中國科學院物理研究所
INSTITUTE OF PHYSICS CHINESE ACADEMY OF SCIENCE
SONGSHAN LAKE
MATERIALS LABORATORY
松山湖材料实验室
SF10

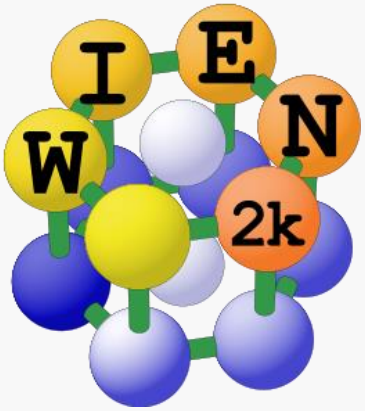
VASP 使用基础及上机实践

Speaker: 王恩

Date: 2019/07/23

1. VASP 介绍

第一性原理计算软件



PySCF, DMol3, Gaussian, Octopus …

https://en.wikipedia.org/wiki/List_of_quantum_chemistry_and_solid-state_physics_software

VASP (Vienna Ab initio Simulation Package)

The Vienna Ab initio Simulation Package (VASP) is a computer program for **atomic scale materials modelling**, e.g. electronic structure calculations and quantum-mechanical molecular dynamics, from **first principles**.

1989, Developed from CASTEP
Currently frequently used in solid-states physics and quantum chemistry

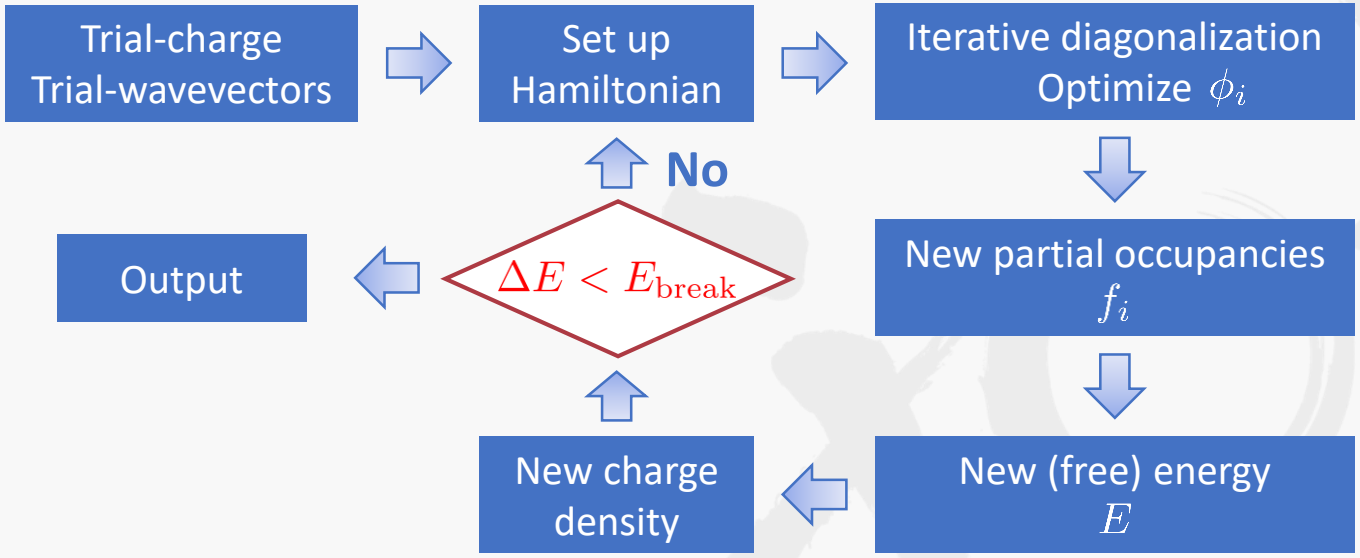
1. **Density Functional Theory**
2. **Plane wave basis set**
3. **Projector augmented wave method (PAW)**

