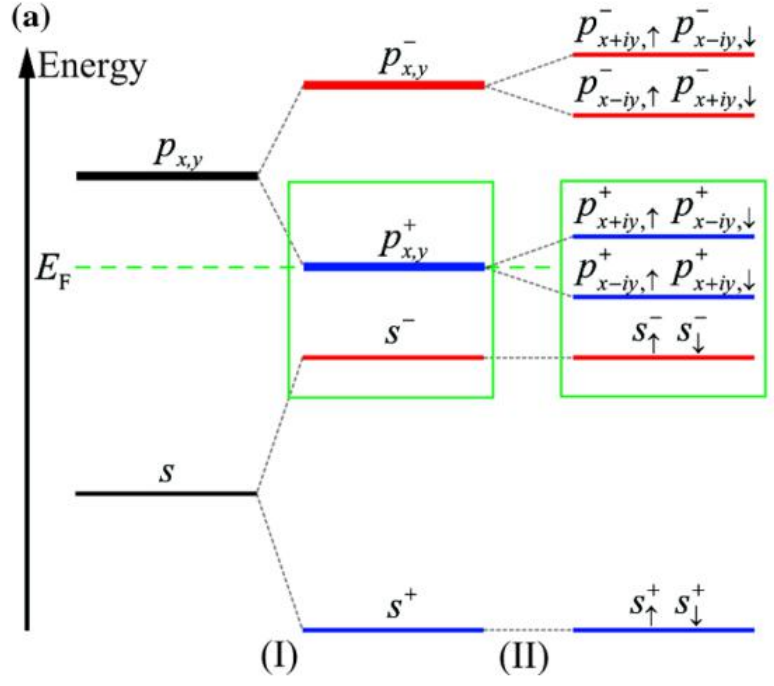


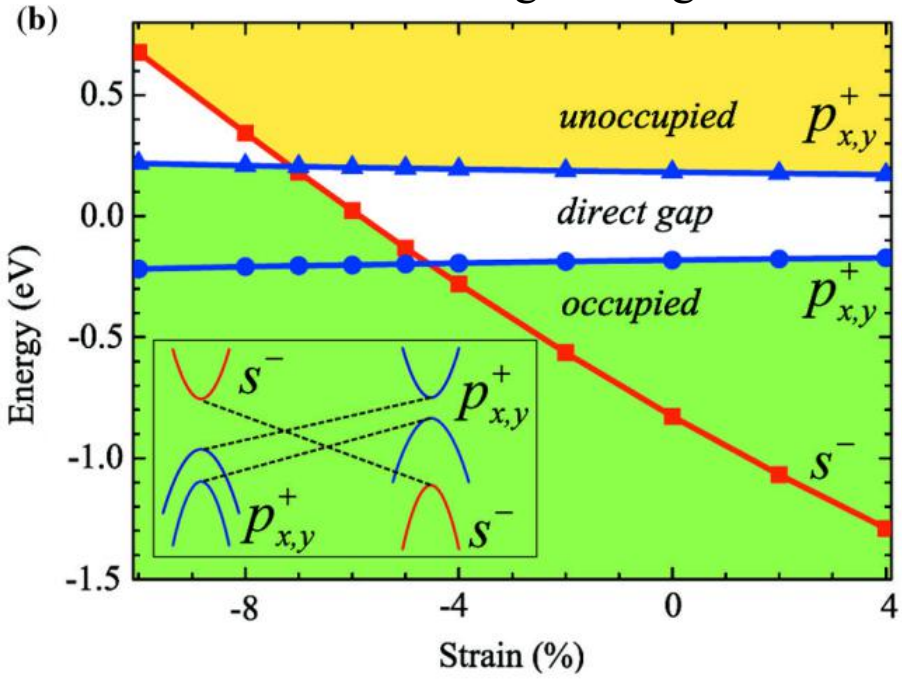
Y. Xu *et al*. PRL **111**, 136804 (2013).

