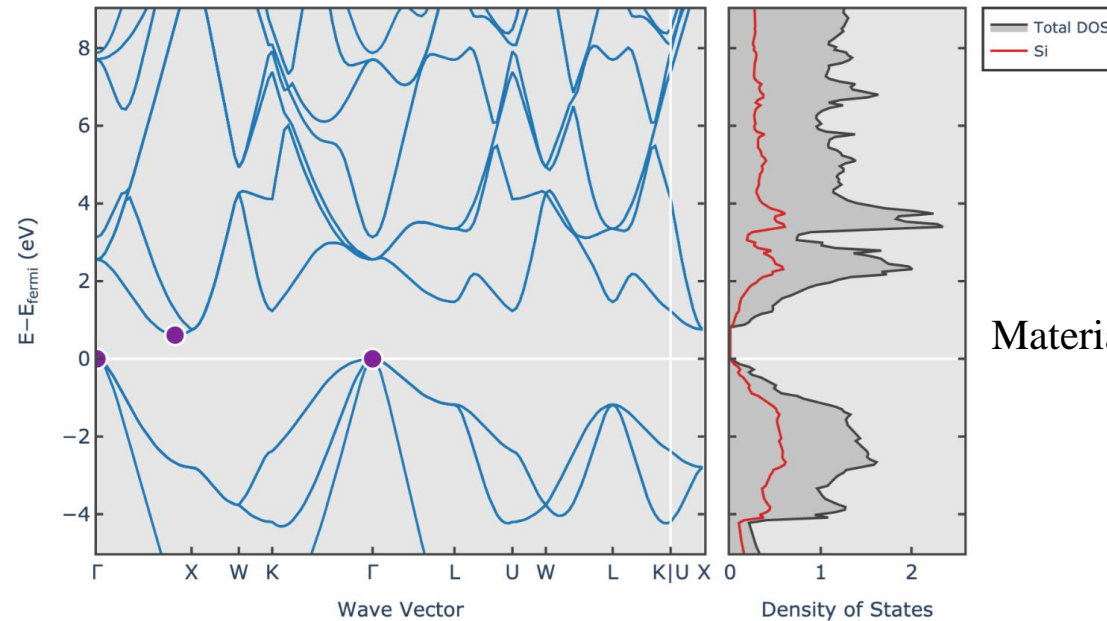


能带结构与态密度计算

Band structure and Density of states

在第一性原理计算中。**能带结构** (band structure) 与**态密度** (density of states, DOS) 是其中**最为常见且具有互补性**的两类表征方法，它们分别强调电子**能量色散关系** $E(k)$ 与电子**能量分布统计** $\rho(E)$ 。

能带和倒空间的k矢量有关，DOS只是和能量相关，两者相互关联



Material Project 中Si的能带和DOS图

态密度计算

态密度计算 (Density of states)

$$\rho(E) = \frac{1}{N_k} \sum_{i,\mathbf{k}} \delta(\varepsilon_{i,\mathbf{k}} - E) = \frac{\Omega_{\text{cell}}}{(2\pi)^d} \int_{\text{BZ}} d\mathbf{k} \delta(\varepsilon_{i,\mathbf{k}} - E)$$

定义： 态密度表示每单位能量和每单位体积中包含的电子状态数
 $\rho(E)dE$ 表示单位体积中能量处于 **$E+dE$ 之间的电子态的数目**

需在布里渊区对波矢 \mathbf{k} 做积分（离散求和），对 \mathbf{k} 点网格有收敛性要求

重要参数：ISMear

SIGMA

NEDOS

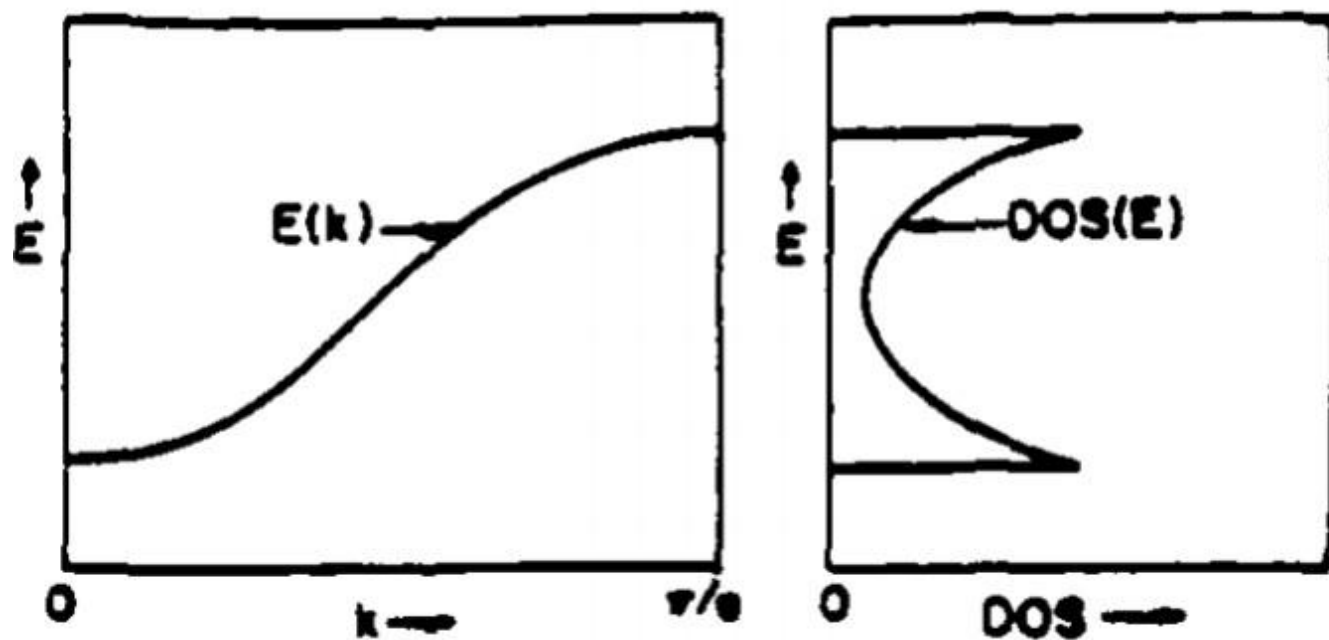
KPOINTS

展宽方法

展宽宽度

DOS的能量点数

足够密的 \mathbf{k} 点

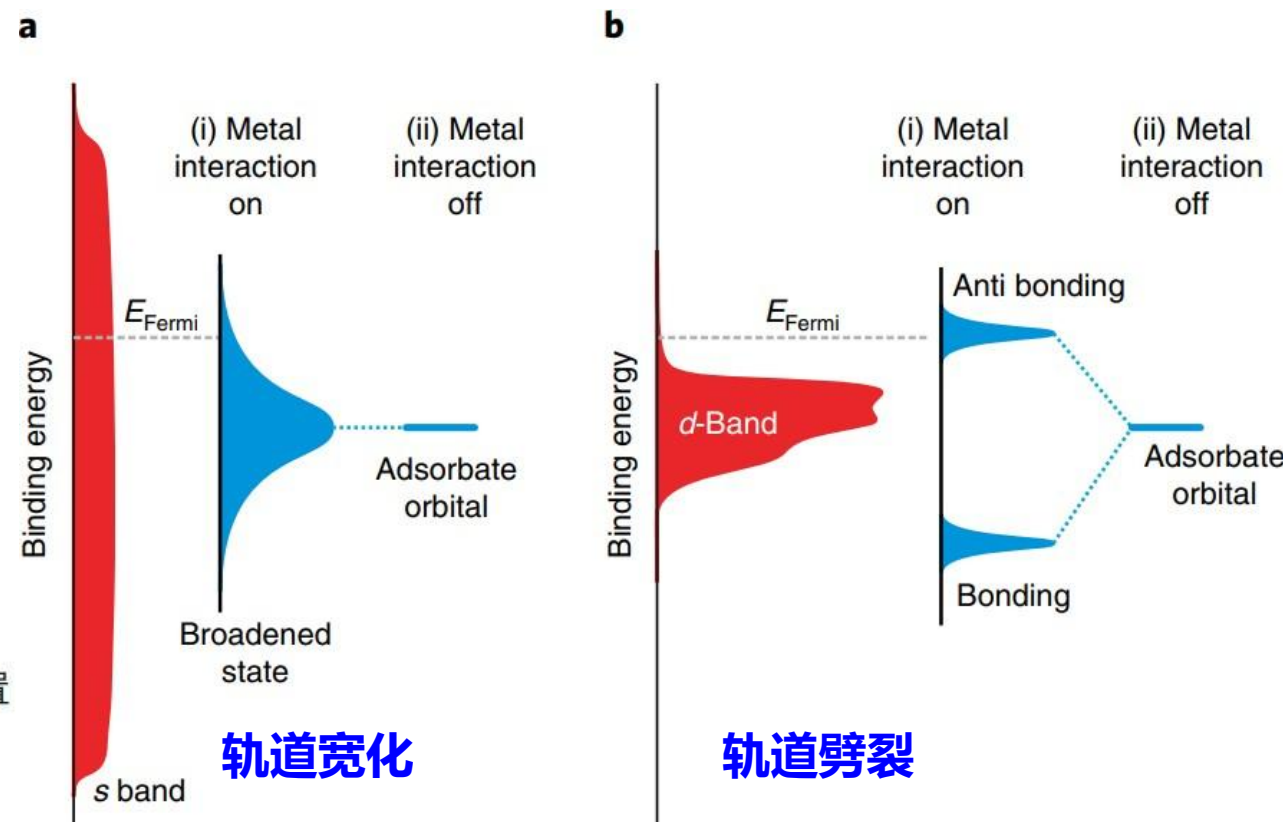
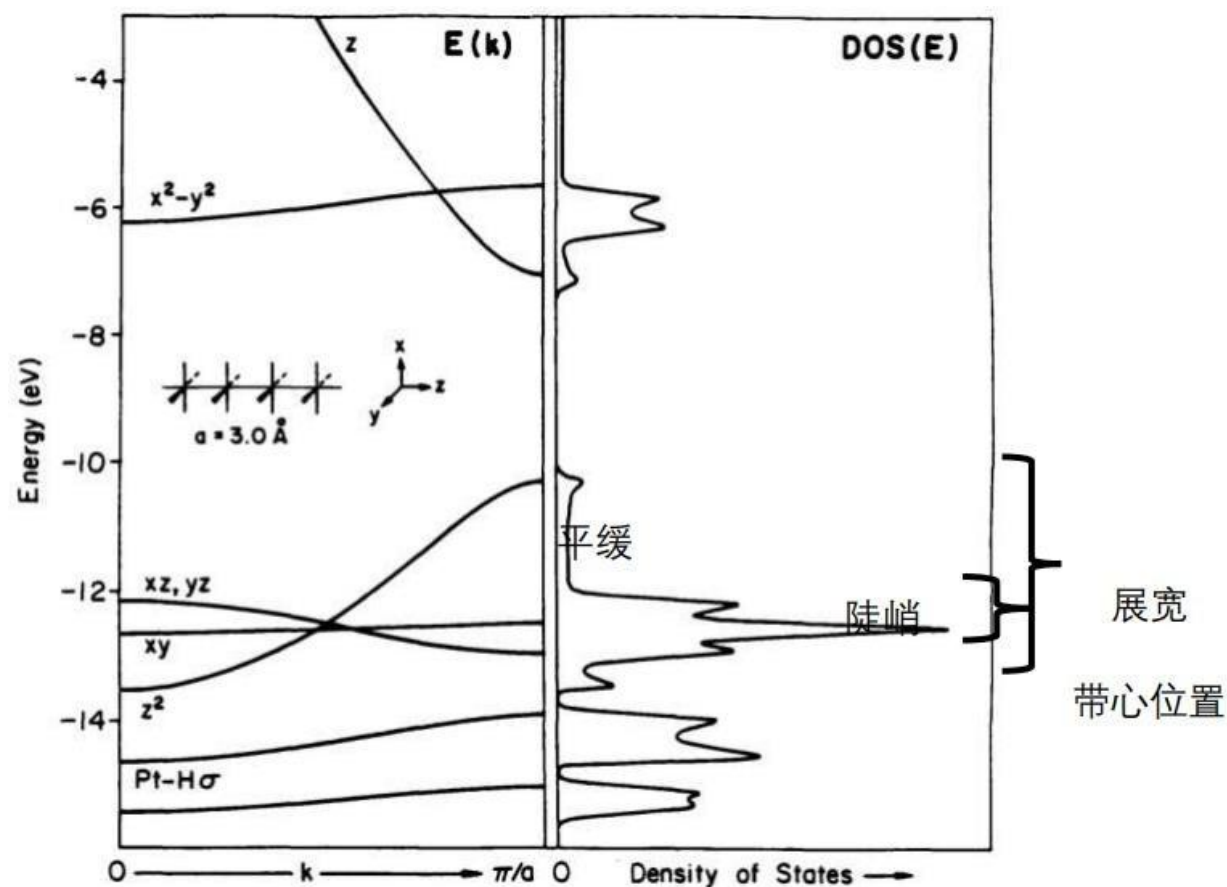


(对能带中的K进行积分 在E上进行投影 DOS)

1. 一般来说能带越密集/平缓的地方，单位能量范围内态越多，所以DOS也越大，能带越稀疏/陡峭的地方态密度就越小。
2. 对DOS积分就能得到电子数目，比如上图只有一条能带，上面占据了两个电子，那么对应的DOS图的积分也会是2，代表这个能量范围里的态上有两个电子。 所以DOS的展宽/位置就成了影响体系性质的关键因素