https://www.vasp.at/index.php/about-vasp/59-about-vasp

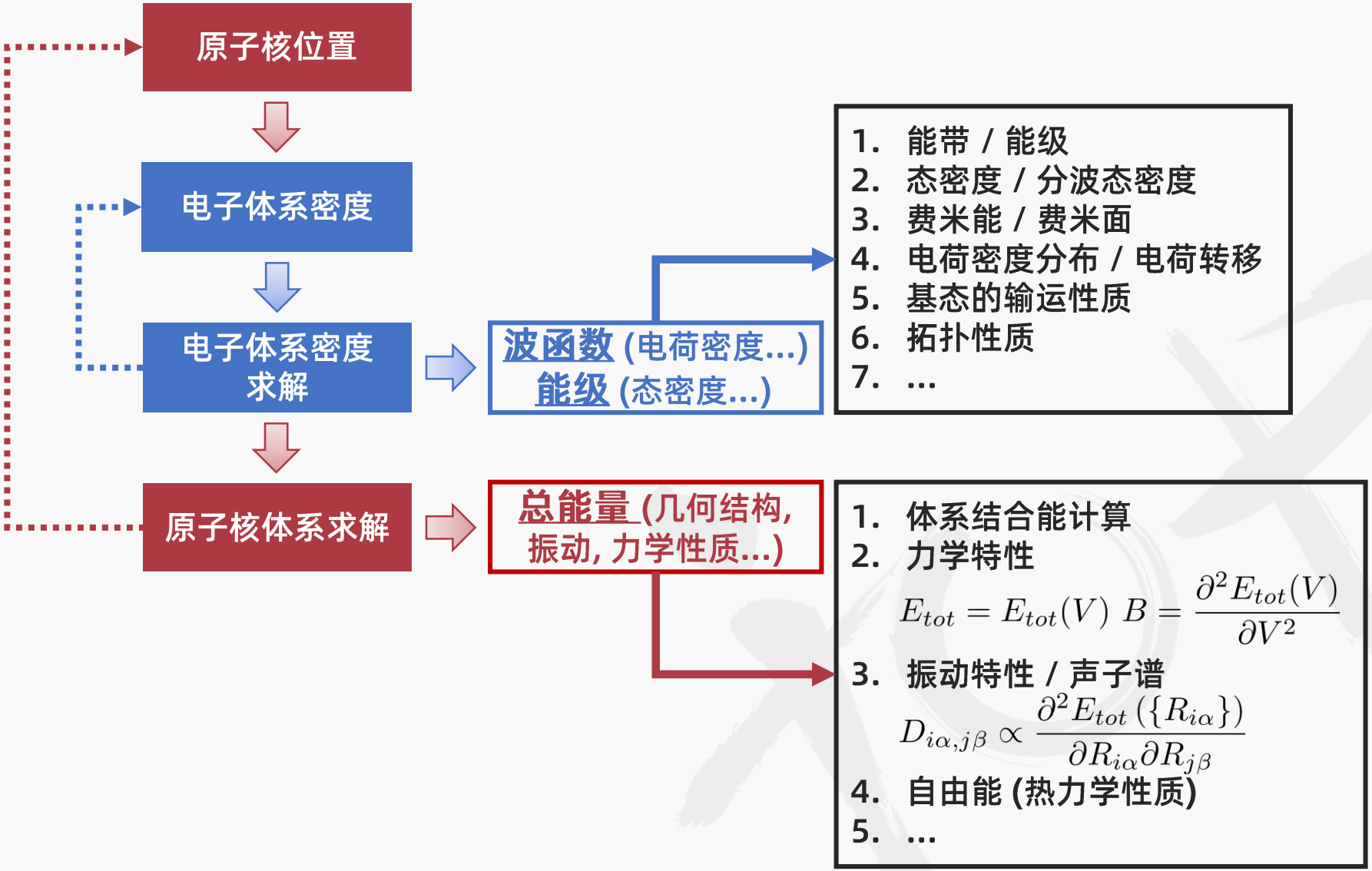
KS-ground-state 计算流程

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + v_{\text{ext}}(\mathbf{r}) + e^2\int\frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}' + \frac{\delta E_{\text{xc}}[\rho]}{\delta\rho(\mathbf{r})}\right)\phi_i(\mathbf{r}) = \varepsilon_i\phi_i(\mathbf{r})$$