✓ Topological properties of stanene: quantum spin Hall insulators



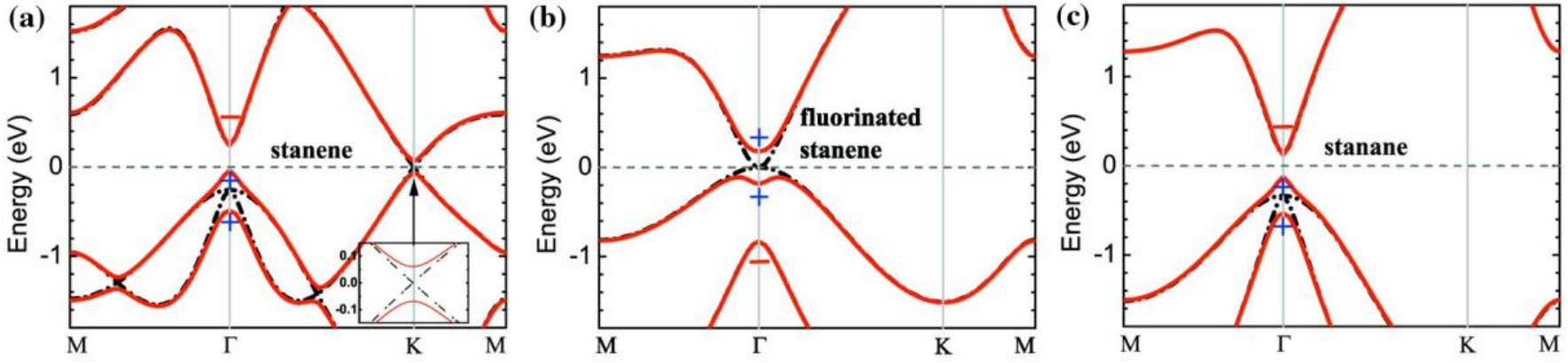
Strain engineering



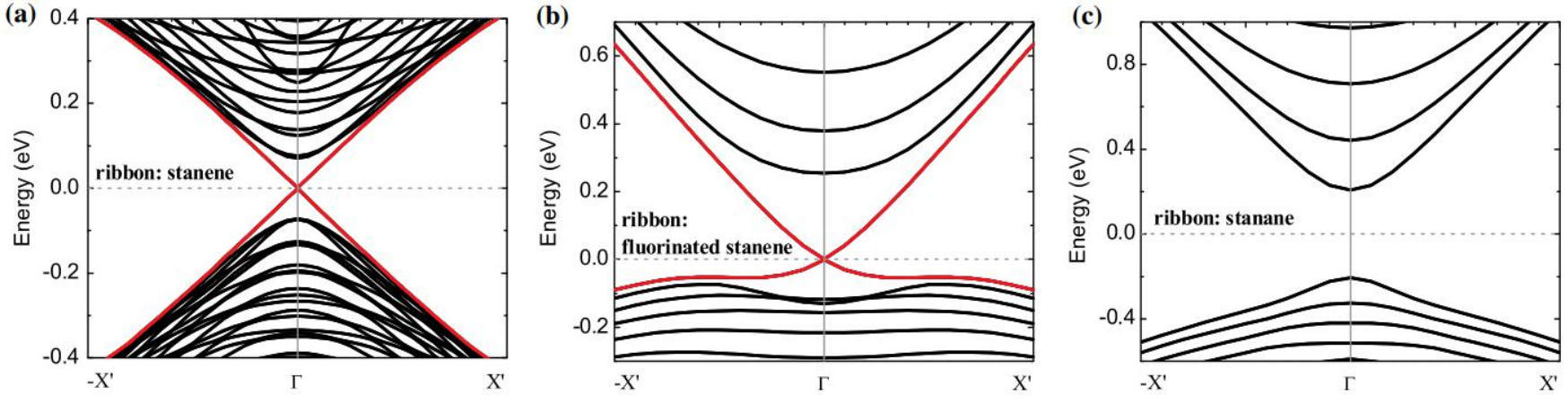


Y. Xu *et al*. PRL **111**, 136804 (2013).

✓ Topological properties of stanene: quantum spin Hall insulators



Sn SnF SnH