例子——判断电子局域和离域: PtH₄一维分子链

s d轨道和吸附物相互作用

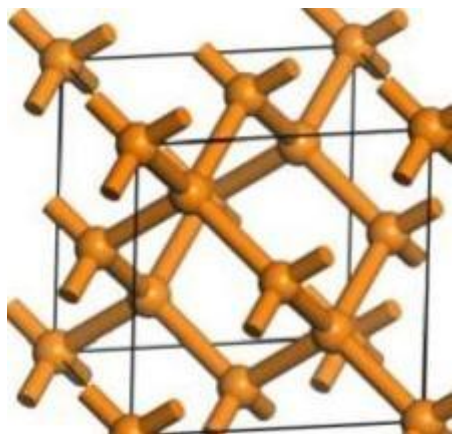


Nature Chemistry | VOL 10 | OCTOBER 2018 | 1008–1015

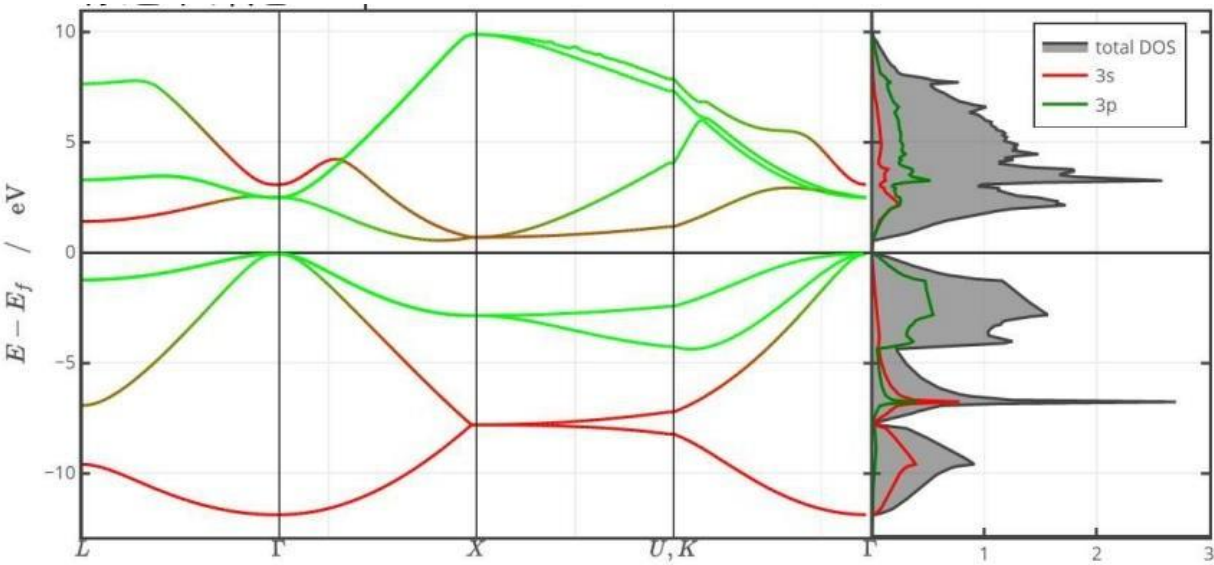
1. 根据DOS的展宽就能判断原子轨道之间的作用强弱程度，带心位置能影响体系和其他分子的相互作用。
2. 比如 dz^2 轨道，能带比较宽，dos能量跨度比较大，轨道离域，相互作用强
3. 比如 dxy dxz 轨道，能带接近于平带，dos峰尖锐，轨道较局域，作用比较弱

案例——DOS的轨道贡献

程序会把 E_{fermi} 对齐到0 eV的位置，所以纵坐标是 $E-E_f$

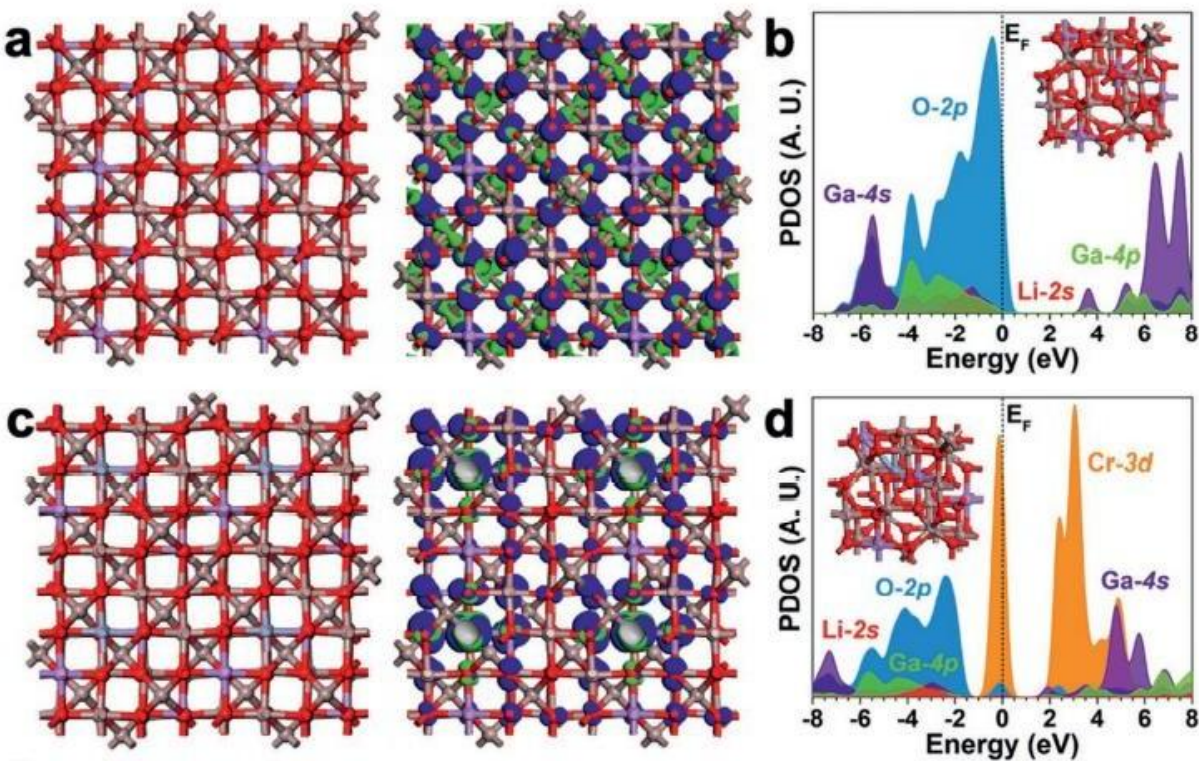


Bulk Si



3s轨道贡献比较小

LiGa₅O₈

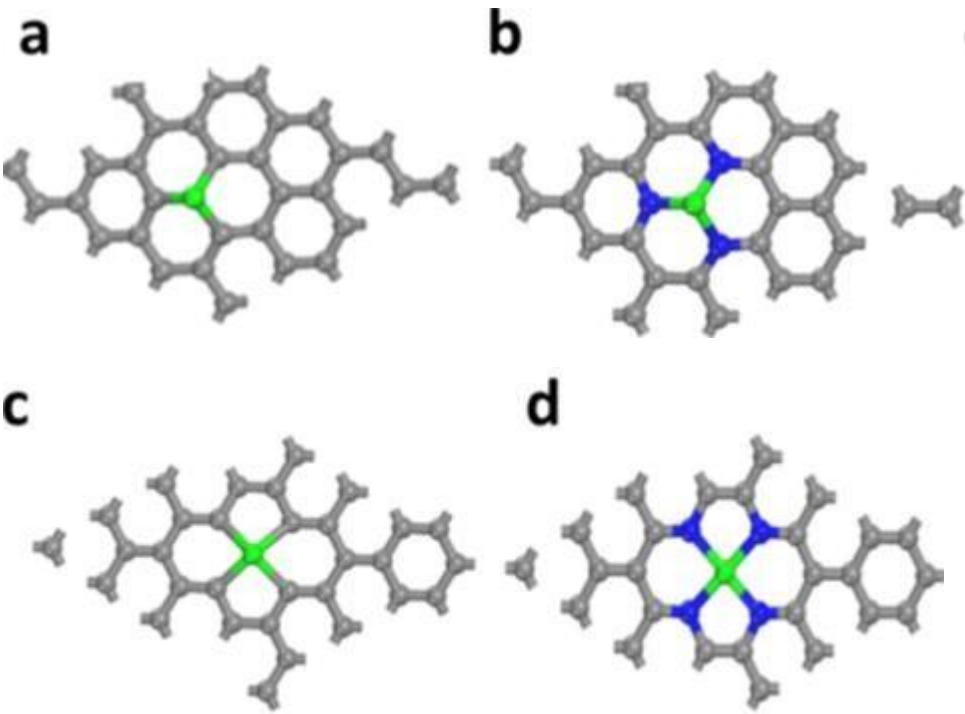
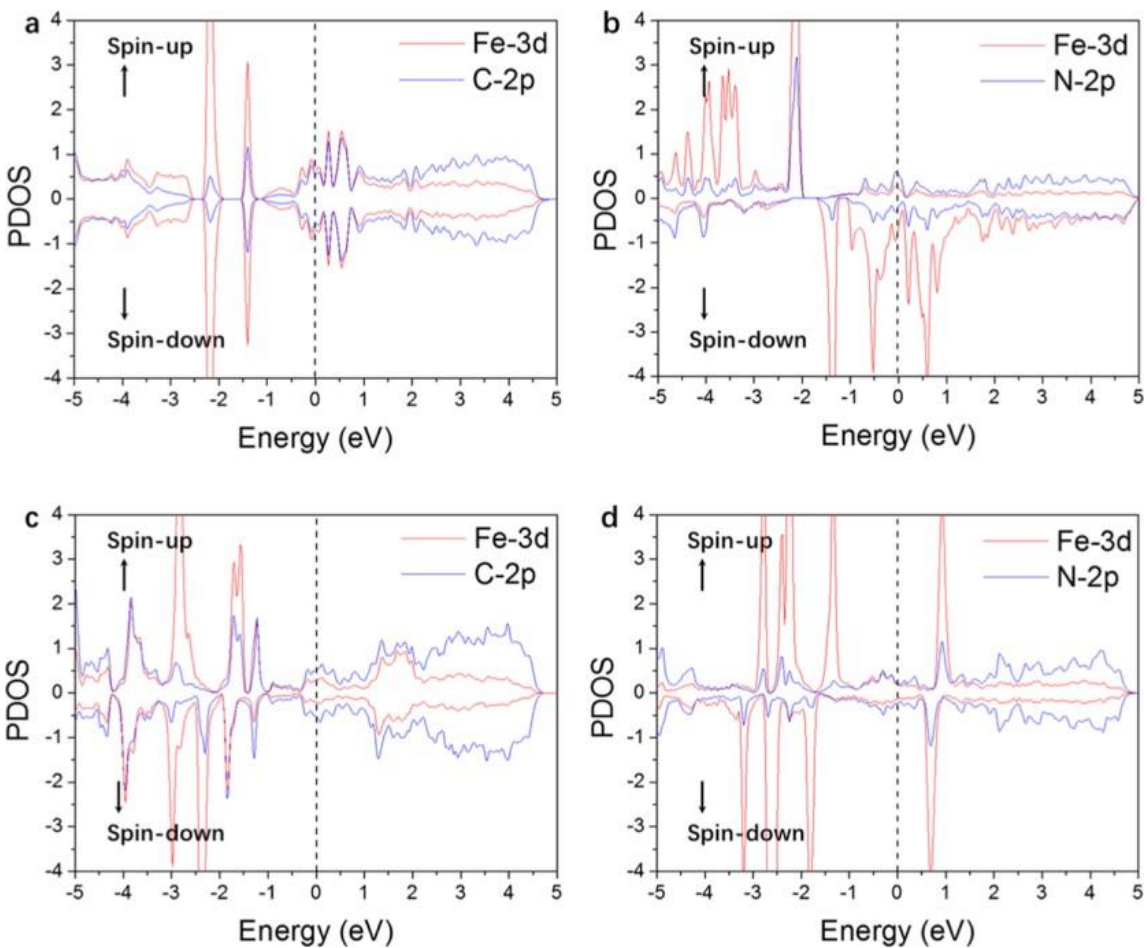


LiGa₅O₈:Cr

Adv. Funct. Mater. 2021, 31, 2010685

不同原子不同轨道对总态密度的贡献

案例——不同自旋电子的态密度



单铁原子 (Fe) 负载在缺陷石墨烯上 (N掺杂或不掺杂)

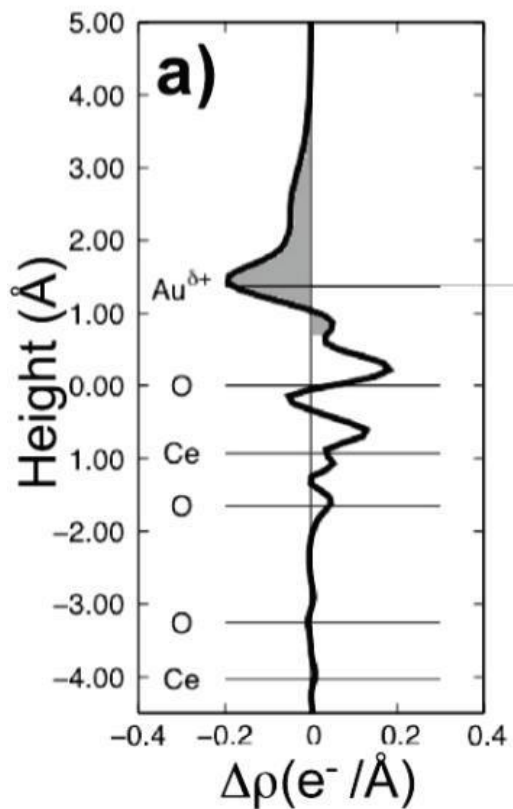
DOS上下自旋对称则无磁矩，不对称则有净磁矩

案例——研究相互作用模型 (1)