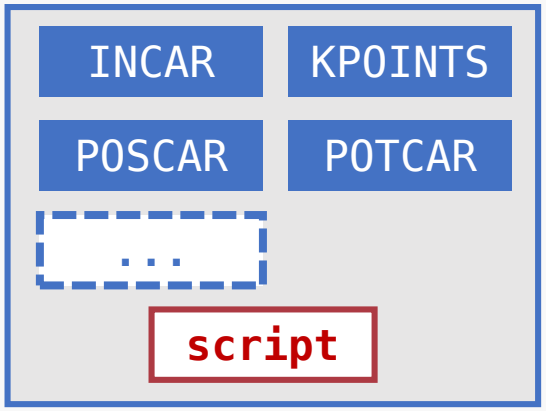
$$\rho(\mathbf{r}) = \sum_i^N |\phi_i(\mathbf{r})|^2 \qquad E = \sum_i^N \varepsilon_i - E_H[\rho] + E_{\text{xc}}[\rho] - \int\frac{\delta E_{\text{xc}}[\rho]}{\delta\rho(\mathbf{r})}\rho(\mathbf{r})d\mathbf{r}$$



求解 K-S 方程以及总能量的重要性



计算流程



1. INCAR
   1. 最为复杂
   2. 控制了「算什么, 怎么算」
2. KPOINTS
   1. 包含 K 点信息用于计算积分
   2. 能带路径
3. POSCAR
   1. 模型结构
   2. 包含原胞以及原子的坐标信息
4. POTCAR
   1. 赝势文件

https://cms.mpi.univie.ac.at/wiki/index.php/The_VASP_Manual

```
SYSTEM = WTe2

# Start parameter for this run:
  PREC   = High
  ISTART = 0
  ICHARG = 2
  LREAL  = .FALSE.

# Ionic Relaxation
#  IBRION = -1
#  ISIF   = 3
#  NSW    = 0
#  EDIFFG = -0.0001
#  POTIM  = 0.1

# Electronic Relaxation
  EDIFF  = 1.0E-06
  ENCUT  = 260 eV
  ALGO   = Fast
  NELMIN = 4
  NELM   = 200

# DOS related values
  ISMEAR = 0
  SIGMA  = 0.05
```

```
# Writing items
  LWAVE  = .FALSE.
  LCHARG = .TRUE.
  LVTOT  = .FALSE.

# Speed up parameters
#  NCORE  = 40
#  LPLANE = .TRUE.
#  LSCALU = .FALSE.
#  NSIM   = 4

# SOC
  LORBIT  = 11
  ISPIN   = 2
  MAGMOM  = 4*0 4*0 4*0 8*0 8*0 8*0
  LSORBIT = .TRUE.
  LMAXMIX = 4
  SAXIS   = 0 0 1
  NBANDS  = 120
  ISYM    = 0
  GGA_COMPAT = .FALSE.
  LORBMOM    = .TRUE.
```

https://cms.mpi.univie.ac.at/wiki/index.php/The_VASP_Manual

在 VASP 的计算过程中，实际上是在 k-空间 (动量空间) 中对 K-S 方程进行求解。(等价于采用平面波作为基底)

$$\sum_{\mathbf{G}'}\left(\frac{1}{2}\left|\mathbf{k}+\mathbf{G}'\right|^2\delta_{\mathbf{G}\mathbf{G}'}+V^{\mathrm{eff}}_{\mathbf{k}\mathbf{G}\mathbf{G}'}\right)\Phi_j\left(\mathbf{G}'\right)=\epsilon_j\Phi_j(\mathbf{G})$$