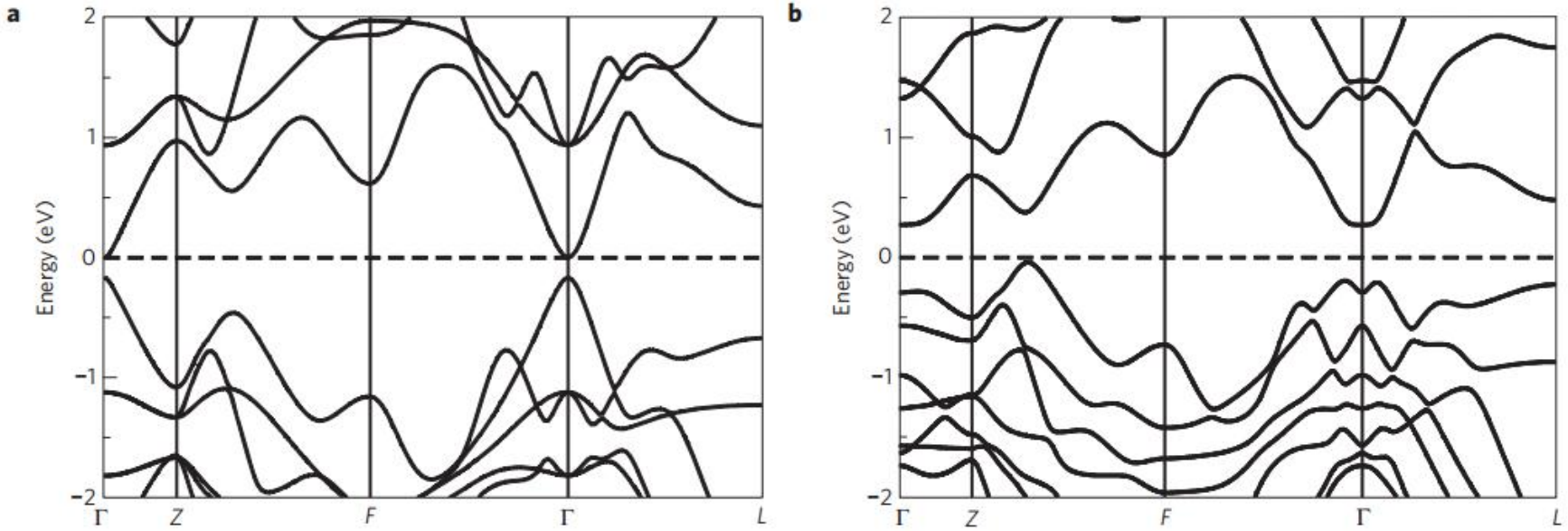
Y. Xu *et al*. PRL **111**, 136804 (2013).

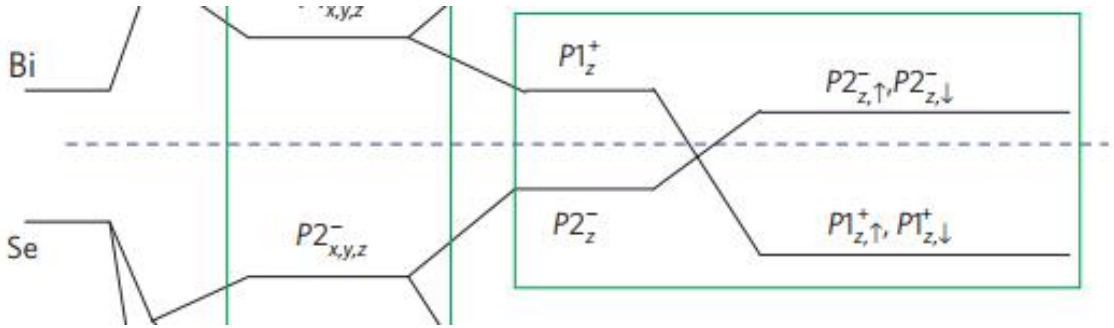
(3) Bi_2Se_3 family: 3D strong TI

✓ SOC induced band inversion

Without SOC

With SOC





Evolution of orbitals at Γ

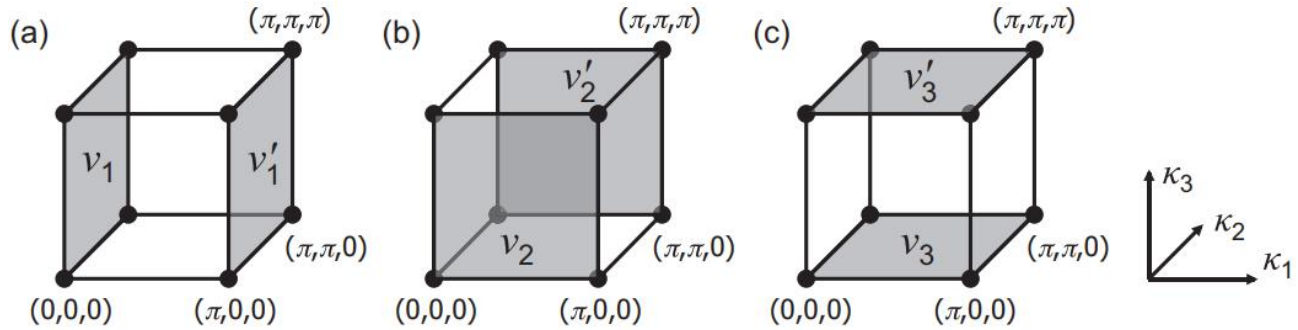
Nat. Phys. **5**, 438 (2009)