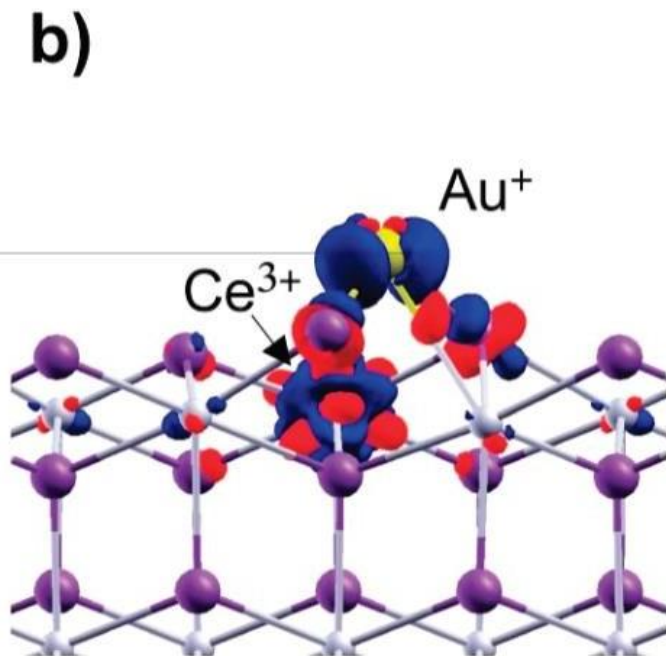
Au@bridge

Ce 4f¹ 5d¹ 6s²
Au 6s¹

Ce的4f空
轨道

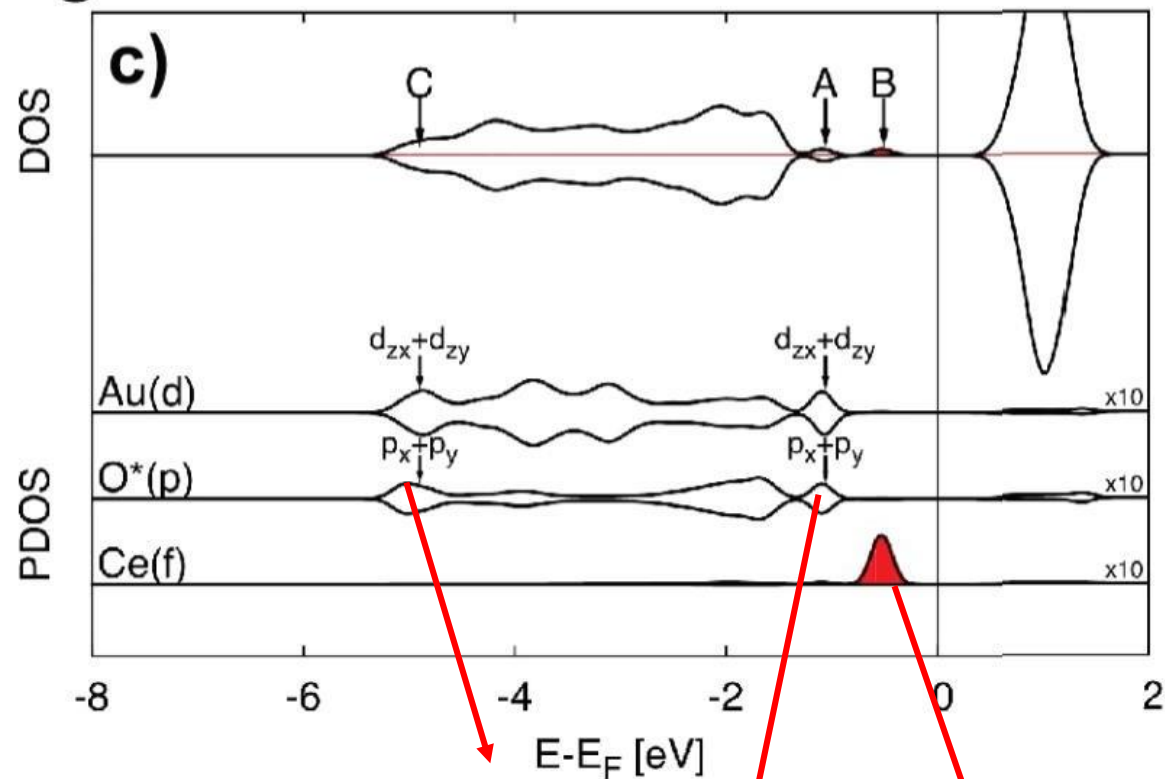


差分电荷密度



金原子在CeO₂(111)表面上催化CO氧化

判断离子键看孤立的峰
判断共价键看重叠的峰



O-Au轨道重叠作用比较大,
共价键

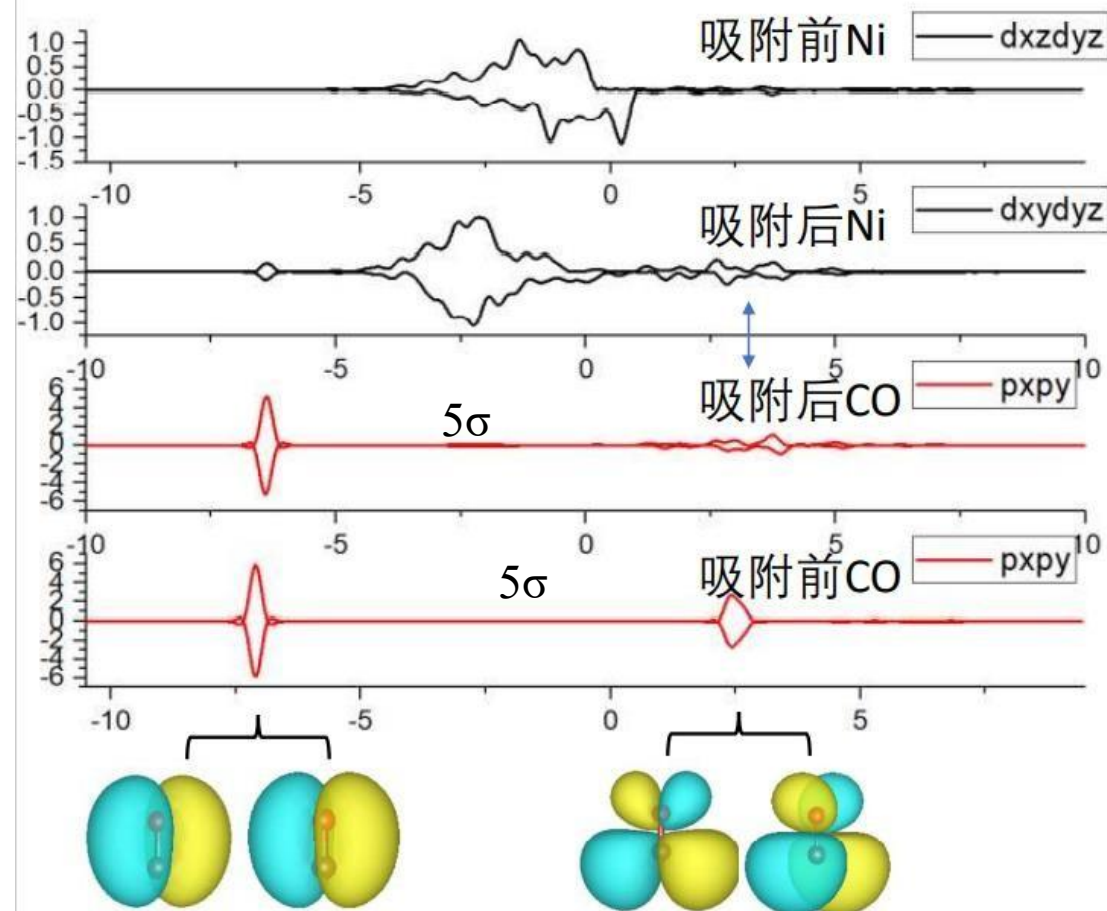
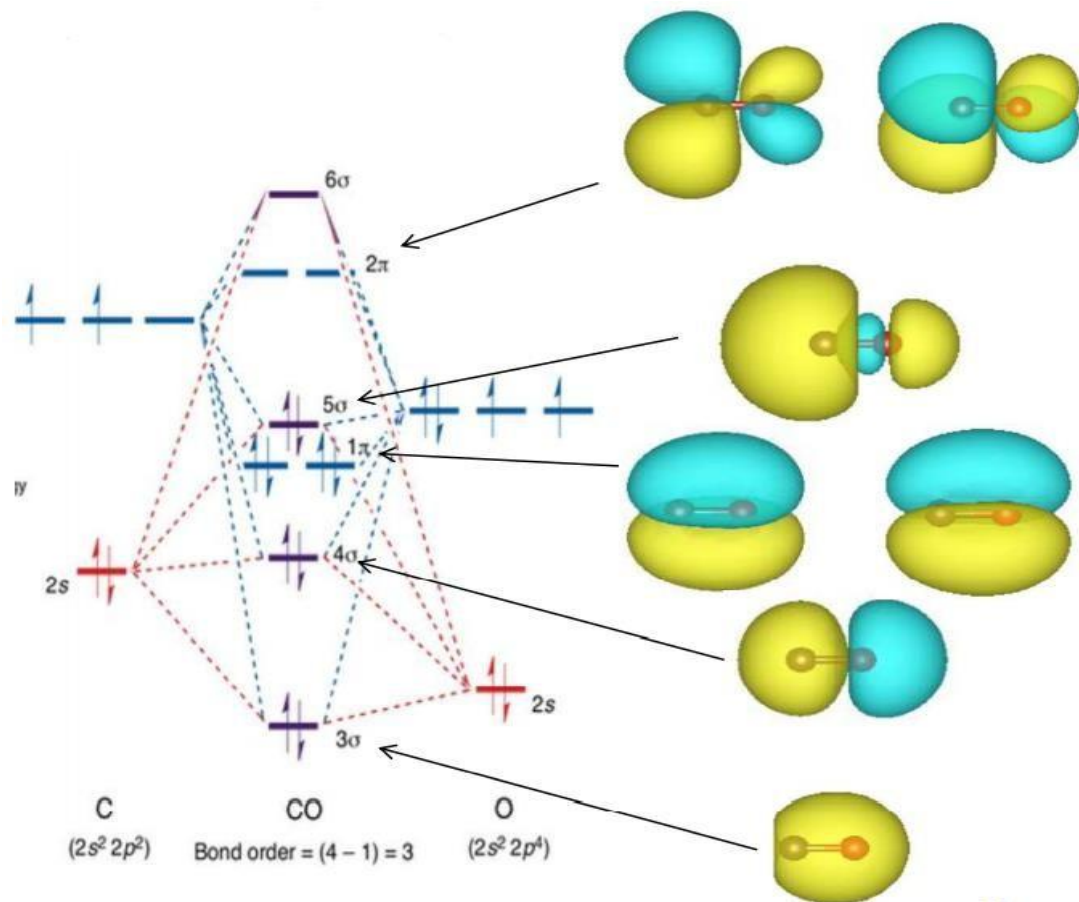
Ce 4f占据一个局
域电子 (电子转移),
Ce⁴⁺ → Ce³⁺

说明Au向CeO₂转移电子, 形成Au⁺和Ce³⁺

J. Am. Chem. Soc. 2009, 131, 10473-10483

案例——研究相互作用模型 (2)

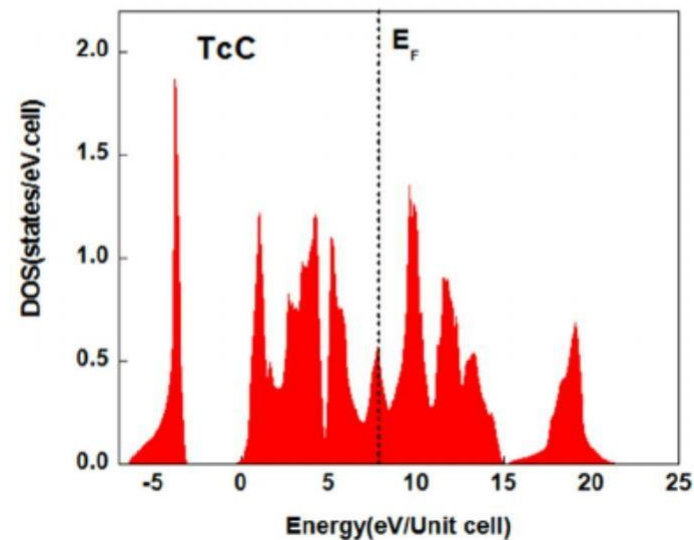
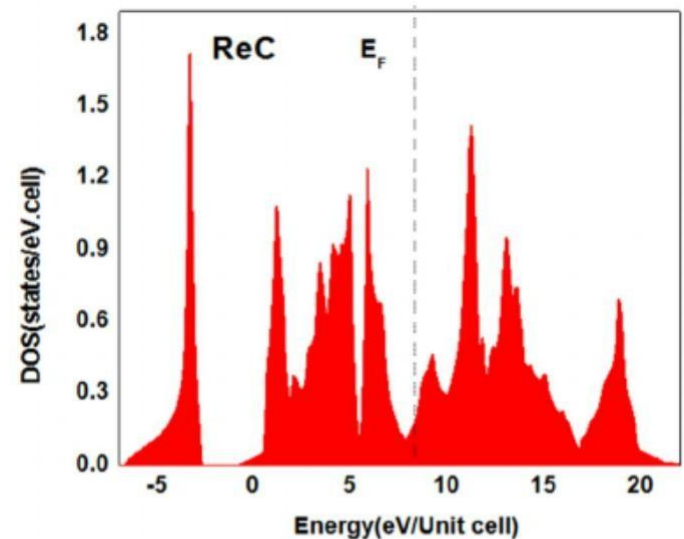
CBM VBM 周期性体系
HOMO LUMO分子体系



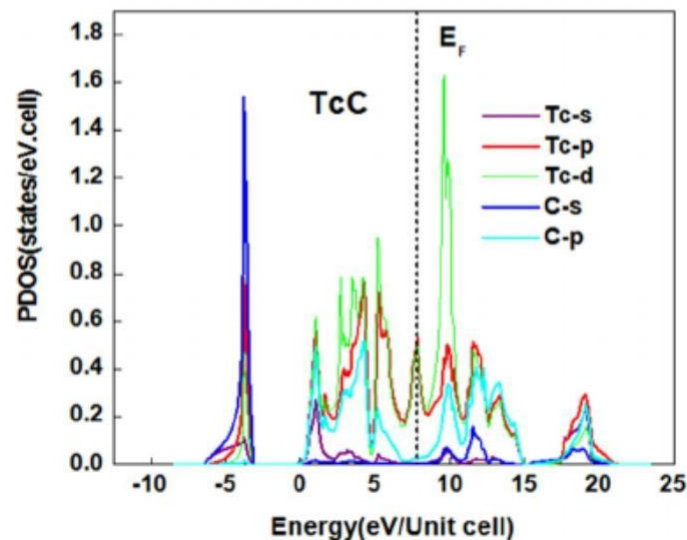
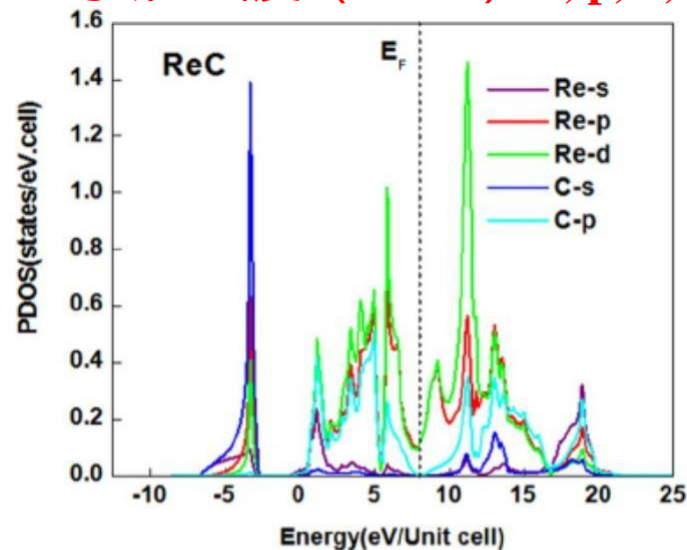
5σ 和 $2\pi^*$ 轨道, 与Ni的d带发生杂化, 形成了 5σ 成键和 Ni- $2\pi^*$ 反键。CO 的 5σ 轨道上的电子转移至Ni的d轨道, 使 5σ 轨道发生左移, Ni的d轨道上的电子转移到CO的 $2\pi^*$ 轨道, 使 $2\pi^*$ 轨道发生分裂, 部分进入成键轨道

Density of states计算 (fermi能级未归0)

