

LOBSTER による COHP解析

K.NAKADA

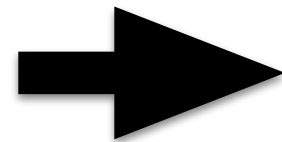
2017.06.13 メモ

2017.06.13

lobster-2.1.0 実行において必要なファイル

symlink でよい(読むだけなので)

CONTCAR
DOSCAR
EIGENVAL
KPOINTS
OUTCAR
POTCAR
WAVECAR
vasprun.xml



出力ファイル

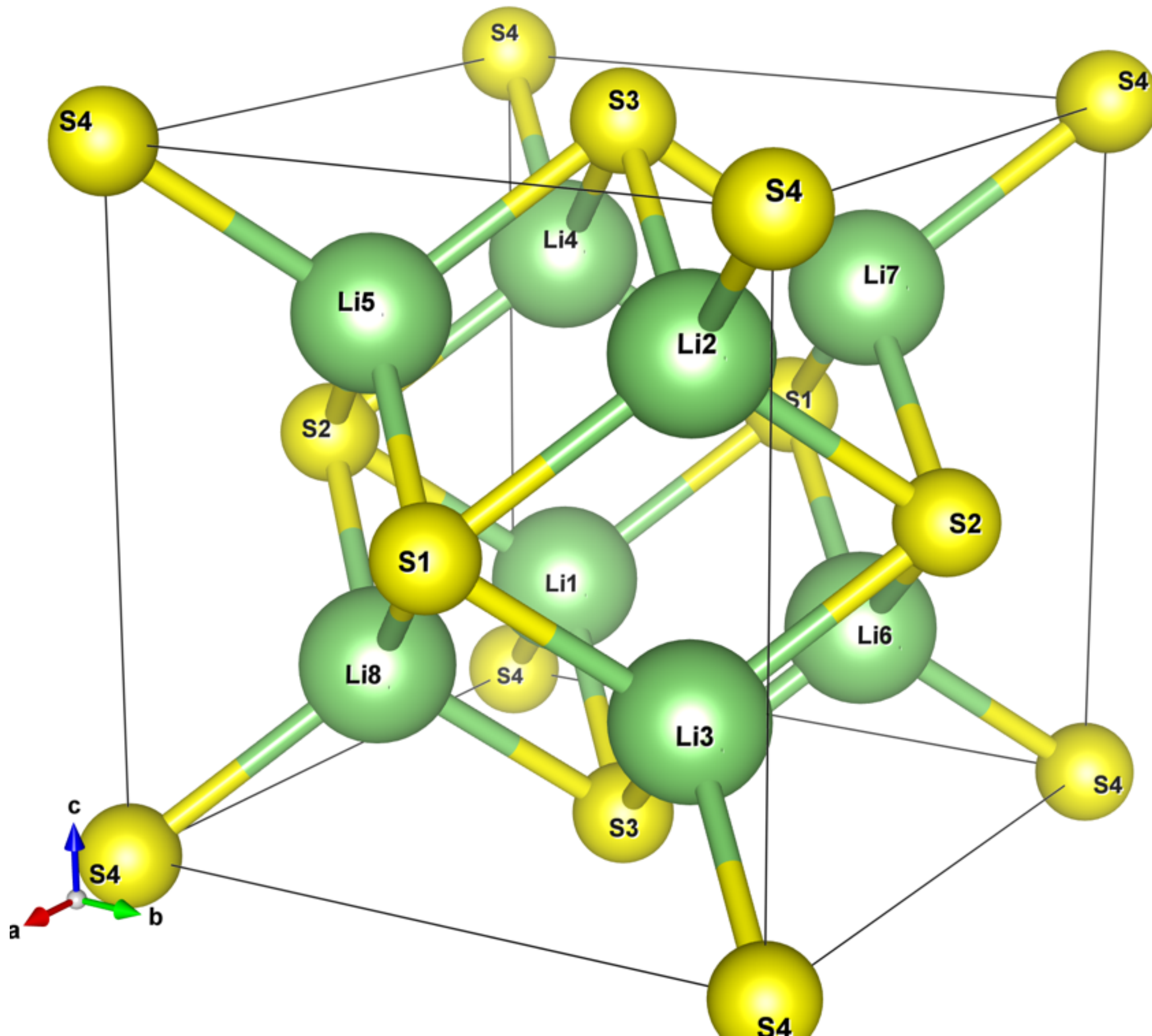
COHPCAR.lobster
COOPCAR.lobster
DOSCAR.lobster
ICOHPLIST.lobster
ICOOPLIST.lobster
bandOverlaps.lobster
lobsterin
lobsterout

2017.06.13

COHP ペア探しについて

例)