(3) Bi_2Se_3 family: 3D strong TI

✓ Z_2 invariant & topological surface states

With inversion symmetry: 2D: $(-1)^{\nu} = \prod_{a=1}^{4} \prod_{m}^{N_{occ}/2} \xi_{am}$

3D:



$$(-)^{\nu_0} = (-)^{\nu_1+\nu_1'} = (-)^{\nu_2+\nu_2'} = (-)^{\nu_3+\nu_3'}$$

$(\nu_0; \nu_1'\nu_2'\nu_3')$ ν_0 odd is known as a *strong TI*

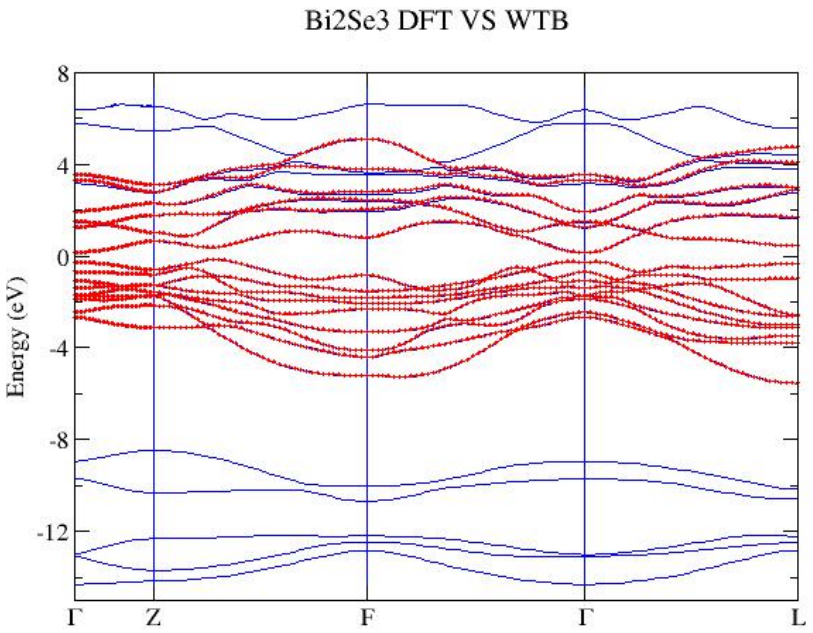
Berry phases in electronic structure theory, book by David Vanderbilt