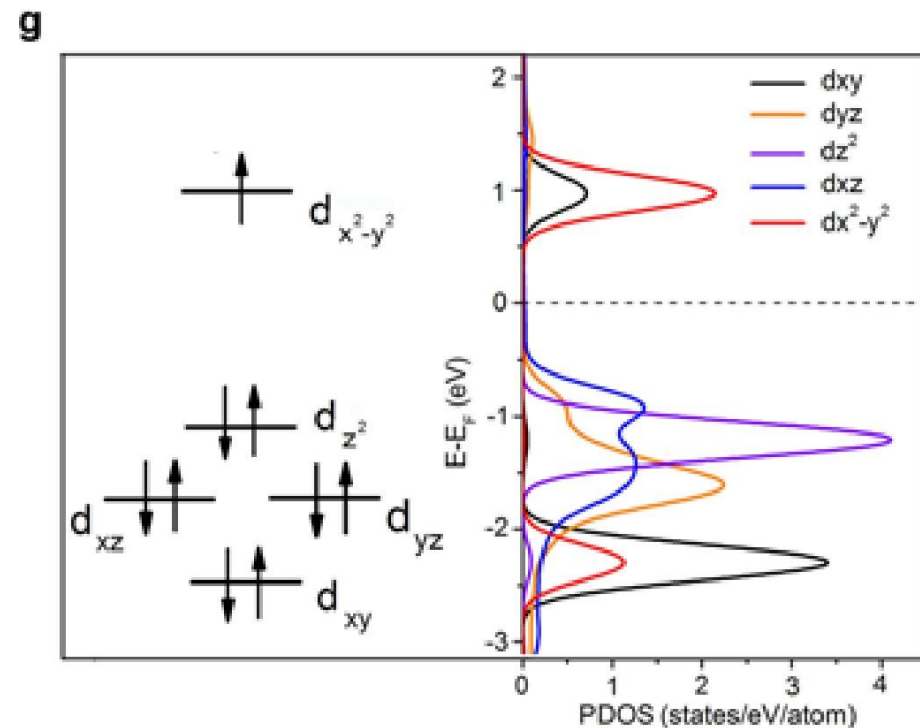
TDOS-total DOS



局域态密度 (LDOS) -s, p, d, f 轨道



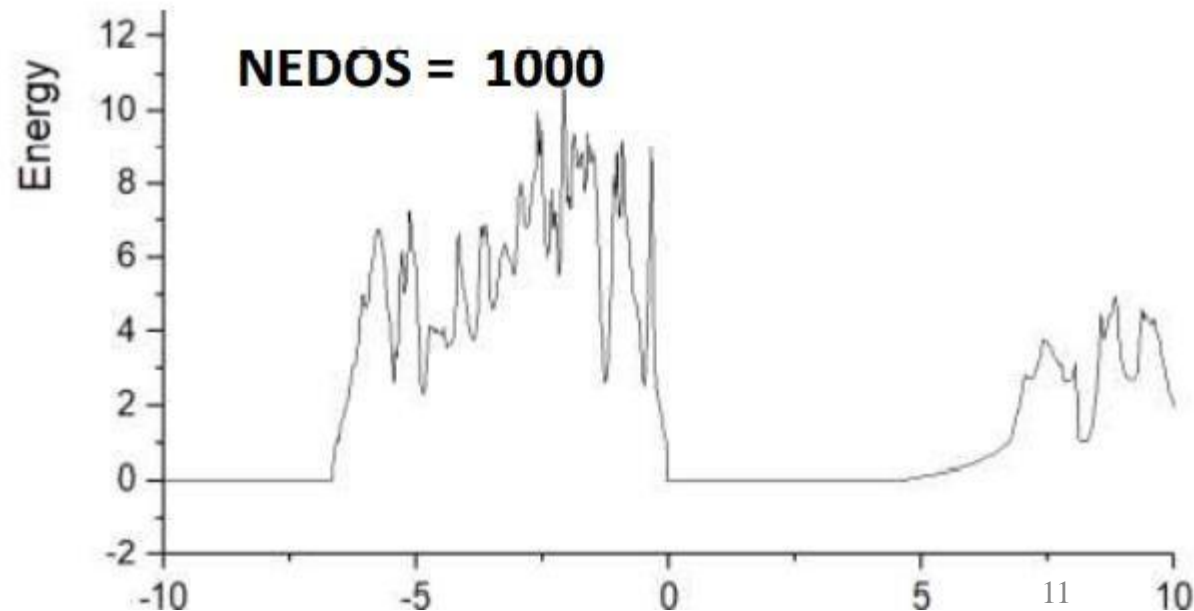
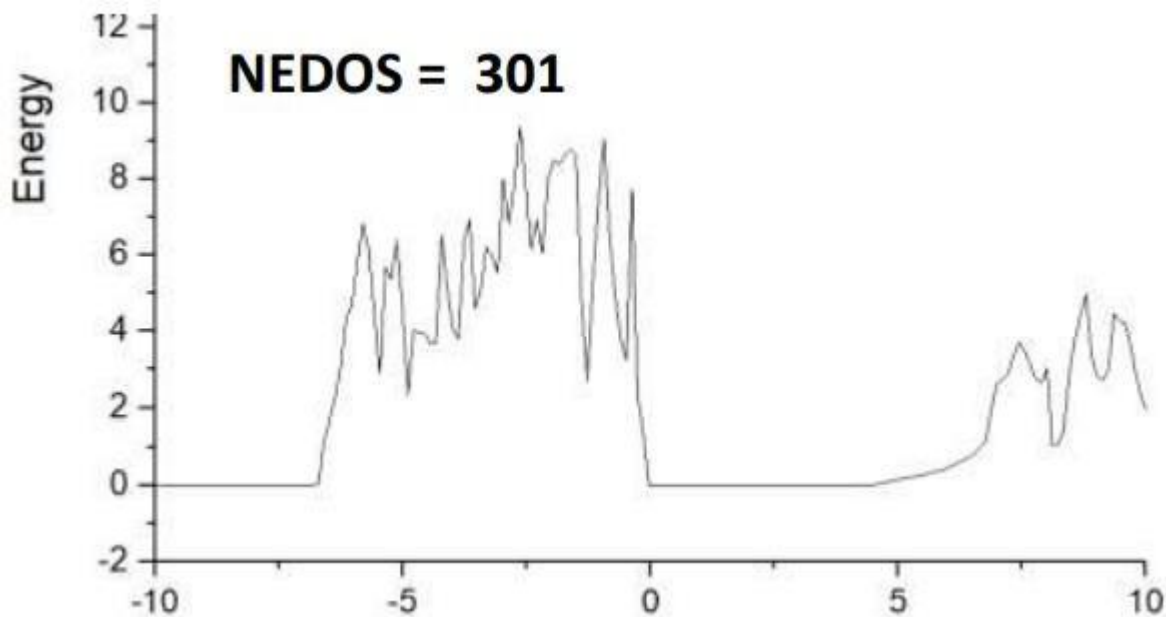
投影态密度 (PDOS)



- LORBIT = 10 把态密度分解到每个原子以及原子的spd轨道上面, 称为局域态密度, Local DOS (LDOS)。
- LORBIT = 11 在10的基础上, 还进一步分解到px, py, pz等轨道上, 称为投影态密度 (Projected DOS) 或者分波态密度 (Partial DOS), 即PDOS。
- 所以LORBIT = 11可以提供我们更多的信息。

态密度DOS计算-KPOINTS, NEDOS

- **KPOINTS**: K点数目的选取, K点数目越高, DOS质量越高, 一般我们 $k*a = 30-45$ 左右就可以了
- **NEDOS**数目越多, DOS质量也越高, 它是把DOS的能量区间 (横坐标) 范围分成NEDOS个点, 然后作图, 一般NEDOS=3001就够了
- NEDOS $\uparrow \rightarrow$ DOSCAR, vasprun.xml \uparrow , 占用空间越大
- 如果DOS的峰太尖, 可以提高NEDOS, 插入更多的点



态密度DOS计算 ISMEAR, SIGMA

1. ISMEAR -5 (四面体方法), 0 (GS方法), 1 (MP方法)

1. ISMEAR=-5适于所有体系DOS的计算, 但是**K点数目绝对不能小于4**, 否则会报错

VERY BAD NEWS! internal error in subroutine IBZKPT:

Tetrahedron method fails for NKPT<4. NKPT= 1

2. ISMEAR=-5, SIGMA可以不用管了

3. ISMEAR=-5, 不能用于体系的优化和能带计算, 因为不能准确处理Fermi能级处的电子占据问题, 导致力的计算出现误差

2. 如果你的体系很大, 直接用的Gamma单点计算, 那么K点数目肯定小于4, 这个时候ISMEAR禁止等于-5,

1. 建议ISMEAR=0或者1, 这个时候SIGMA需要注意了

2. ISMEAR=0, 适用于**所有体系**的计算, SIGMA = 0.01~0.05就可以了

3. ISMEAR=1, 适于**金属体系**的计算, 需要很高精度的SIGMA, 一般SIGMA = 0.2就够了

3. **一般我们直接用ISMEAR = 0了, 因为这个方法得到的DOS谱图相比于ISMEAR=-5更光滑, 更好看**

态密度DOS计算方法

一步计算

NSW=0

LORBIT=11/10

ISMEAR=0

SIGMA=0.05

NEDOS=3001, 高密度K点

二步计算

步骤一：静态计算(scf获得电荷文件CHGCAR):

NSW=0

ISMEAR=0

LORBIT=11

LCHARG=T

步骤二：读入CHGCAR

ISTART=1

ICHARG=11

LCHAGR=F

SIGMA=0.05

NEDOS=3001, 高密度K点

后处理vaspkit → 11

Vaspkit处理DOS的步骤

vaspkit → 11

```
[CMS@doge Cu]$ cd dos/
[CMS@doge dos]$ ls
INCAR KPOINTS LORBIT10 LORBIT11 POSCAR POTCAR vasp.5.4.4.pbs
```

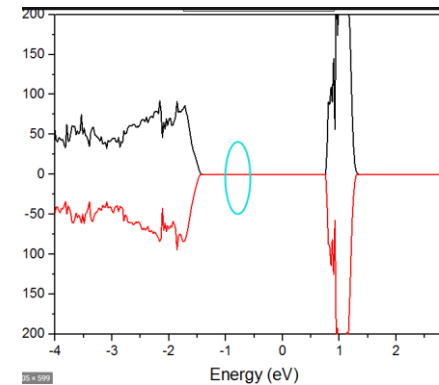
```
[CMS@doge LORBIT10]$ vaspkit

      \\\///
      /  ( )  \      Hey, you must know what you are doing.
    (| (.) (.) |)    Otherwise you might get wrong results!
+-----0000--()--0000-----+
|                               |
|   A Pre- and Post-Processing Program for VASP Code   |
|                               |
|   VASPKIT Version: 0.73 (20 Apr. 2019)              |
|   Developed by Vei WANG (wangvei@me.com)            |
|   Contributor: Nan XU (tamas@zju.edu.cn)            |
|                               |
+-----0000-----+
|   ( )   0000.   |
|   \ (   ( )   |
|   \_)  ) /   |
|   (/_         |
|===== Structural Options =====|
| 1) VASP Input Files Generator      2) Elastic-Properties |
| 3) K-Path Generator                4) Structure Editor  |
| 5) Catalysis-ElectroChemi Kit      6) Symmetry Search   |
| lobsterin" 6L, 123C                |
|===== Electronic Options =====|
| 11) Density-of-States               21) DFT Band-Structure |
| 23) 3D Band-Structure               25) Hybrid-DFT Band-Structure |
| 26) Fermi-Surface                   28) Band-Structure Unfolding |
```

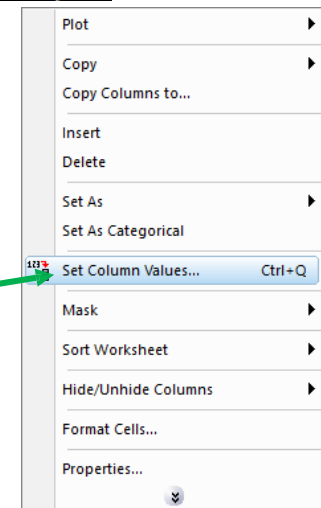
```
----->>
11
===== DOS Options =====
111) Total Density-of-States
112) Projected Density-of-States for Selected Atoms
113) Projected Density-of-States for Each Element
114) The Sum of Projected Density-of-States for Selected Atoms
115) The Sum of Projected DOS for Selected Atoms and Orbitals

0) Quit
9) Back
----->>

111
-->> (01) Reading Input Parameters From INCAR File...
-->> (02) Reading Fermi Energy from DOSCAR File...
00000000 The Fermi Energy will be set to zero eV 0000000000000000
-->> (03) Reading DOS Data From DOSCAR File...
-->> (04) Written TDOS.dat and ITDOS.dat Files!
```



Vaspkit自动把fermi能级平移到0，就是把横坐标的能量直接减去 E_{fermi} ，如果想要得到没减过fermi能级的图，则把现在得到的图横坐标加上fermi能级能量（origin直接可以操作，设置列值加上 E_{fermi} ）



vaspkit处理DOS的步骤，计算DOS前查看OSZICAR最后一列mag是不是等于0，如果等于0则没有自旋，DOS可以关了ISPIN，如果有的话则一定要开

```

----->>
11
===== DOS Options =====
111) Total Density-of-States
112) Projected Density-of-States for Selected Atoms
113) Projected Density-of-States for Each Element
114) The Sum of Projected Density-of-States for Selected Atoms
115) The Sum of Projected DOS for Selected Atoms and Orbitals

0) Quit
9) Back
----->>
111
-->> (01) Reading Input Parameters From INCAR File...
-->> (02) Reading Fermi Energy from DOSCAR File...
(ooooooooo The Fermi Energy will be set to zero eV ooooooooooooooooooooo)
-->> (03) Reading DOS Data From DOSCAR File...
-->> (04) Written TDOS.dat and ITDOS.dat Files!

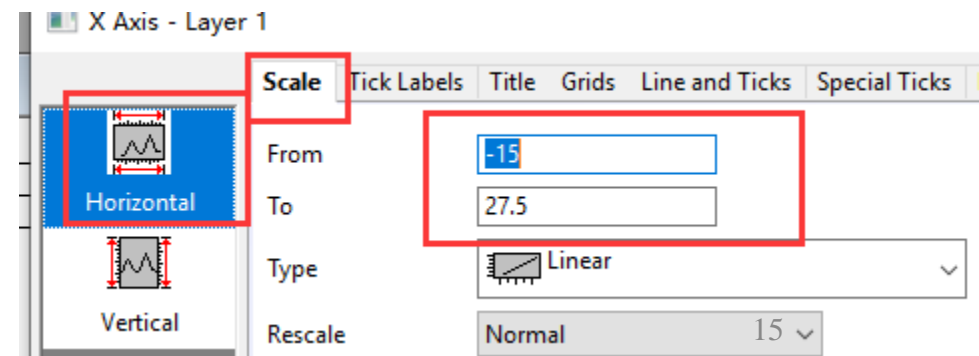
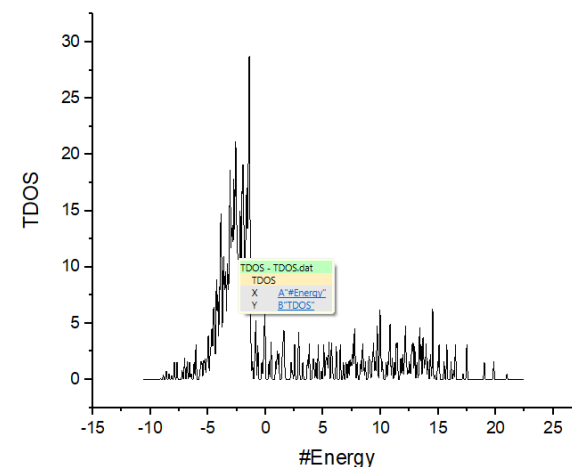
```

111 → 体系总DOS，直接用TDOS.dat文件作图即可，这里第一列是横坐标能量，第二列是纵坐标态密度，因为Cu是没有磁矩的，所以我关了ISPIN，直接删除就可→得到的TDOS直接拖入origin作图

	Energy	TDOS
1	-10.63672	0.00000
2	-10.62572	0.00000
3	-10.61472	0.00000
4	-10.60372	0.00000
5	-10.59272	0.00000
6	-10.58172	0.00000
7	-10.57072	0.00000
8	-10.55872	0.00000
9	-10.54772	0.00000
10	-10.53672	0.00000
11	-10.52572	0.00000
12	-10.51472	0.00000
13	-10.50372	0.00000