Li_2S



COHPCAR.lobster: ペア情報と COHP 情報

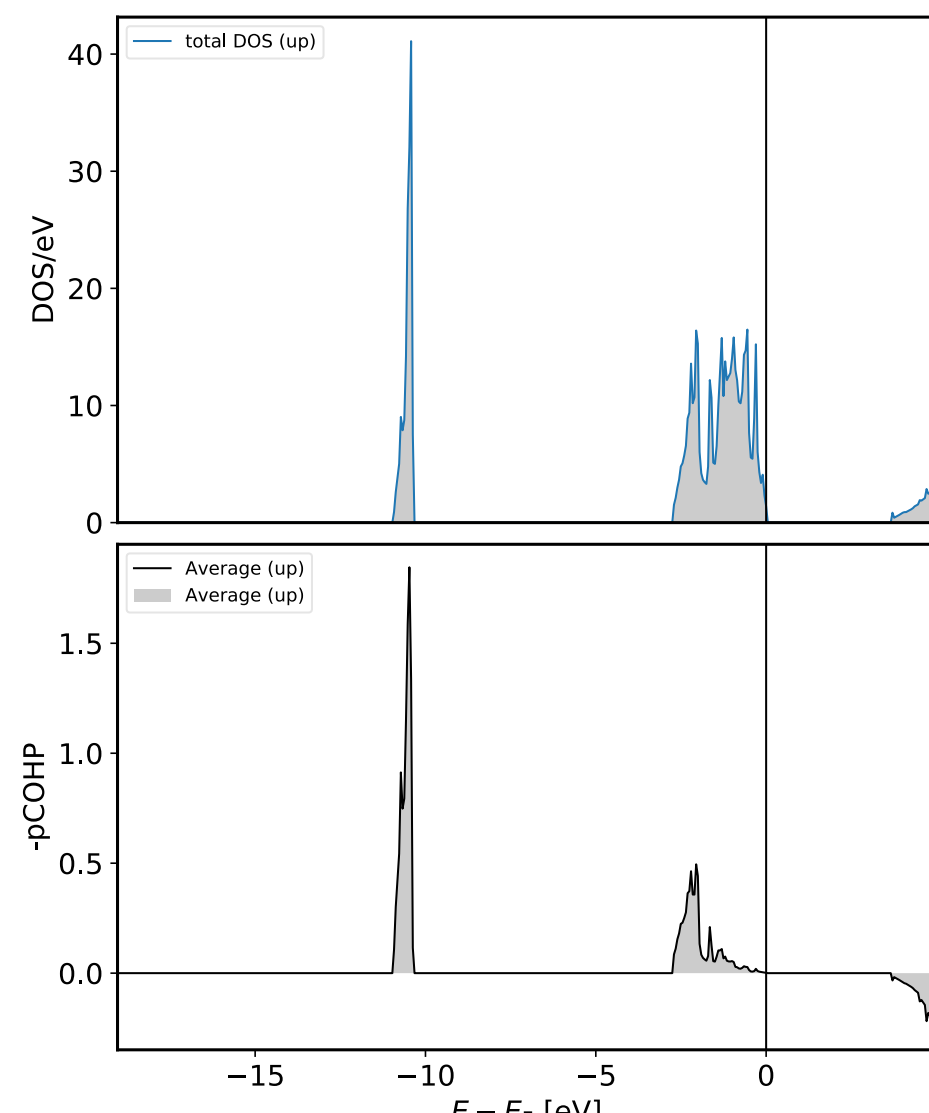
cohpbetween atom 1 atom 12

(cohpGenerator を使わない場合, between 間のatomの結合)

Average

No.1:**S1**->**Li12**(2.4750139185536151)