我们不可能把所有的 G’ 都考虑到，因此上述计算必须有一个截断。截断选取越大，计算越精确，更加消耗计算资源。

$$\phi_j(\mathbf{r})=\sum_{\mathbf{G}}\Phi_j\left(\mathbf{k}+\mathbf{G}\right)e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}$$

```
WTe2
   1.00000000000000
     3.4770    0.0000    0.0000
     0.0000    6.2490    0.0000
     0.0000    0.0000   14.0180
   W    Te
     4     8
Direct
  0.0000000000000000  0.595643170692812  0.5000000000000000
  0.5000000000000000  0.404244811428892  0.0000000000000000
  0.0000000000000000  0.044664776428891  0.0152200010000030
  0.5000000000000000  0.955223213692813  0.5152199770000010
  0.0000000000000000  0.852633176692814  0.6552499920000017
  0.5000000000000000  0.147254786428891  0.1552499579999989
  0.0000000000000000  0.651174767428894  0.1111200010000033
  0.5000000000000000  0.348713214692809  0.6111200010000033
  0.0000000000000000  0.303314777428891  0.8598300089999995
  0.5000000000000000  0.696573204692813  0.3598300089999995
  0.0000000000000000  0.202243209692812  0.4038699939999972
  0.5000000000000000  0.797644734428889  0.9038699939999972
```

Direct

$$\tilde{\mathbf{R}} = x_1\tilde{a}_1 + x_2\tilde{a}_2 + x_3\tilde{a}_3$$

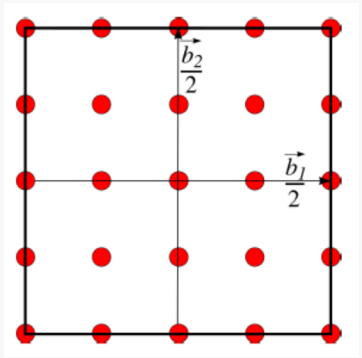
Cartesian

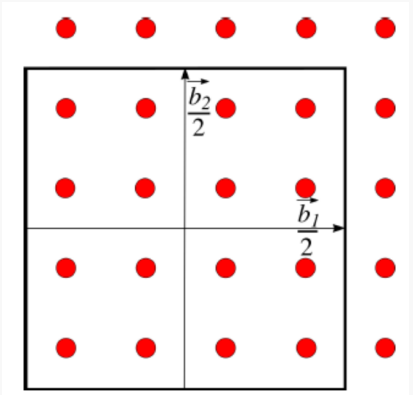
$$\tilde{\mathbf{R}} = s\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

https://cms.mpi.univie.ac.at/wiki/index.php/POSCAR

```
Automatic generation
0
Monhkorst-Pack
12   10   6
0.0  0.0  0.0
```

$$\tilde{k} = x_1\tilde{b}_1 + x_2\tilde{b}_2 + x_3\tilde{b}_3$$





Automatic k-mesh

$$\tilde{k} = \tilde{b}_1\frac{n_1}{N_1} + \tilde{b}_2\frac{n_2}{N_2} + \tilde{b}_3\frac{n_3}{N_3}$$

Gamma centered

$$\tilde{k} = \tilde{b}_1\frac{n_1 + 1/2}{N_1} + \tilde{b}_2\frac{n_2 + 1/2}{N_2} + \tilde{b}_3\frac{n_3 + 1/2}{N_3}$$

K-抽样

$$n(\mathbf{r}) = \frac{1}{N_k}\sum_{\mathbf{k},i}^{occ} n_{i,\mathbf{k}}(\mathbf{r})$$