	A(X)	B(Y)
Long Name	#Energy	TDOS
Units		
Comments		
F(x)=		
Sparklines		
1	-10.63672	0
2	-10.62572	0
3	-10.61472	0
4	-10.60372	0
5	-10.59272	0
6	-10.58172	0
7	-10.57072	0
8	-10.55872	0
9	-10.54772	0
10	-10.53672	0
11	-10.52572	0
12	-10.51472	0
13	-10.50372	0
14	-10.49272	0
15	-10.48172	0
16	-10.47072	0
17	-10.45972	0
18	-10.44872	0
19	-10.43772	0
20	-10.42672	0
21	-10.41572	0
22	-10.40472	0
23	-10.39372	0
24	-10.38272	0
25	-10.37172	0
26	-10.36072	0
27	-10.34972	0
28	-10.33872	0
29	-10.32772	0
30	-10.31672	0
31	-10.30572	0
32	-10.29372	0
33	-10.28272	0
34	-10.27172	0
35	-10.26072	0
36	-10.24972	0
37	-10.23872	0
38	-10.22772	0
39	-10.21672	0
40	-10.20572	0
41	-10.19472	0
42	-10.18372	0
43	-10.17272	0
44	-10.16172	0
45	-10.15072	0
46	-10.13972	0
47	-10.12872	0

- 1.选中数据
2. 作图
3. 双击很横坐标或者纵坐标，修改横纵坐标取值范围，一般改横坐标比较多，因为我们只考虑fermi能级附近的态密度（-5~5之内大致可以，具体情况视实际情况定）



PDOS讲白了就是投影得到某个原子的DOS LDOS就是投影到具体轨道上的DOS

```
----->>
11
===== DOS Options =====
111) Total Density-of-States
112) Projected Density-of-States for Selected Atoms
113) Projected Density-of-States for Each Element
114) The Sum of Projected Density-of-States for Selected Atoms
115) The Sum of Projected DOS for Selected Atoms and Orbitals
```

112 → 得到选中原子的PDOS，基本就是直接给出所有原子的PDOS，自己选自己需要的

```
[CMS@dodge dos]$ head POSCAR
graphite\ (2)\ (\0\0\1)\ (2)
1.000000000000000
 7.380000114399996    0.000000000000000    0.000000000000000
-3.690000057199998    6.391267579000000    0.000000000000000
 0.000000000000000    0.000000000000000   10.000000000000000
C      Cu      H
17      1      1
Direct
-0.0095713766827253 -0.0056505244885387  0.0848699638956381
 0.0951535004651247  0.2164065235231978  0.0816850869779018
[CMS@dodge dos]$ vaspkit
```

```
----->>
112
-->> (01) Reading Input Parameters From INCAR File...
-->> (02) Reading Fermi-Energy from DOSCAR File...
oooooooo The Fermi Energy will be set to zero eV oooooooooooooooooo
-->> (03) Reading DOS Data From DOSCAR File...
-->> (04) Reading Structural Parameters from POSCAR File...
|-----|
Input the element-symbol and/or atom-index to SUM [Total-atom: 19]
(Free Format is OK, e.g., C Fe H 1-4 7 8 24)
----->>
C Cu H
-->> (05) Written SELECTED_ATOM_LIST File!
-->> (06) Written PDOS_A1.dat Files!
-->> (07) Written Integrated IPDOS_A1.dat Files!
-->> (08) Written PDOS_A2.dat Files!
-->> (09) Written Integrated IPDOS_A2.dat Files!
-->> (10) Written PDOS_A3.dat Files!
-->> (11) Written Integrated IPDOS_A3.dat Files!
-->> (12) Written PDOS_A4.dat Files!
-->> (13) Written Integrated IPDOS_A4.dat Files!
-->> (14) Written PDOS_A5.dat Files!
-->> (15) Written Integrated IPDOS_A5.dat Files!
-->> (16) Written PDOS_A6.dat Files!
```

113 → 得到按原子种类分类的DOS，比如体系有Cu，C，O三种元素，数目都不一定，那么可以得到这些元素的总PDOS

```
----->>
113
-->> (01) Reading Input Parameters From INCAR File...
-->> (02) Reading Fermi-Energy from DOSCAR File...
oooooooo The Fermi Energy will be set to zero eV oooooooooooooooooo
-->> (03) Reading DOS Data From DOSCAR File...
-->> (04) Reading Structural Parameters from POSCAR File...
-->> (05) Written PDOS_C.dat Files!
-->> (06) Written Integrated IPDOS_C.dat Files!
-->> (07) Written PDOS_Cu.dat Files!
-->> (08) Written Integrated IPDOS_Cu.dat Files!
-->> (09) Written PDOS_H.dat Files!
-->> (10) Written Integrated IPDOS_H.dat Files!
+-----+
```

114 → 得到选中原子的DOS之和，有的时候并不要所有的原子总和，只要局部，这个时候，只需要输入局部的原子序数，eg.这里我只要石墨烯中1,2,3号元素的DOS之和，就可以这样输

```
----->>
114
-->> (01) Reading Input Parameters From INCAR File...
-->> (02) Reading Fermi-Energy from DOSCAR File...
oooooooo The Fermi Energy will be set to zero eV oooooooooooooooooo
-->> (03) Reading DOS Data From DOSCAR File...
-->> (04) Reading Structural Parameters from POSCAR File...
|-----|
Input the element-symbol and/or atom-index to SUM [Total-atom: 19]
(Free Format is OK, e.g., C Fe H 1-4 7 8 24)
----->>
C 1-3
-->> (05) Written SELECTED_ATOM_LIST File!
-->> (06) Written PDOS_SUM.dat Files!
-->> (07) Written Integrated IPDOS_SUM.dat Files!
```


LORBIT=10, 只能得到 s p d tot总能量,

1	#Energy	s	p	d	tot
2	-10.63672	0.00000	0.00000	0.00000	0.00000
3	-10.62572	0.00000	0.00000	0.00000	0.00000
4	-10.61472	0.00000	0.00000	0.00000	0.00000
5	-10.60372	0.00000	0.00000	0.00000	0.00000
6	-10.59272	0.00000	0.00000	0.00000	0.00000

LORBIT=11。可以得到px py pz具体轨道的能量, 如果想得到p轨道总能量, 可以把px+py+pz轨道能量之和加在一起, (origin操作) 就免去再计算的麻烦

1	#Energy	s	py	pz	px	dxy	dyz	dz2	dxz	dx2	tot
2	-10.63672	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
3	-10.62572	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
4	-10.61472	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
5	-10.60372	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
6	-10.59272	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
7	-10.58172	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
8	-10.57072	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
9	-10.55872	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
10	-10.54772	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

	A(X)	B(Y)	C(Y)	D(Y)	E(Y)	F(Y)	G(Y)	H(Y)	I(Y)	J(Y)	K(Y)	L(Y)
Long Name	#Energy	s	py	pz	px	dxy	dyz	dz2	dxz	dx2	tot	
Units												
Comments												
F(x)=												
Sparklines												F+G+H+I+J
18	-8.07869	0	0	0	0	0	0	0	0	0	0	0
19	-8.01269	0	0	0	0	0	0	0	0	0	0	0
20	-7.94669	0	0	0	0	0	0	0	0	0	0	0
21	-7.88169	0	0	0	0	0	0	0	0	0	0	0
22	-7.81569	-1E-5	0	0	0	0	0	0	0	0	-1E-5	0
23	-7.75069	-8E-5	0	0	0	0	0	0	0	0	-8E-5	0
24	-7.68469	-3.5E-4	0	-1E-5	0	0	0	0	0	0	-3.6E-4	0

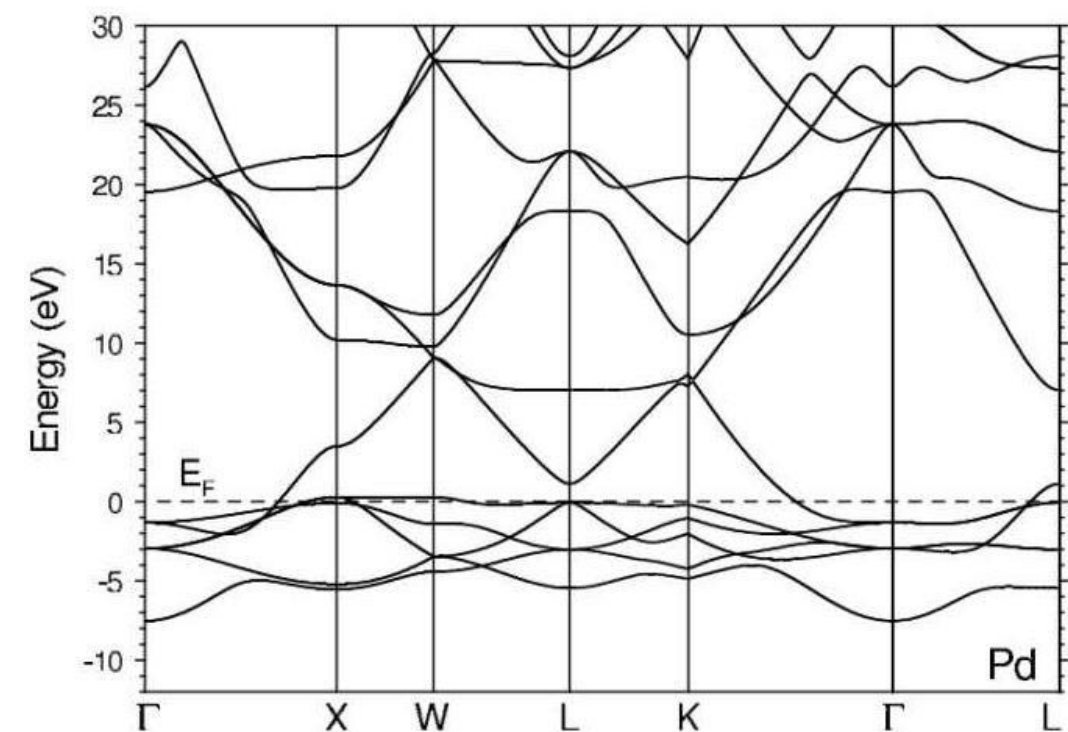
能带计算

Band计算

1. 金属？半金属？半导体？

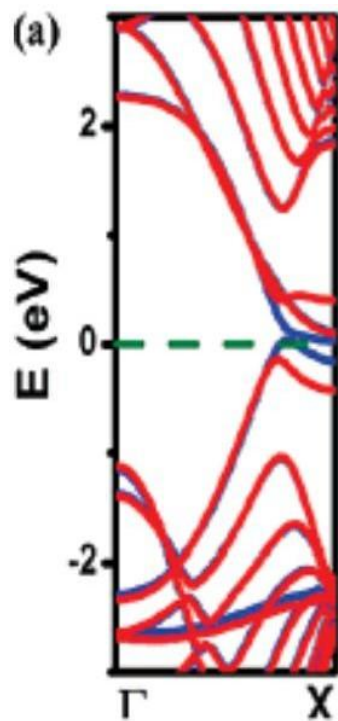
2. 直接带隙？间接带隙？

1. 金属：能带穿过fermi能级
2. 半金属：自旋向上 (or向下) 存在带隙，半导体性质，但是自旋向下 (or向上) 没有带隙，金属性质
3. 半导体：存在明显的带隙 E_g