原子選択で、特定のペア
をplotする場合はこの方法が吉



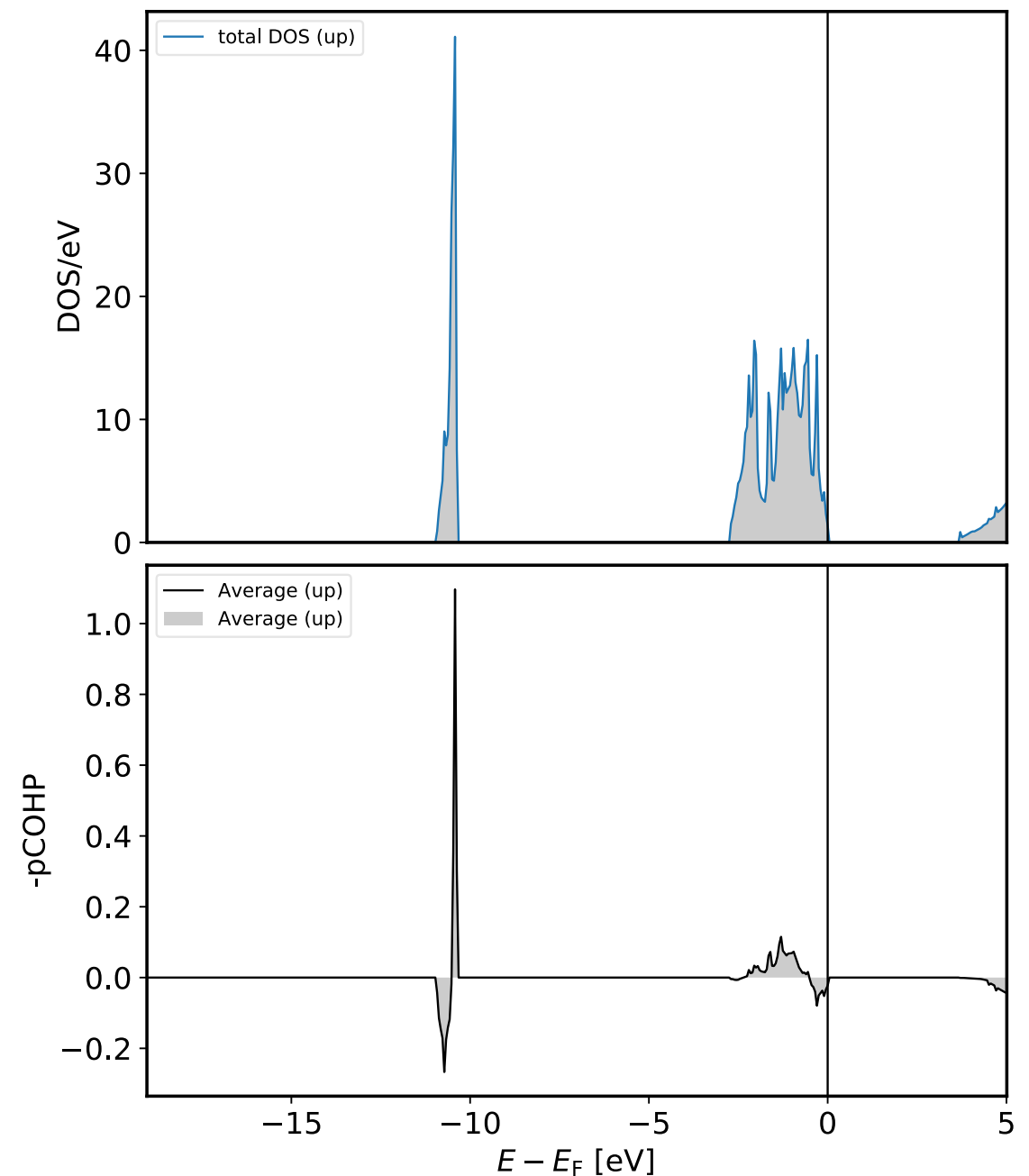
cohpbetween atom 1 atom 2

(cohpgenerator を使わない場合, between 間のatomの結合)

Average

No.1:**S1**->**S2**(4.0416808044951198)

原子選択で、特定のペア
をplotする場合はこの方法が吉



(cohpbetween を使わない)

(cohpGenerator も使わない) → 完全にデフォルト

WARNING: You did not specify any COHP pairs in the lobsterin file. As default

WARNING: I will try to find any pairs between 1.0 and 3.0 Å distance,

WARNING: but that might be wrong. If you want pCOHPs or pCOOPs, change the lobsterin!

found 44 interactions.

Average

No.1:S1->Li5(2.4750139185536151)

No.2:S1->Li6(2.4750139185536151)

No.3:S1->Li7(2.4750139185536151)

..

..

..

No.43:Li9->Li12(2.85789990425)

No.44:Li10->Li11(2.85789990425)