需要将积分离散化处理

$$\frac{1}{\Omega_{BZ}}\int_{BZ} d\vec{k} f_i(\vec{k}) \Rightarrow \frac{1}{N_k}\sum_{\vec{k}} f_i(\vec{k})$$

https://cms.mpi.univie.ac.at/wiki/index.php/KPOINTS

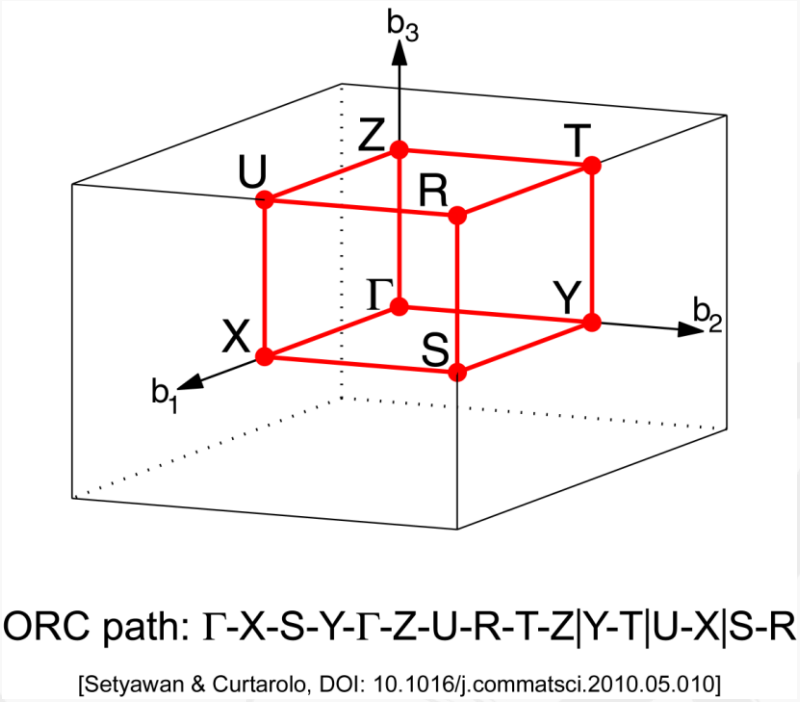
```
WTe2
50   ! 50 grids
Line-mode
reciprocal
   0.0000   0.0000   0.0000   ! Gamma
   0.0000   0.5000   0.0000   ! Y

   0.0000   0.5000   0.0000   ! Y
   0.5000   0.5000   0.0000   ! S

   0.5000   0.5000   0.0000   ! S
   0.5000   0.0000   0.0000   ! X

   0.5000   0.0000   0.0000   ! X
   0.0000   0.0000   0.0000   ! Gamma

   0.0000   0.0000   0.0000   ! Gamma
   0.0000   0.0000   0.5000   ! Z
```

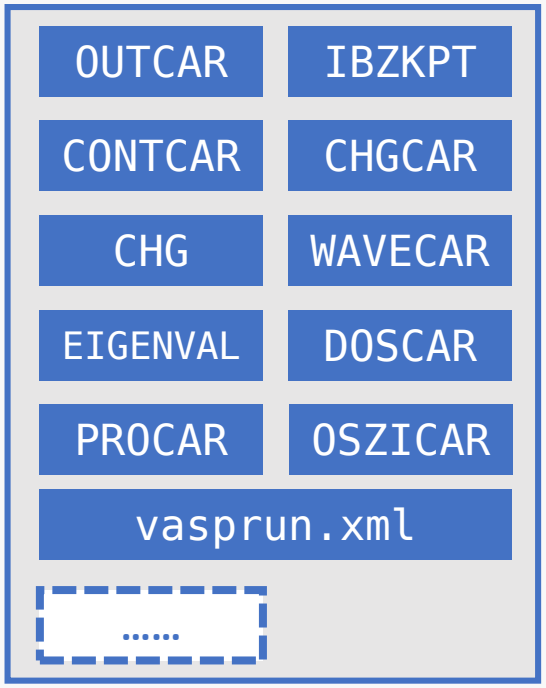


ORC path: Γ-X-S-Y-Γ-Z-U-R-T-Z|Y-T|U-X|S-R

[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]

https://cms.mpi.univie.ac.at/wiki/index.php/KPOINTS
https://en.wikipedia.org/wiki/Brillouin_zone