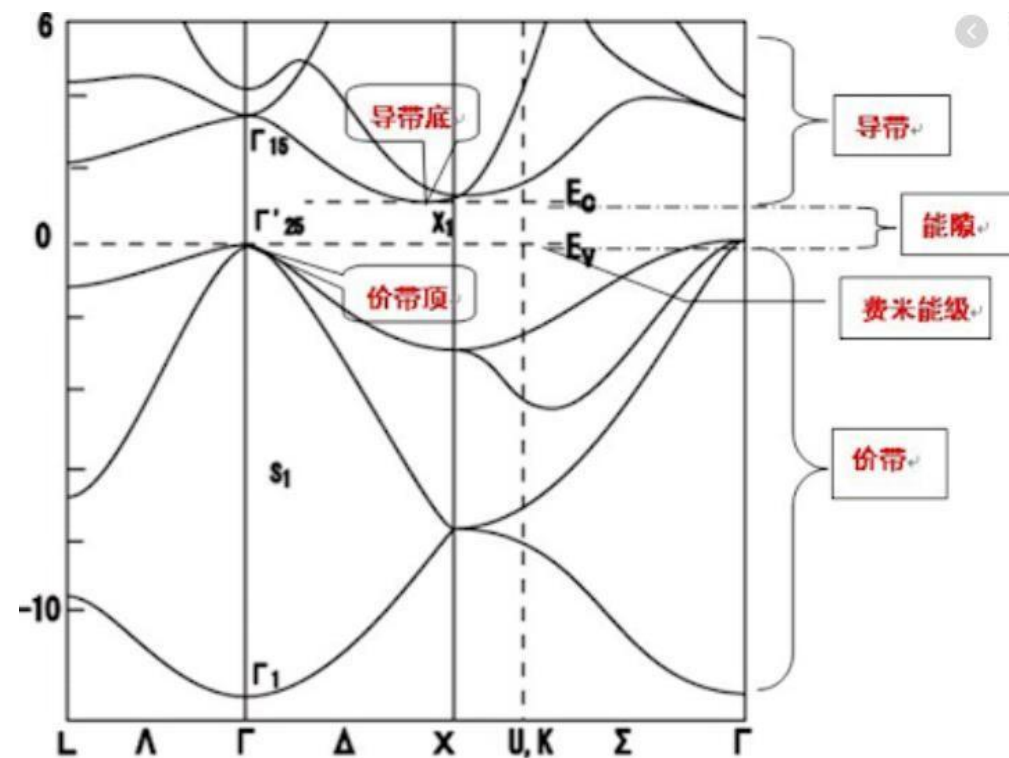


高对称点

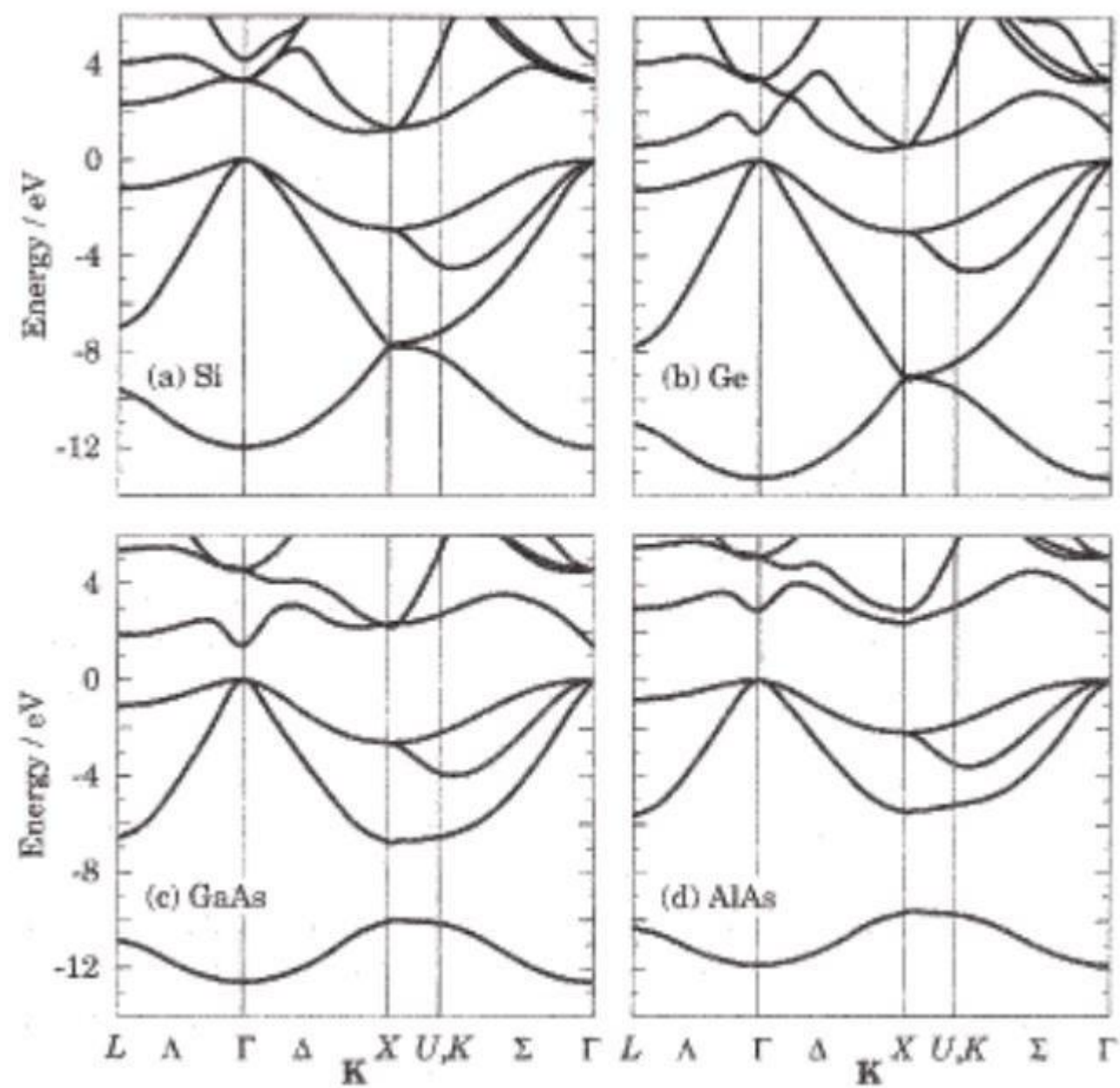
金属



半金属

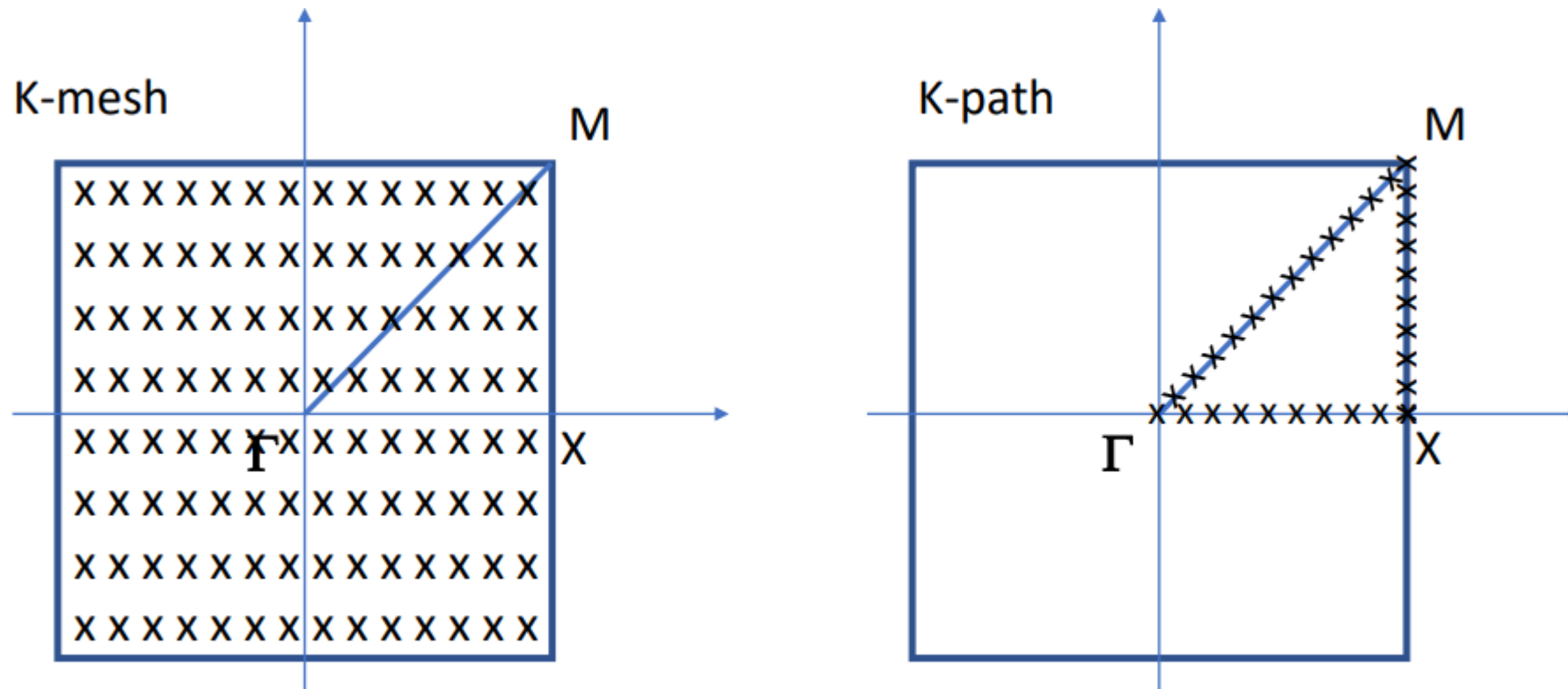


半导体



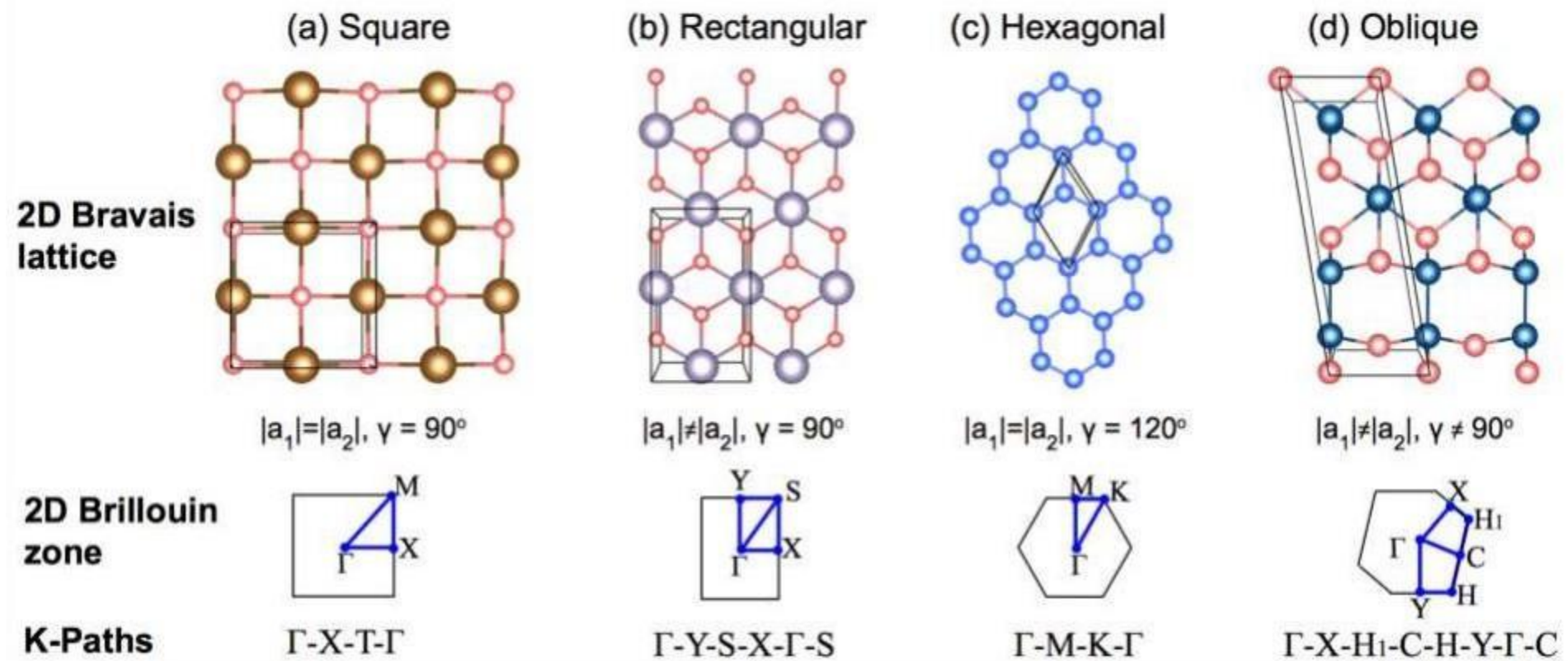
能带计算k点选取

1. (自洽) 非能带计算，K点都是在布里渊区均匀撒点的，这样可以较好的还原实空间中的电荷密度等信息。
2. 但是，能带计算的K点的选择是在布里渊区的边界上的，这些K点不能很好的体现实空间的电荷密度，所以我们要选一些高对称的k点，所谓的算能带结构，就是算这些高对称点的连线上的能级。



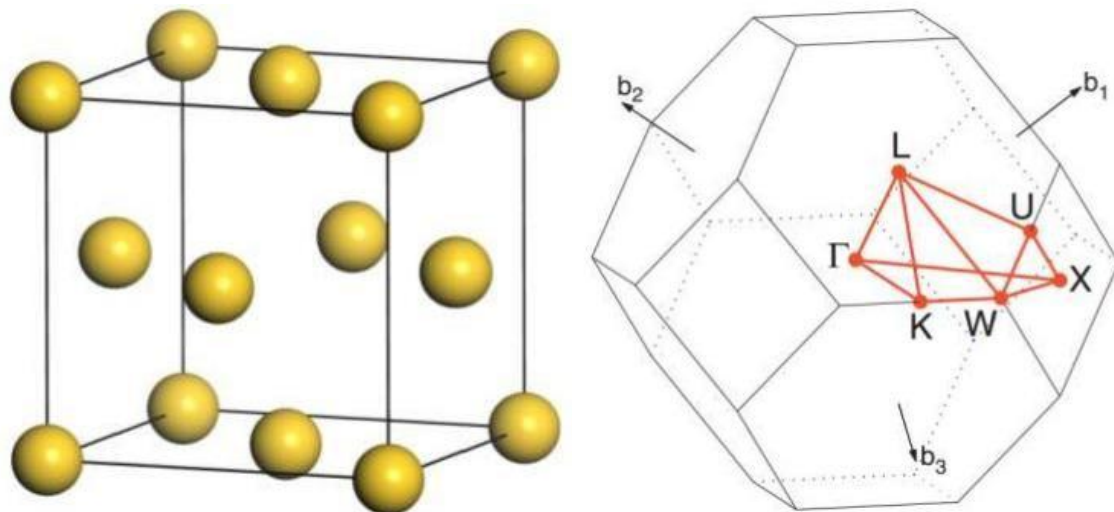
二维体系布里渊区

二维体系，那么K 点的取值就是两个数字的组合： k_x k_y



三维体系的布里渊区

此时，倒空间和布里渊区是三维的，K点的取值就是三个数字的组合： $k_x k_y k_z$ 。三维布里渊区边界不可能一笔画完，所以能带图中会出现“断点”，用“|”标记。



$\Gamma-X-U \mid K-\Gamma-L-W-X$

K-Path Generated by VASPKIT.

20 #表示每小段路径中插值的K点的数目，如果默认数值都算不动的话，可以考虑将其设小

Line-Mode

Reciprocal

0.0000000000	0.0000000000	0.0000000000	GAMMA
0.5000000000	0.0000000000	0.5000000000	X
0.5000000000	0.0000000000	0.5000000000	X
0.6250000000	0.2500000000	0.6250000000	U
0.3750000000	0.3750000000	0.7500000000	K
0.0000000000	0.0000000000	0.0000000000	GAMMA
0.0000000000	0.0000000000	0.0000000000	GAMMA
0.5000000000	0.5000000000	0.5000000000	L
0.5000000000	0.5000000000	0.5000000000	L
0.5000000000	0.2500000000	0.7500000000	W
0.5000000000	0.5000000000	0.7500000000	W
0.5000000000	0.2500000000	0.7500000000	W
0.5000000000	0.0000000000	0.5000000000	X

BCC金属Fe的第一布里渊区，高对称点路径

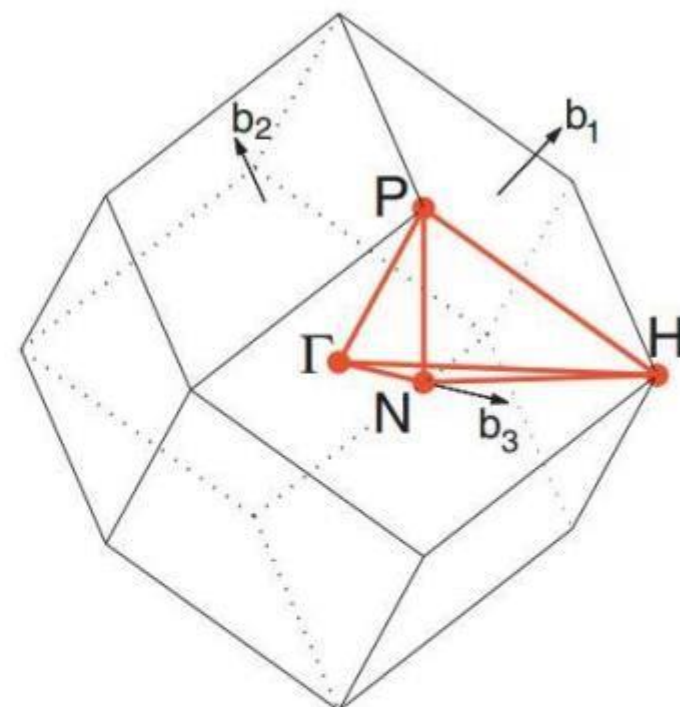
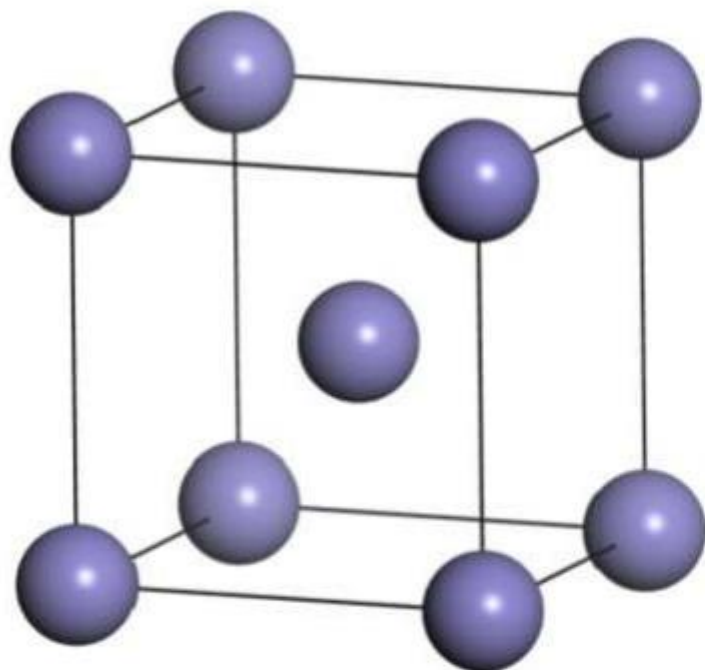


Table 4
Symmetry **k**-points of BCC lattice.