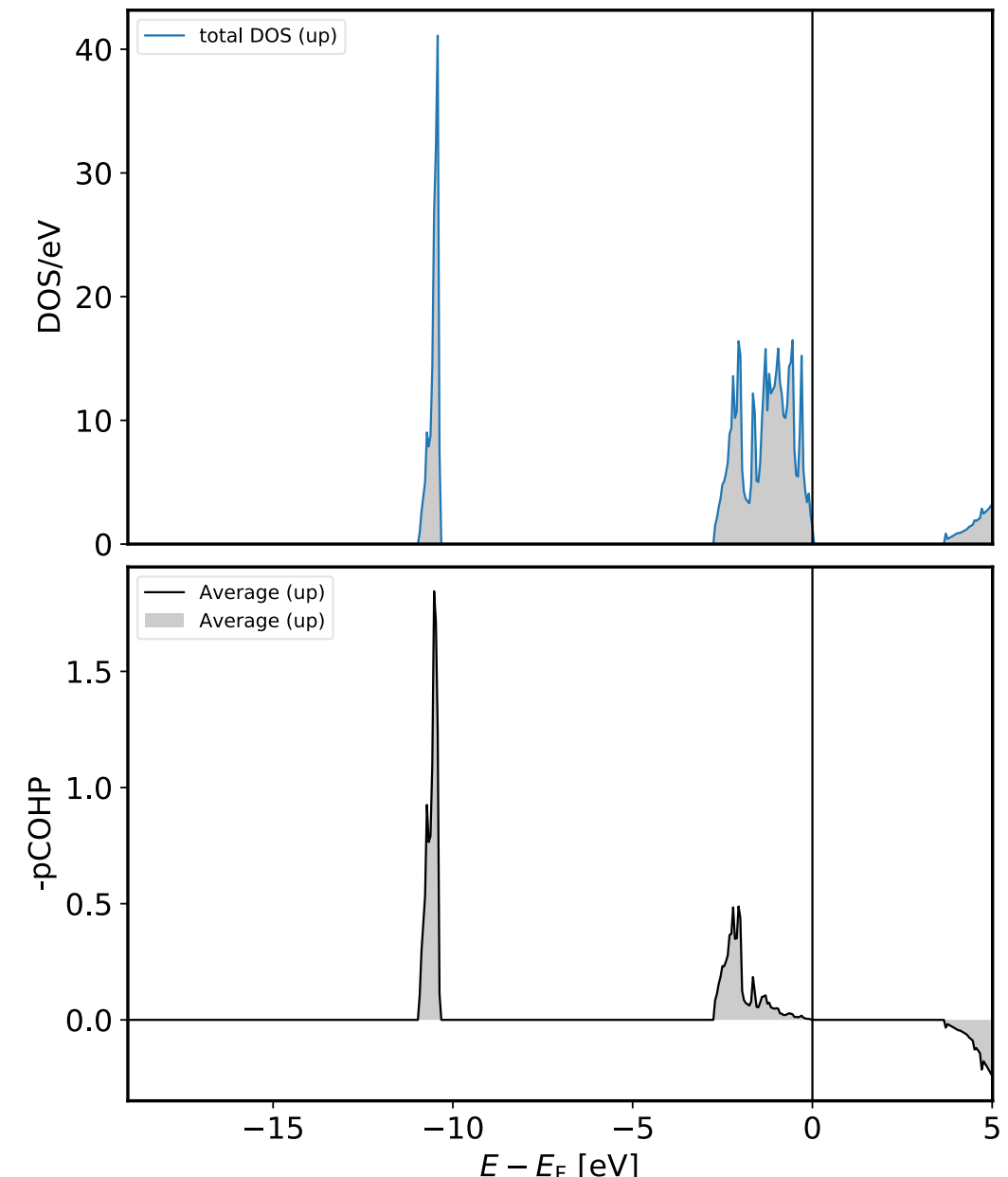
全部で44の結合

cohpbetween と cohpGenerator の両方あるときは cohpGenerator が優先される

cohpbetween atom 1 atom 36
cohpGenerator from 1.0 to 2.5

WARNING: There is a syntax error in a cohpbetween line in the lobsterin file.
WARNING: ignoring line "cohpbetween atom 1 atom 36" found 32 interactions.

cohpGenerator from 1.0 to 2.5
にて検索されたもの



ペア捜しの注意

必ず **lobsterout** の **found 数** と近傍ログを確認する

INFO: the PAW bands from 1009 and upwards will be ignored.
setting up CO interactions... found 691 interactions.

INFO: the PAW bands from 1009 and upwards will be ignored.
setting up CO interactions... found 1 interaction.

注意事項まとめ

!!!!必ず行うこと!!!!

- 1) on-site でボンドの議論は出来ないなのでプリミティブセルの時は注意する（例えばFCCはSCセルを4つ用意して計算するなど）
- 2) lobsterout に出てくるワーニングで BAND の数について怒られたら NBANDS 増やして計算し直す
- 3) 対称化されたSymmetryではBZ内のすべてのMeshを計算出来ないで(waveの情報は対称化されている)、KPOINTSを手動でMeshを切るか、 $ISYM = -1$ (or 0) で対称性なしで一回だけ計算して、フルゾーンの波動関数を出力させること
- 4) USPP だと動かない。PAW にすること

MD後ではダメ (NSW=0)

WAVECARが必要(LWAVE = .TRUE.)

規約ゾーンではなくてフルゾーン計算

(もしトラブったら、symmetry のスイッチを **ISYM = -1** に)

USPP では動かない

NBANDSを上げておくべき

Gammna バージョンのVASP では動かない！！

complex が必要

並列計算の時は、NPAR =1 をセットしておくべき
(バンドの計算は基本それ)