输出文件



1. OSZICAR
   1. 关于收敛速度的信息
2. OUTCAR
   1. 主要输出文件
   2. 包含每一步计算细节
3. vasprun.xml
   1. 以 xml 格式保存的输出文件
   2. 基于这个进行进一步的处理
4. CHGCAR/CHG
   1. 电荷密度
   2. 还有诸如 PARCHG, PROCHG
5. WAVECAR
6. EIGENVAL
7. ……

https://cms.mpi.univie.ac.at/wiki/index.php/The_VASP_Manual

```
running on   36 total cores
distrk:  each k-point on   36 cores,    1 groups
distr:  one band on    1 cores,   36 groups
using from now: INCAR
vasp.5.4.1 05Feb16 (build Apr 16 2019 13:49:49) complex

POSCAR found type information on POSCAR  Si
POSCAR found :  1 types and       2 ions
scaLAPACK will be used

 -----------------------------------------------------------------------------
|                                                                             |
|           W    W    AA    RRRRR   N    N  II  N    N   GGGG   !!!          |
|           W    W   A  A   R    R  NN   N  II  NN   N  G    G  !!!          |
|           W    W  A    A  R    R  N N  N  II  N N  N  G       !!!          |
|           W WW W  AAAAAA  RRRRR   N  N N  II  N  N N  G  GGG   !           |
|           WW  WW  A    A  R   R   N   NN  II  N   NN  G    G                |
|           W    W  A    A  R    R  N    N  II  N    N   GGGG   !!!          |
|                                                                             |
|      For optimal performance we recommend to set                            |
|        NCORE= 4 - approx SQRT( number of cores)                             |
|      NCORE specifies how many cores store one orbital (NPAR=cpu/NCORE).     |
|      This setting can  greatly improve the performance of VASP for DFT.     |
|      The default, NPAR=number of cores might be grossly inefficient         |
|      on modern multi-core architectures or massively parallel machines.     |
|      Do your own testing !!!!                                               |
|      Unfortunately you need to use the default for GW and RPA calculations. |
|      (for HF NCORE is supported but not extensively tested yet)             |
|                                                                             |
 -----------------------------------------------------------------------------

LDA part: xc-table for Pade appr. of Perdew
POSCAR, INCAR and KPOINTS ok, starting setup
WARNING: small aliasing (wrap around) errors must be expected
FFT: planning ...
WAVECAR not read
entering main loop
      N       E                     dE             d eps       ncg     rms          rms(c)
DAV:   1    -0.783658338415E+01   -0.78366E+01   -0.28159E+03 28584   0.127E+02
DAV:   2    -0.107787138244E+02   -0.29421E+01   -0.29376E+01 39708   0.119E+01
DAV:   3    -0.107812122938E+02   -0.24985E-02   -0.24984E-02 26496   0.408E-01
DAV:   4    -0.107812134979E+02   -0.12041E-05   -0.12044E-05 51480   0.865E-03
DAV:   5    -0.107812134982E+02   -0.30587E-09   -0.14769E-11 26568   0.706E-06    0.298E+00
DAV:   6    -0.106605343453E+02    0.12068E+00   -0.81721E-02 39924   0.335E-01    0.175E+00
DAV:   7    -0.106060806802E+02    0.54454E-01   -0.14312E-01 42228   0.470E-01    0.157E-01
DAV:   8    -0.106070970134E+02   -0.10163E-02   -0.23873E-03 35280   0.780E-02    0.264E-02
DAV:   9    -0.106071950600E+02   -0.98047E-04   -0.72605E-05 45720   0.161E-02
   1 F= -.10607195E+02 E0= -.10606766E+02  d E =-.106072E+02
```