$\times \mathbf{b}_1$	$\times \mathbf{b}_2$	$\times \mathbf{b}_3$		$\times \mathbf{b}_1$	$\times \mathbf{b}_2$	$\times \mathbf{b}_3$	
0	0	0	Γ	1/4	1/4	1/4	P
1/2	-1/2	1/2	H	0	0	1/2	N

$\Gamma-H-N-\Gamma-P-H \mid P-N$

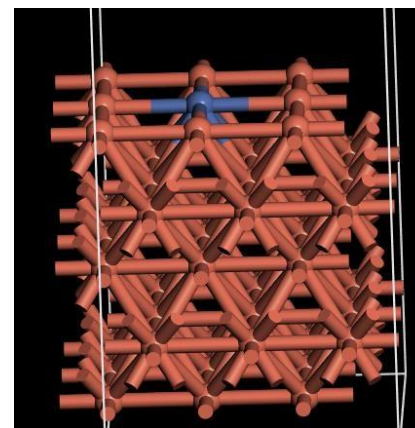
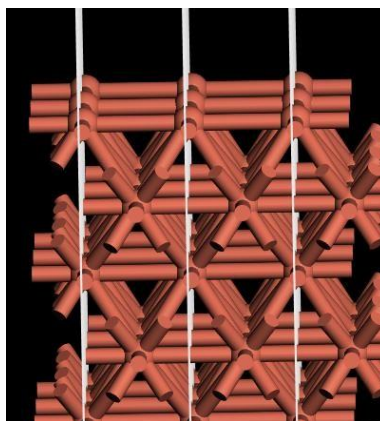
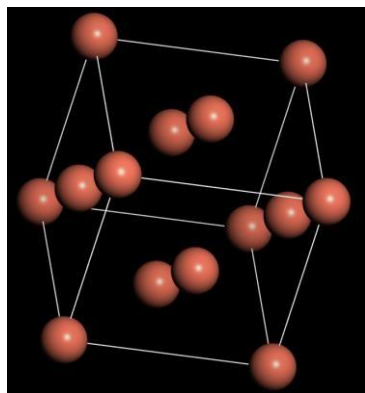
生成高对称点路径

- ① 结构网站生成<https://www.materialscloud.org/work/tools/seekpath>
- ② 判断体系的布里渊区形状自己生成，参考论文High-throughput electronic band structure calculations: Challenges and tools
- ③ 一些脚本，如VASPKIT
- ④ 建议使用后两种方法生成K点后，与结构网站对应一下

注意:

能带是材料的本征性质，一般我们用原胞计算就行

1. 比如我们想知道Cu111 Cu100的能带，那么我们直接算cubic Cu的能带就行；如果我们想算石墨烯的band, 那么我们直接算最小的胞就行
2. 如果计算Cu111面掺杂Fe之后的band，那么这个掺杂后的体系其实就是原胞；如果计算掺Cu后的石墨烯的band，那么这个掺Cu石墨烯就是原胞



能带计算方法

- **只能分步计算**：由于在能带计算时 k 点是一些在倒空间高对称线上的点，不能进行自洽计算。
- 参考网址：<https://blog.shishiruqi.com/2019/07/11/band2/>
- 也就是计算能带的时候，**自洽计算是必须的一步**；

BAND计算步骤

以体相Cu为例：

- 步骤一：优化体相 (opt)
- 步骤二：静态计算(scf, 得到电荷文件CHGCAR)

NSW=0 LCHARG=T

- 步骤三：非自洽计算, 读入CHGCAR
- cp INCAR POTCAR CONTCAR CHGCAR band

ISTART=1

ICHARG=11

LCHARG=F

ISMEAR=0

准备高对称点KPOINTS, 使用 vaspkit 得到 vaspkit → 3 →根据自己的实际情况选择1D 2D 3D材料), 将生成的KPATH.in 文件名改为KPOINTS

步骤四：提交作业计算, 完成后数据处理, 输入vaspkit → 21

```
K-Path Generated by VASPKIT.
20
Line-Mode
Reciprocal
0.0000000000 0.0000000000 0.0000000000 GAMMA
0.5000000000 0.0000000000 0.5000000000 X

0.5000000000 0.0000000000 0.5000000000 X
0.6250000000 0.2500000000 0.6250000000 U

0.3750000000 0.3750000000 0.7500000000 K
0.0000000000 0.0000000000 0.0000000000 GAMMA

0.0000000000 0.0000000000 0.0000000000 GAMMA
0.5000000000 0.5000000000 0.5000000000 L

0.5000000000 0.5000000000 0.5000000000 L
0.5000000000 0.2500000000 0.7500000000 W

0.5000000000 0.2500000000 0.7500000000 W
0.5000000000 0.0000000000 0.5000000000 X
```

```

21)
===== Band Options =====
211) Band-Structure
212) Projected Band-Structure for Selected Atoms
213) Projected Band-Structure for Each Element
214) The Sum of Projected Band-Structure for Selected Atoms

0) Quit
9) Back
----->>
211
-->> (01) Reading Input Parameters From INCAR File...
-->> (02) Reading Fermi-Energy from DOSCAR File...
00000000 The Fermi Energy will be set to zero eV 0000000000000000
-->> (03) Reading Energy-Levels From EIGENVAL File...
-->> (04) Reading Structural Parameters from POSCAR File...
-->> (05) Reading K-Paths From KPOINTS File...
-->> (06) Written BAND.dat File!
-->> (07) Written BAND_REFORMATTED.dat File!
-->> (08) Written KLINEs.dat File!
-->> (09) Written KLABELS File!
-->> (10) Written BAND_GAP File!

```

BAND.dat文件就是总的能带图，横坐标是横坐标（高对称点位于每隔20个点数据处，因为我们之前设的是每隔20个点插入一个高对称点，纵坐标是能带

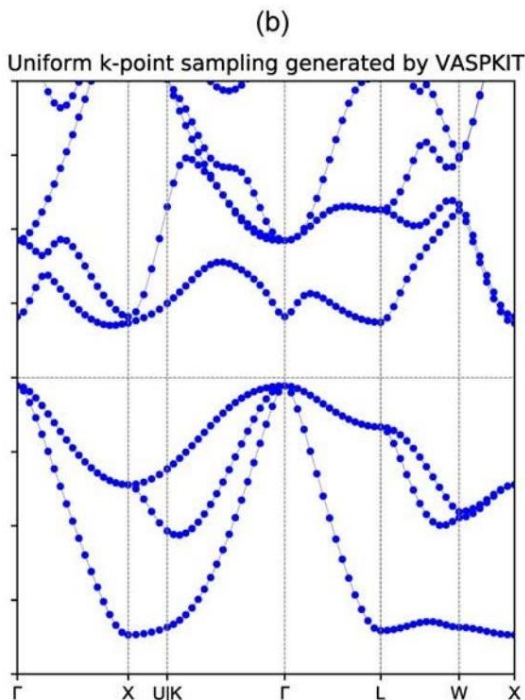
```

[CMS@doge band]$ vi KLINEs.dat
[CMS@doge band]$ vi KLABELS

1  K-Label      K-Coordinate in band-structure plots
2  GAMMA        0.000
3  X            1.229
4  U|K          1.761
5  GAMMA        3.358
6  L            4.863
7  W            5.478
8  X            6.092
9
10
11 * Give the label for each high symmetry point in KPOINTS (KPATH.in) file. Otherwise, they will be identified as 'Undefined' in KLABELS file

```

KLABELS文件给出第一列高对称点的排序。第二列给出这些高对称点出现的横坐标，其实直接看这个文件就可以顺利插入高对称点



```

[CMS@doge band]$ vi BAND_GAP

----- Summary -----
Band Character:      Indirect
Band Gap (eV):       0.6677
Eigenvalue of VBM (eV): 5.8258
Eigenvalue of CBM (eV): 6.4936
HOMO & LUMO Bands:   16      17
Location of VBM:     0.000000  0.000000  0.000000
Location of CBM:     0.019737  0.019737  0.039474

```

BAND_GAP文件可以直接得出：

- (1) 半导体是什么类型半导体？直接带隙？间接带隙？
- (2) 半导体的带隙值
- (3) CBM, VBM的值以及位置

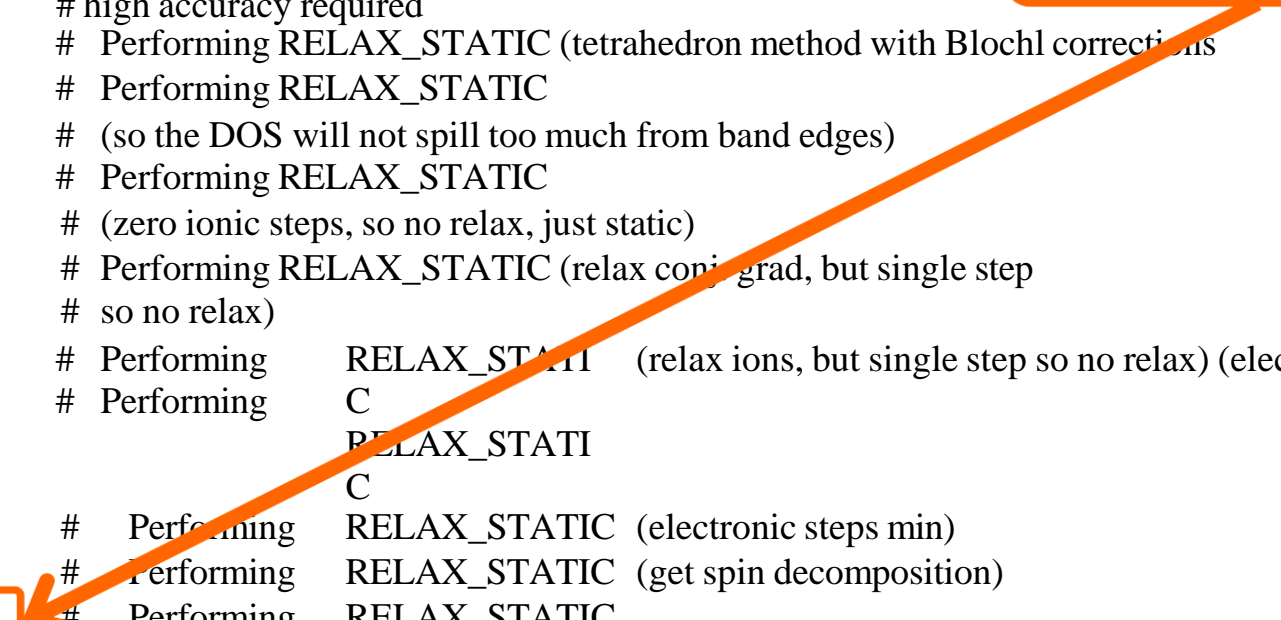
K-Path	Energy-Level
#Band-index	1
0.000	-9.1516
0.065	-9.1348
0.129	-9.0842
0.194	-9.0002
0.259	-8.8832
0.323	-8.7337
0.388	-8.5525
0.453	-8.3405
0.518	-8.0992
0.582	-7.8301

Example 1: Si DOS calculations

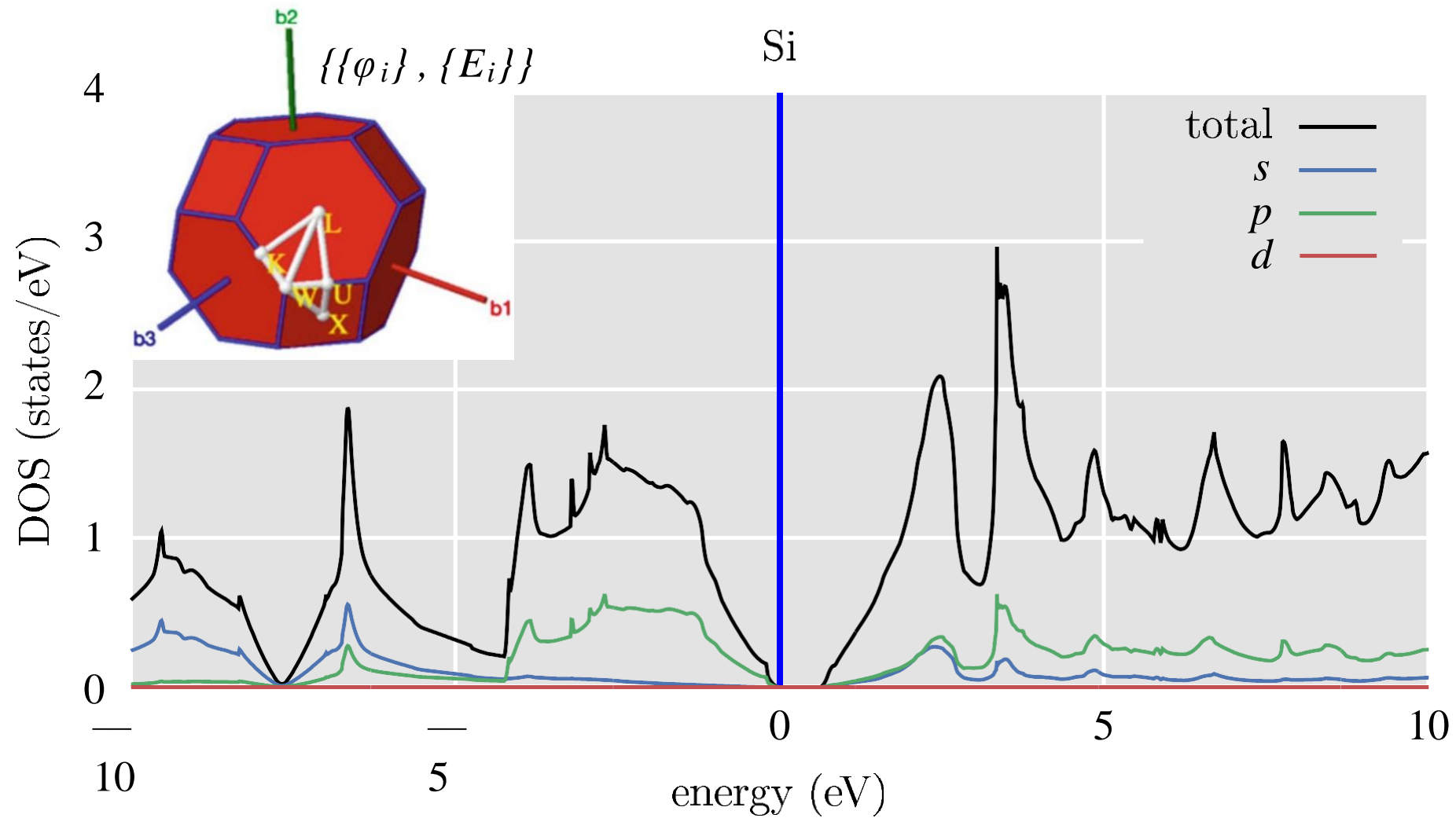
INCAR (Si DOS):

```
SYSTEM=Si
NBANDS=39      # KBIN::XVASP_INCAR_GetNBANDS #
ISYM=2         SYMMETRY=ON
ENMAX=343.483  # 1.4*ENMAX (245.345) of pseudopotentials
EDIFF=1E-6     # high accuracy required
ISMEAR=-5      # Performing RELAX_STATIC (tetrahedron method with Blochl corrections)
SIGMA=0.05     # Performing RELAX_STATIC
               # (so the DOS will not spill too much from band edges)
NSW=0          # Performing RELAX_STATIC
               # (zero ionic steps, so no relax, just static)
IBRION=2       # Performing RELAX_STATIC (relax conjugate grad, but single step
               # so no relax)
ISIF=2         # Performing RELAX_STATIC (relax ions, but single step so no relax) (electronic steps max)
NELM=12        # Performing C
0              RELAX_STATIC
               C
NELMIN=2       # Performing RELAX_STATIC (electronic steps min)
LORBIT=10      # Performing RELAX_STATIC (get spin decomposition)
LCHARG=.TRUE. # Performing RELAX_STATIC
               # Performing RELAX_STATIC (Bader ON)
#LAECHG=.TRUE. # Performing RELAX_STATIC
LWAVE=.FALSE.  # Performing RELAX_STATIC
PREC=ACCURATE  # Performing RELAX_STATIC (aleksey)
E
EMIN= -30.0    # Performing RELAX_STATIC (aleksey) force search for EMIN (DOS E min)
EMAX= 45.0     # Performing RELAX_STATIC (aleksey) (DOS E max)
NEDOS= 5000    # Performing RELAX_STATIC (aleksey) (number of E steps)
```