ただし、新しい LOBSTER では関係ない

実は OpenMP なので OMP_NUM_THREADS を変えれば並列できる

env OMP_NUM_THREADS=16 lobster-1.2.0

実行方法

- 1) VASP計算する(固定計算などが要求、次項での注意を参照)
- 2) **lobsterin** を用意
- 3) lobster-1.2.0 実行

DOSCAR.lobster  DOSCAR.lobster: **EF->0 したVASPのDOS**
projection している DOS

ICOHPLIST.lobster

ICOOPLIST.lobster

COHPCAR.lobster  pCOHP の結果

COOPCAR.lobster  COOP の結果

lobsterout

擬ポテンシャルに注意 (valence electron)

period	group												group					
	IA	IIA											IIIA	IVA	VA	VIA	VIIA	VIIIA
1	1 1.036 2.1 H Hydrogen																	2 4.00 He Helium
2	3 6.94 1.0 Li Lithium	4 9.01 1.5 Be Beryllium											5 10.81 2.0 B Boron	6 12.01 2.5 C Carbon	7 14.007 3.0 N Nitrogen	8 15.999 3.5 O Oxygen	9 18.998 4.0 F Fluorine	10 20.18 Ne Neon
3	11 22.99 0.9 Na Sodium	12 24.31 1.2 Mg Magnesium	group										13 26.98 1.5 Al Aluminum	14 28.09 1.8 Si Silicon	15 30.97 2.1 P Phosphorus	16 32.06 2.5 S Sulfur	17 35.45 3.0 Cl Chlorine	18 39.95 Ar Argon
4	19 39.10 0.8 K Potassium	20 40.08 1.0 Ca Calcium	21 44.96 1.3 Sc Scandium	22 47.90 1.5 Ti Titanium	23 50.94 1.6 V Vanadium	24 51.996 1.6 Cr Chromium	25 54.94 1.5 Mn Manganese	26 55.85 1.8 Fe Iron	27 58.93 1.8 Co Cobalt	28 58.70 1.8 Ni Nickel	29 63.55 1.9 Cu Copper	30 65.38 1.6 Zn Zinc	31 69.72 1.6 Ga Gallium	32 72.59 1.8 Ge Germanium	33 74.92 2.0 As Arsenic	34 78.96 2.4 Se Selenium	35 79.90 2.8 Br Bromine	36 83.80 Kr Krypton
5	37 85.47 0.8 Rb Rubidium	38 87.62 1.0 Sr Strontium	39 88.91 1.3 Y Yttrium	40 91.22 1.4 Zr Zirconium	41 92.91 1.6 Nb Niobium	42 95.94 1.8 Mo Molybdenum	43 [97] Tc Technetium	44 101.07 2.2 Ru Ruthenium	45 102.91 2.2 Rh Rhodium	46 106.87 2.2 Pd Palladium	47 107.87 1.9 Ag Silver	48 112.41 1.7 Cd Cadmium	49 114.82 1.7 In Indium	50 118.69 1.8 Sn Tin	51 121.75 1.9 Sb Antimony	52 127.60 2.1 Te Tellurium	53 126.90 2.5 I Iodine	54 131.30 Xe Xenon
6	55 132.91 0.7 Cs Caesium	56 137.33 0.9 Ba Barium	57 138.91 1.1 La Lanthanum	72 178.49 1.3 Hf Hafnium	73 180.95 1.5 Ta Tantalum	74 183.85 1.7 W Tungsten	75 186.21 1.9 Re Rhenium	76 190.2 2.2 Os Osmium	77 192.22 2.2 Ir Iridium	78 195.22 2.2 Pt Platinum	79 196.97 2.4 Au Gold	80 200.59 1.9 Hg Mercury	81 204.37 1.8 Tl Thallium	82 207.2 1.8 Pb Lead	83 208.98 1.9 Bi Bismuth	84 [209] Po Polonium	85 [210] At Astatine	86 [222] Rn Radon
7	87 [223] Fr Francium	88 [226] Ra Radium	89 [227] Ac Actinium	104 [261] Rf Rutherfordium	105 [262] Db Dubnium	106 [263] Sg Seaborgium	107 [262] Bh Bohrium	108 [265] Hs Hassium	109 [268] Mt Meitnerium	110 [269] Ds Darmstadtium	111 [290] Rg Roentgenium	112 [277] Cn Copernicium	113 [297] Uut Ununtrium	114 [289] Fl Flerovium	115 [288] Uup Ununpentium	116 [289] Lv Livermorium	117 [?] Uus Ununseptium	118 [294] Uuo Ununoctium

Lanthanides	58 140.12 1.1 Ce Cerium	59 140.91 1.1 Pr Praseodymium	60 144.24 1.1 Nd Neodymium	61 [145] Pm Promethium	62 150.35 1.2 Sm Samarium	63 151.96 1.2 Eu Europium	64 157.93 1.2 Gd Gadolinium	65 158.92 1.2 Tb Terbium	66 162.50 1.2 Dy Dysprosium	67 164.93 1.2 Ho Holmium	68 167.26 1.2 Er Erbium	69 168.93 1.2 Tm Thulium	70 173.04 1.2 Yb Ytterbium	71 174.97 1.2 Lu Lutetium
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Actinides	90 232.04 Th Thorium	91 231.04 Pa Protactinium	92 238.03 U Uranium	93 237.05 Np Neptunium	94 [244] Pu Plutonium	95 [243] Am Americium	96 [247] Cm Curium	97 [247] Bk Berkelium	98 [251] Cf Californium	99 [254] Es Einsteinium	100 [257] Fm Fermium	101 [258] Md Mendelevium	102 [259] No Nobelium	103 [260] Lr Lawrencium
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lobsterin
入力のサンプル

! This is an example for the lobster control file lobster.in.