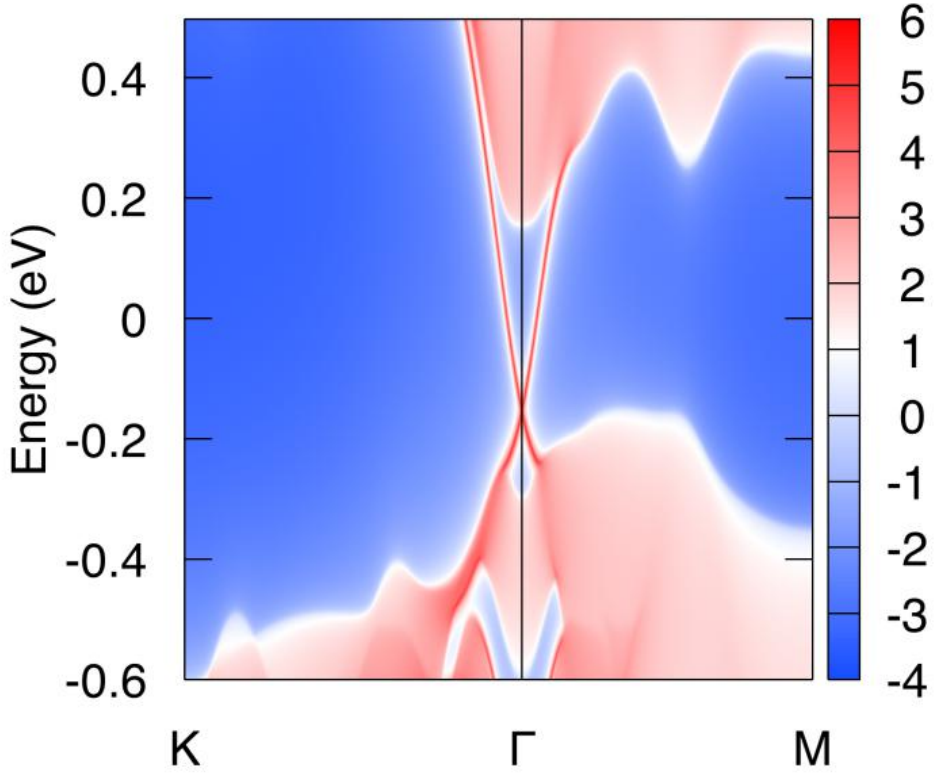
- calculate parity at TRIM using irvsp

(3) Bi_2Se_3 family: 3D strong TI

✓ Z_2 invariant & topological surface states

- calculate surface states using Wannier90 + WannierTools:





WannierTools教程之拓扑绝缘体---Bi2Se3

(4) $MnBi_2Te_4$ family: magnetic topological materials

➢ DFT study of magnetism

https://www.vasp.at/wiki/index.php/Magnetism_-_Tutorial

- spin-polarized calculation

AFM

```
ISPIN = 2
MAGMOM = 2.0 -2.0 2*0
```

FM

```
ISPIN = 2
MAGMOM = 2.0 2.0 2*0
```

- DFT+*U* method

```
LDAU = .TRUE.
LDAUTYPE = 2
LDAUL = 2 -1
LDAUU = 3.0 0.0
LDAUJ = 0.0 0.0
LDAUPRINT = 2
```

- Noncollinear magnetism

```
LNONCOLLINEAR = .TRUE.
MAGMOM = 1 0 0 0 1 0
```

- Effect of SOC: magnetocrystalline anisotropy

```
LSORBIT = .TRUE.
MAGMOM = 0 0 2 0 0 -2 6*0
SAXIS = 1.0 0.0 0.0
```

(4) $MnBi_2Te_4$ family: magnetic topological materials

➢ Tunable magnetic topological properties in $MnBi_2Te_4$

- interlayer magnetic coupling

- dimension /thickness

维度/厚度	层间磁序	
	反铁磁	铁磁
体相	反铁磁 拓扑绝缘体	磁性拓扑外尔半金属
奇数层薄膜	陈绝缘体	陈绝缘体
偶数层薄膜	轴子绝缘体	陈绝缘体

- magnetic orientation-dependent topological propreties

Sci. Adv. **5**, eaaw5685 (2019)
Phys. Rev. B **100**, 121103(R) (2019)

总结：计算流程

1.Relax步（非必选）

INCAR（重点检查IBRION, NSW, ISIF）

KPOINTS（Gamma/MP格式）

POTCAR（例：cat /pot_paw/PBE/B/POTCAR /pot_paw/PBE/N/POTCAR > POTCAR）

POSCAR（记住原子和POTCAR一一对应)

run.sh（修改前几行）然后qsub run.sh

如何检查relax步？

```
reached required accuracy - stopping structural energy minimisation
```

grep TOTEN OUTCAR |tail

在OUTCAR中寻找原子受力 (TOTAL-FORCE)

最后得到的弛豫完成的文件 CONTCAR

2.sc步

修改INCAR文件（重点检查 LCHARG, NSW, IBRION）

必要时修改KPOINTS

记住cp CONTCAR POSCAR

提取费米能用于后续绘制能带

3.Band 步

修改INCAR文件（重点检查ICHARG=11）

修改KPOINTS文件（查询晶体对称性vaspkit，确定高对称路径KPATH）

4.绘制能带

vaspkit -task 211

安装xftp或用sz命令，传文件到自己的电脑上， 画图!

5.报错怎么办?

报错有多种可能，报错信息写在output*以及*.o*, *.e* 中，自行翻译，有问题先想想，一般都能解决!

Appendix 辅助网站

(1) 材料数据库

https://mp.weixin.qq.com/s/gJJhMYKrRqHfbYyJI4mwhg

(2) 晶体对称性相关, BZ, 高对称路径

https://mp.weixin.qq.com/s/Ptnj_oDZl-_foaAPcp6imA

http://www.cryst.ehu.es/cgi-bin/cryst/programs/nph-kv-list

(3) 晶体结构建模相关: crystaltoolkit

https://crystaltoolkit.org/

(4) 其它学习资料

https://mp.weixin.qq.com/s/ZCgC5Rw3898Za_ejMF1xIw