print well-converged
CHGCAR for BANDS



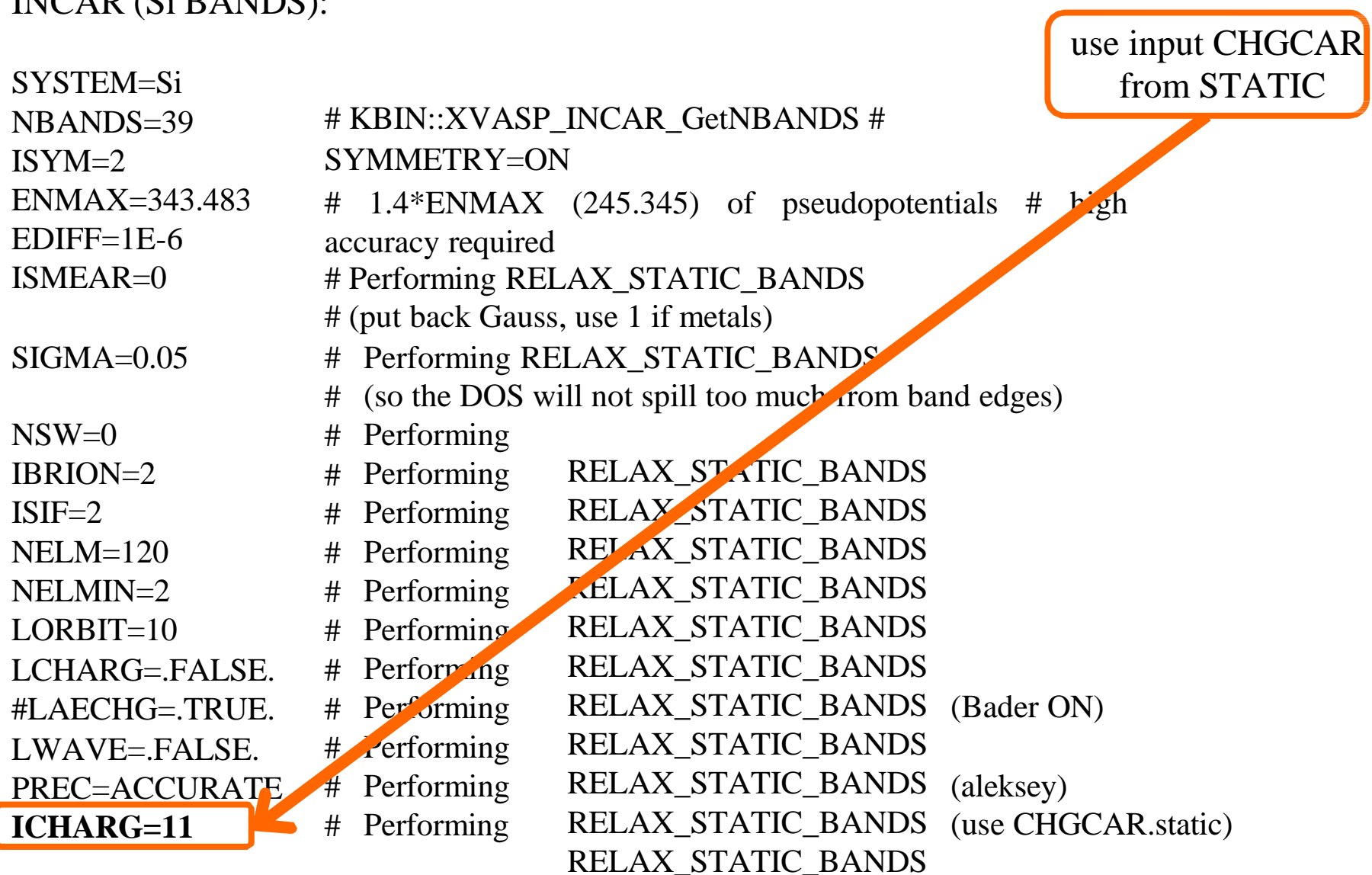
Example 1: Si DOS calculations



Example 2: Si band structure calculations

INCAR (Si BANDS):

```
SYSTEM=Si
NBANDS=39      # KBIN::XVASP_INCAR_GetNBANDS #
ISYM=2         SYMMETRY=ON
ENMAX=343.483  # 1.4*ENMAX (245.345) of pseudopotentials # high
EDIFF=1E-6     accuracy required
ISMEAR=0       # Performing RELAX_STATIC_BANDS
              # (put back Gauss, use 1 if metals)
SIGMA=0.05     # Performing RELAX_STATIC_BANDS
              # (so the DOS will not spill too much from band edges)
NSW=0          # Performing
IBRION=2       # Performing RELAX_STATIC_BANDS
ISIF=2         # Performing RELAX_STATIC_BANDS
NELM=120       # Performing RELAX_STATIC_BANDS
NELMIN=2       # Performing RELAX_STATIC_BANDS
LORBIT=10      # Performing RELAX_STATIC_BANDS
LCHARG=.FALSE. # Performing RELAX_STATIC_BANDS
#LAECHG=.TRUE. # Performing RELAX_STATIC_BANDS (Bader ON)
LWAVE=.FALSE.  # Performing RELAX_STATIC_BANDS
PREC=ACCURATE  # Performing RELAX_STATIC_BANDS (aleksey)
ICHARG=11    # Performing RELAX_STATIC_BANDS (use CHGCAR.static)
              RELAX_STATIC_BANDS
```



Example 2: Si band structure calculations

KPOINTS (Si):

FCC (face-centered cubic) G-X-W-K-G-L-U-W-L-K U-X 20! 20 grids

Line-mode
reciprocal

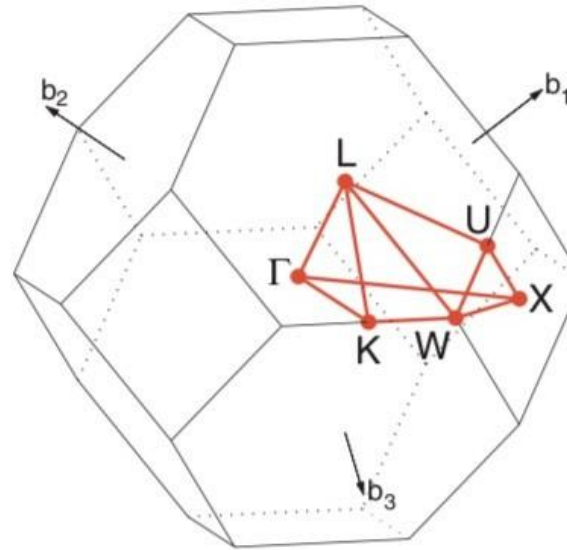


Fig. 2. Brillouin zone of FCC lattice. Path: Γ -X-W-K- Γ -L-U-W-L-K|U-X. An example of band structure using this path is given in Fig. 27.

Table 3
Symmetry \mathbf{k} -points of FCC lattice.

$\times \mathbf{b}_1$	$\times \mathbf{b}_2$	$\times \mathbf{b}_3$		$\times \mathbf{b}_1$	$\times \mathbf{b}_2$	$\times \mathbf{b}_3$	
0	0	0	Γ	5/8	1/4	5/8	U
3/8	3/8	3/4	K	1/2	1/4	3/4	W
1/2	1/2	1/2	L	1/2	0	1/2	X

Example 2: Si band structure calculations

KPOINTS (Si BANDS):

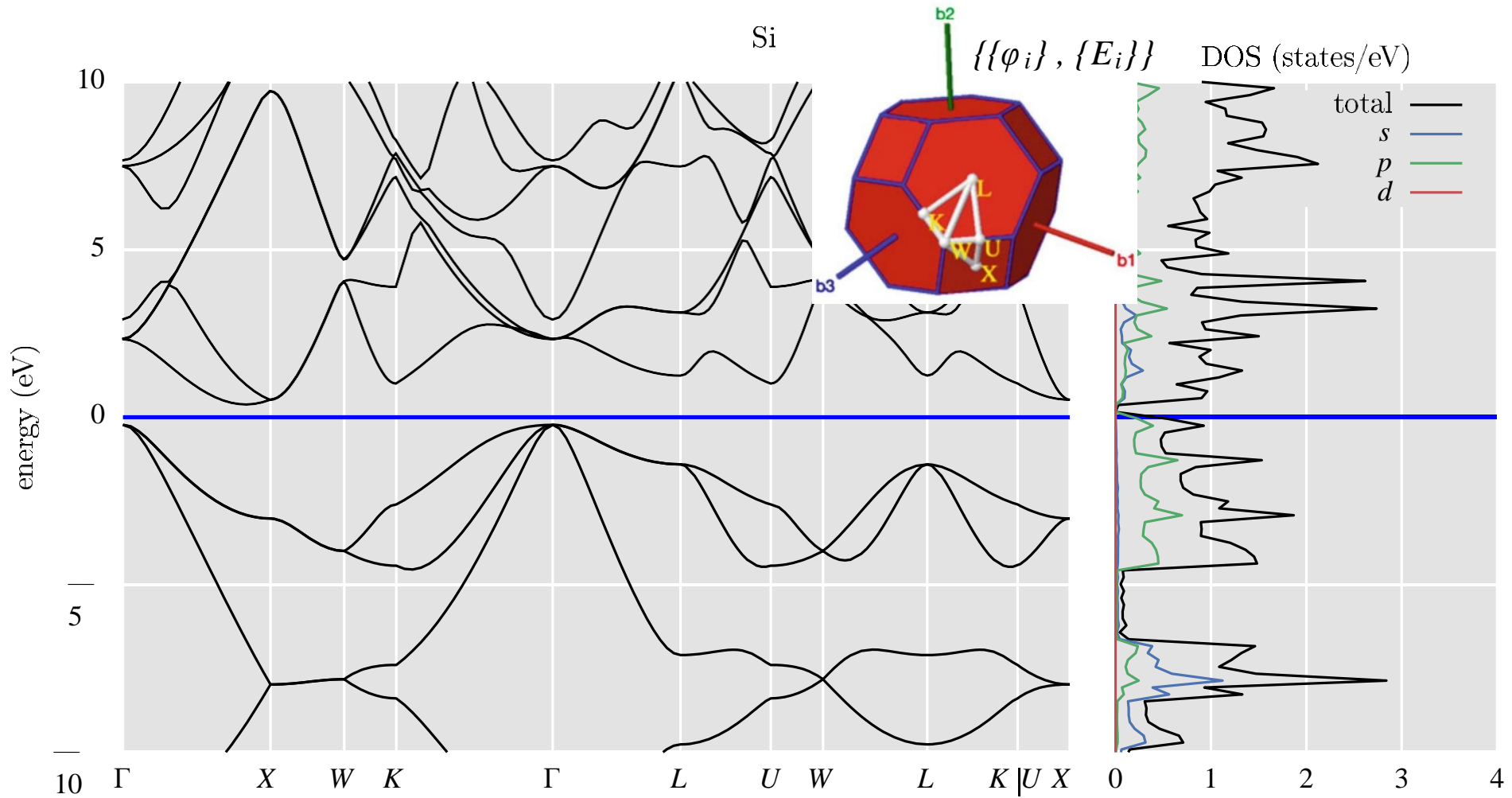
FCC (face-centered cubic) G-X-W-K-G-L-U-W-L-K U-X

20 ! 20 grids

Line-mode reciprocal

0.0000	0.0000	0.0000	! \Gamma
0.5000	0.0000	0.5000	! X
0.5000	0.0000	0.5000	! X
0.5000	0.2500	0.7500	! W
0.5000	0.2500	0.7500	! W
0.3750	0.3750	0.7500	! K
0.3750	0.3750	0.7500	! K
0.0000	0.0000	0.0000	! \Gamma
0.0000	0.0000	0.0000	! \Gamma
0.5000	0.5000	0.5000	! L
0.5000	0.5000	0.5000	! L
0.6250	0.2500	0.6250	! U
0.6250	0.2500	0.6250	! U
0.5000	0.2500	0.7500	! W
0.5000	0.2500	0.7500	! W
0.5000	0.5000	0.5000	! L
0.5000	0.5000	0.5000	! L
0.5000	0.5000	0.5000	! L
0.3750	0.3750	0.7500	! K
0.6250	0.2500	0.6250	! U
0.5000	0.0000	0.5000	! X

Example 2: Si band structure calculations



练习

- 计算体相Cu的态密度，比较参数ISMEAR=0, 1, -5的区别，并分析体相Cu的态密度主要由哪个轨道贡献。
- 计算体相Si和Cu的能带，比较分析。与实验值比较，带隙类型一致吗？DFT低估还是高估带隙？
- **可选做：**计算Cu(111), Cu(100)表面吸附CO分子的吸附能，根据吸附能判断最稳定构型（是hollow, top, 还是bridge? ），计算吸附CO的Cu位点和CO的态密度变化。

吸附位点解释：<https://zhuanlan.zhihu.com/p/646095577>