! (See, here we are using the comment function!)

! First enter the energetic window in eV (relative to the Fermi level):

COHPstartEnergy -10

COHPendEnergy 5

! Then, specify which types of valence orbitals to use:

includeorbitals s p d

! You can also specify the basis functions per element manually, e.g.:

! basisfunctions Ga 4s 4p

! basisfunctions Sr 5s 4s 4p ! Sr_sv potential

! Now define the pairs for which COHP analysis etc. should be done.

! The atoms are numbered as per order in the POSCAR file.

cohpbetween atom 1 atom 10

! If you are interested in single orbital COHPs, you can get all the pairs

! like s-s, s-p_x, ..., p_z-p_z. Uncomment this line to switch it on:

! cohpbetween atom 1 atom 2 orbitalwise

! If you want to generate the COHPPairs automatically, use this to include

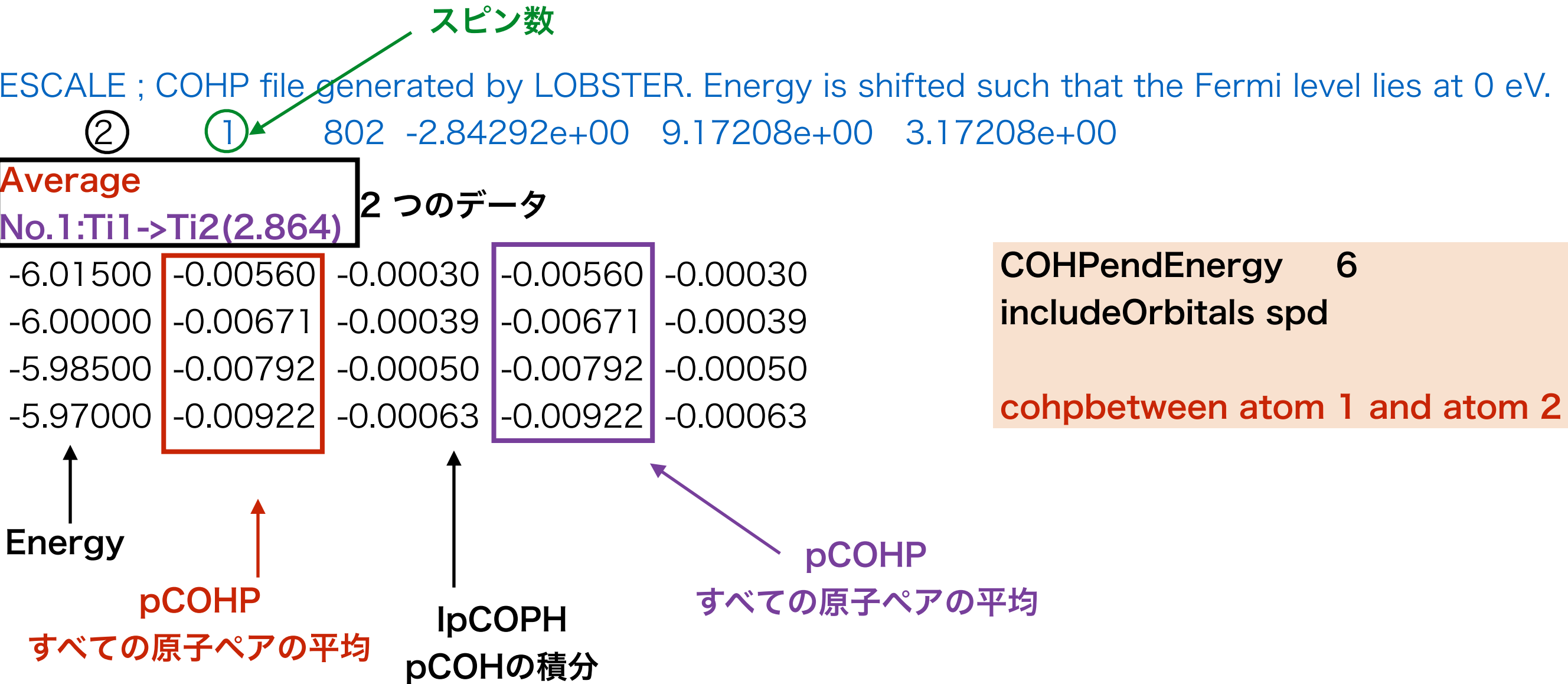
! all pairs in a given distance range (in Angstrom, not in atomic units):

! cohpGenerator from 1.4 to 1.5

COHPCAR.lobster

COHPCAR.lobster のデーター構造

- Starting in line 3, the labels for the interactions are presented, followed by the actual data.
- Column 1: energy axis, shifted such that the Fermi level lies at zero eV.
- **Column 2: pCOHP averaged over all atom pairs specified**
- Column 3: integrated pCOHP (IpCOHP) *averaged* over all atom pairs
- Column 4: pCOHP of the 1st interaction
- Column 5: integrated pCOHP of the 1st interaction
- and so on...