OSZICAR

IOP, CAS

```
      N       E                     dE             d eps       ncg     rms          rms(c)
DAV:   1    -0.783658338415E+01   -0.78366E+01   -0.28159E+03 28584   0.127E+02
DAV:   2    -0.107787138244E+02   -0.29421E+01   -0.29376E+01 39708   0.119E+01
DAV:   3    -0.107812122938E+02   -0.24985E-02   -0.24984E-02 26496   0.408E-01
DAV:   4    -0.107812134979E+02   -0.12041E-05   -0.12044E-05 51480   0.865E-03
DAV:   5    -0.107812134982E+02   -0.30587E-09   -0.14769E-11 26568   0.706E-06    0.298E+00
DAV:   6    -0.106605343453E+02    0.12068E+00   -0.81721E-02 39924   0.335E-01    0.175E+00
DAV:   7    -0.106060806802E+02    0.54454E-01   -0.14312E-01 42228   0.470E-01    0.157E-01
DAV:   8    -0.106070970134E+02   -0.10163E-02   -0.23873E-03 35280   0.780E-02    0.264E-02
DAV:   9    -0.106071950600E+02   -0.98047E-04   -0.72605E-05 45720   0.161E-02
   1 F= -.10607195E+02 E0= -.10606766E+02  d E =-.106072E+02
      N       E                     dE             d eps       ncg     rms          rms(c)
DAV:   1    -0.108088048239E+02   -0.20171E+00   -0.40261E+00 26424   0.277E+00    0.499E-01
DAV:   2    -0.108077991090E+02    0.10057E-02   -0.13136E-02 33408   0.287E-01    0.294E-01
DAV:   3    -0.108073160668E+02    0.48304E-03   -0.33572E-03 43488   0.822E-02    0.387E-02
DAV:   4    -0.108073087793E+02    0.72875E-05   -0.11941E-04 32760   0.185E-02
   2 F= -.10807309E+02 E0= -.10807249E+02  d E =-.200114E+00
      N       E                     dE             d eps       ncg     rms          rms(c)
DAV:   1    -0.108318292908E+02   -0.24513E-01   -0.99303E-01 26424   0.137E+00    0.239E-01
DAV:   2    -0.108318071683E+02    0.22123E-04   -0.31379E-03 32976   0.140E-01    0.143E-01
DAV:   3    -0.108317677206E+02    0.39448E-04   -0.62480E-04 44676   0.355E-02
   3 F= -.10831768E+02 E0= -.10831764E+02  d E =-.224573E+00
      N       E                     dE             d eps       ncg     rms          rms(c)
DAV:   1    -0.108461782908E+02   -0.14371E-01   -0.32774E-01 26532   0.788E-01    0.137E-01
DAV:   2    -0.108461689488E+02    0.93420E-05   -0.10083E-03 32724   0.809E-02    0.823E-02
DAV:   3    -0.108461544627E+02    0.14486E-04   -0.20180E-04 45216   0.202E-02
   4 F= -.10846154E+02 E0= -.10846154E+02  d E =-.143867E-01
      N       E                     dE             d eps       ncg     rms          rms(c)
DAV:   1    -0.108474886190E+02   -0.13197E-02   -0.59630E-02 27216   0.336E-01    0.589E-02
DAV:   2    -0.108474879599E+02    0.65911E-06   -0.17674E-04 32616   0.338E-02
   5 F= -.10847488E+02 E0= -.10847488E+02  d E =-.157202E-01
```

```
vasp.5.4.1 05Feb16 (build Apr 16 2019 13:49:49) complex

executed on           IFC91_ompi date 2019.07.21  17:08:26
running on   36 total cores
distrk:  each k-point on   36 cores,    1 groups
distr:  one band on NCORES_PER_BAND=   1 cores,   36 groups
```

```
→ 21:27:55 enwang@login2 ~/diamondSi/5-2_diamondSi_relax_select cat OUTCAR | grep 'fermi'
   ISMEAR =     0;   SIGMA  =   0.10  broadening in eV -4-tet -1-fermi 0-gaus
 E-fermi :   6.1067     XC(G=0):  -9.3420     alpha+bet :-11.7364
 E-fermi :   6.0986     XC(G=0):  -9.3305     alpha+bet :-11.7364
 E-fermi :   6.0315     XC(G=0):  -9.3294     alpha+bet :-11.7364
 E-fermi :   5.9628     XC(G=0):  -9.3290     alpha+bet :-11.7364
 E-fermi :   5.9484     XC(G=0):  -9.3290     alpha+bet :-11.7364
```

```
<structure name="finalpos" >
 <crystal>
  <varray name="basis" >
   <v>       0.00000000       2.73400000       2.73400000 </v>
   <v>       2.73400000       0.00000000       2.73400000 </v>
   <v>       2.73400000       2.73400000       0.00000000 </v>
  </varray>
  <i name="volume">     40.87196581 </i>
  <varray name="rec_basis" >
   <v>      -0.18288222       0.18288222       0.18288222 </v>
   <v>       0.18288222      -0.18288222       0.18288222 </v>
   <v>       0.18288222       0.18288222      -0.18288222 </v>
  </varray>
 </crystal>
 <varray name="positions" >
  <v>       0.00000000       0.00000000       0.00000000 </v>
  <v>       0.25070655       0.25070655       0.24719722 </v>
 </varray>
 <varray name="selective"  type="logical" >
  <v type="logical" >  F  F  F </v>
  <v type="logical" >  T  T  T </v>
```