ESCALE ; COHP file generated by LOBSTER. Energy is shifted such that the Fermi level lies at 0 eV.

251 1 1501 -2.22622e+01 5.75646e+00 -2.58218e-01

Average

- No.1: Pd1->Zr23(2.7103)
- No.2: Pd1->O68(2.69174)
- No.3: Pd1->O69(2.10771)
- No.4: Pd2->Zr5(2.70084)
- No.5: Pd2->O27(2.10564)
- No.6: Pd2->O30(2.70242)

結合距離

- ..
- ..
- No.242: O66->O71(2.63785)
- No.243: O66->O72(2.63312)
- No.244: O67->O73(2.51636)
- No.245: O68->O69(2.77625)
- No.246: O69->O71(2.59936)
- No.247: O71->O73(2.74209)
- No.248: O71->O74(2.70153)
- No.249: O72->O73(2.64276)
- No.250: O72->O74(2.73522)

ZrO2 111 06-layer ad on 67(O),25(O)				
1.0000000000000000				
7.3204563553100970 0.000000000000000000 0.000000000000000000				
-3.1057370385276810 6.7584013041189932 0.000000000000000000				
0.00000000000000000000 0.00000000000000000000 46.6				
Pd Zr O				
2 24 48				
Selective dynamics				



O原子の74番目ではなく
トータルで74番目のO原子の意味

DOSCAR.lobster

基本はDOSCARと同じ構造だが、

原子種ごとに軌道成分の射影が異なるので注意する
DOSCAR中で確認するか、対応する lobsterout を参照

6.01468	37.64482	798.91476								
6.01467645	-22.00400267	1501	-0.25821758	1.000000000						
4d_xy 4d_yz 4d_z^2 4d_xz 4d_x^2-y^2					Z= 46; 4s 4p_y 4p_z 4p_x					
-22.00400	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-21.98532	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
...										
9.99333	0.66586	14.06648								
10.01668	0.67006	14.08207								
10.01667779	-25.00667111	1501	-2.12269405	1.000000000						
Z= 6; 2s 2p_y 2p_z 2p_x										
-25.00667	0.00000	0.00000	0.00000	0.00000						
-24.98332	0.00000	0.00000	0.00000	0.00000						
-24.95997	0.00000	0.00000	0.00000	0.00000						

VASP オリジナルの DOSCAR には
存在しない表示項目

lobsterin の設定項目でプロジェクションする軌道を変更するので
COHP解析に対応する軌道成分はここを参照する必要がある

initializing LCAO-system...

setting up local basis functions...

O (Bunge) 2s 2p_y 2p_z 2p_x

Pd (Bunge) 4s 4p_y 4p_z 4p_x 4d_xy 4d_yz 4d_z^2 4d_xz 4d_x^2-y^2

Zr (Bunge) 5s 4p_y 4p_z 4p_x 4d_xy 4d_yz 4d_z^2 4d_xz 4d_x^2-y^2

lobsterout

lobsterout ファイルに対応する軌道が書いてある

解析手順、虎の巻

lobsterin で、適当な距離で結合を探すように指定したとき

Pd原子が対となっている COHP解析した結合成分の抽出

```
cat COHPCAR.lobster | grep No | grep Pd
```

No.1: Pd1->Zr24(2.68368)

No.2: Pd1->O70(2.07237)

No.3: Pd2->Zr6(2.68683)

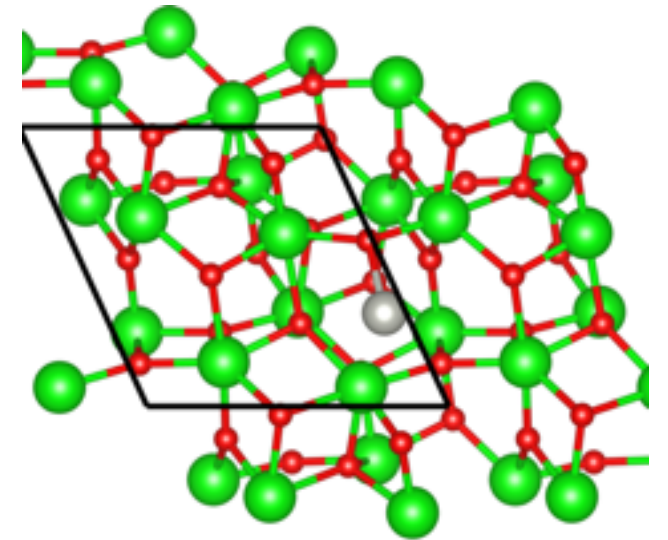
No.4: Pd2->O28(2.07382)