CHGCAR

IOP, CAS

```
diamond Si
   5.46800000000000
     0.000000    0.500000    0.500000
     0.500000    0.000000    0.500000
     0.500000    0.500000    0.000000
   Si
     2
Direct
  0.000000  0.000000  0.000000
  0.250707  0.250707  0.247197

   36   36   36
 -.75104562538E+01 -.60941966784E+01 -.22283260366E+01 0.30821564078E+01 0.85681370110E+01
 0.13102897043E+02 0.15995266134E+02 0.17091152929E+02 0.16698263854E+02 0.15400066785E+02
 0.13803751840E+02 0.12205084943E+02 0.10735705389E+02 0.94755169266E+01 0.84579751852E+01
 0.76859148403E+01 0.71484955459E+01 0.68323973482E+01 0.67275665560E+01 0.68303039105E+01
 0.71444571661E+01 0.76802726885E+01 0.84512039397E+01 0.94680775083E+01 0.10727972428E+02
 0.12197373312E+02 0.13796253841E+02 0.15392671674E+02 0.16690660026E+02 0.17083388450E+02
 0.15988044438E+02 0.13097218988E+02 0.85645433110E+01 0.30803619951E+01 -.22290562710E+01
 -.60944471832E+01 -.60941966784E+01 -.32640858693E+01 0.16106008357E+01 0.72695757717E+01
 0.12427080702E+02 0.16155099972E+02 0.18068019830E+02 0.18300194420E+02 0.17345312865E+02
 0.15836792026E+02 0.14224921153E+02 0.12675332861E+02 0.11289455494E+02 0.10123918517E+02
 0.91996774218E+01 0.85167288049E+01 0.80674016648E+01 0.78442212341E+01 0.78429719398E+01
 0.80636018620E+01 0.85104781094E+01 0.91915177690E+01 0.10114556506E+02 0.11279288889E+02
 0.12664498267E+02 0.14213664580E+02 0.15825385199E+02 0.17333573335E+02 0.18287716404E+02
 0.18055068234E+02 0.16142890050E+02 0.12416890091E+02 0.72617350692E+01 0.16047165390E+01
 -.32680600912E+01 -.60956565929E+01 -.22283260366E+01 0.16106008357E+01 0.67958624582E+01
 0.12022060982E+02 0.16197839637E+02 0.18722785361E+02 0.19536996057E+02 0.19000070294E+02
```

2. VASP 计算实例

0_diamond_a	晶格常数测试.
1_diamondSi_encut	截断能测试.
2_diamondSi_kpoint	k-网格密度测试.
3_diamondSi_sigma	sigma 参数测试.
4_diamondSi_vol_rex	利用 VASP 内置算法优化晶格常数.
5-1_diamondSi_relax	利用 VASP 内置算法优化原子位置.
5-2_diamondSi_relax_select	利用 VASP 内置算法优化原子位置.
6_diamondSi_self_c	自洽计算, 为后续能带和态密度计算准备电荷密度文件.
7-1_diamondSi_band	Si 能带计算.
7-2_diamondSi_dos	Si 态密度计算.

3. 使用 Materials Project