Pd1 と O70 の局所状態密度
&COHP をチェックする

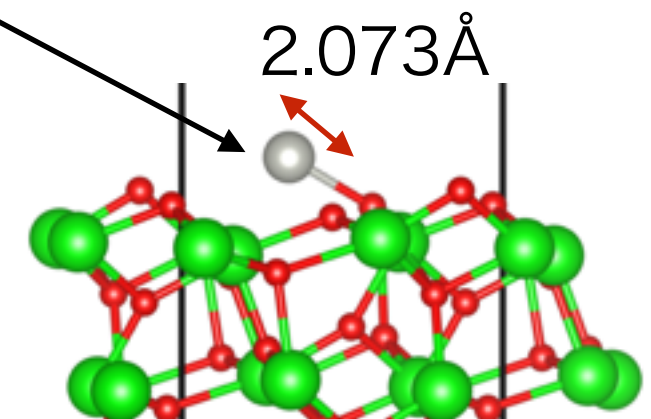
NSW=50

ad_on_68

(b-1)



(b-2)

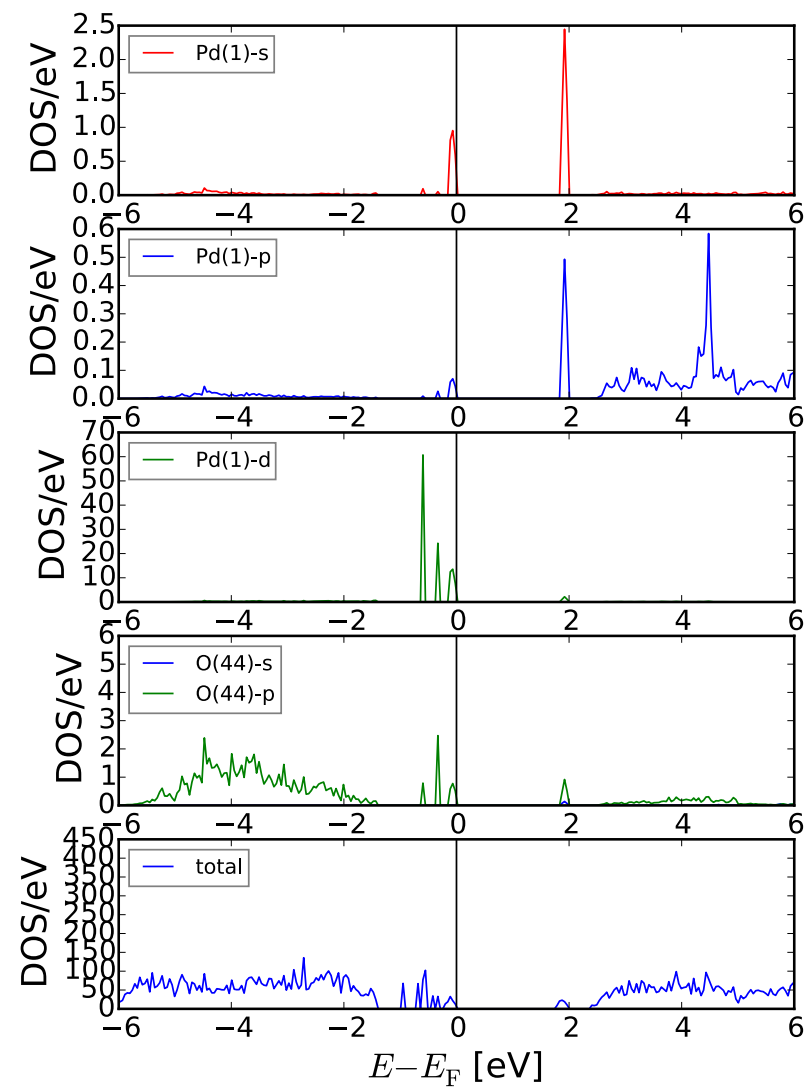


O70 (ローカルではO44)

生 DOSCAR から

on 68(0)

O44 (70)



DOSCAR.lobster の解析

COHP解析と対になる電子状態のプロジェクトションを確認

拙作: [VgetCOHPinfo.py](#)

O :[4] 2s 2p_y 2p_z 2p_x

Pd :[9] 4s 4p_y 4p_z 4p_x 4d_xy 4d_yz 4d_z^2 4d_xz 4d_x^2-y^2

Zr :[9] 5s 4p_y 4p_z 4p_x 4d_xy 4d_yz 4d_z^2 4d_xz 4d_x^2-y^2

Pd は、s,p,d 軌道ともに計算

O は sp 軌道で計算

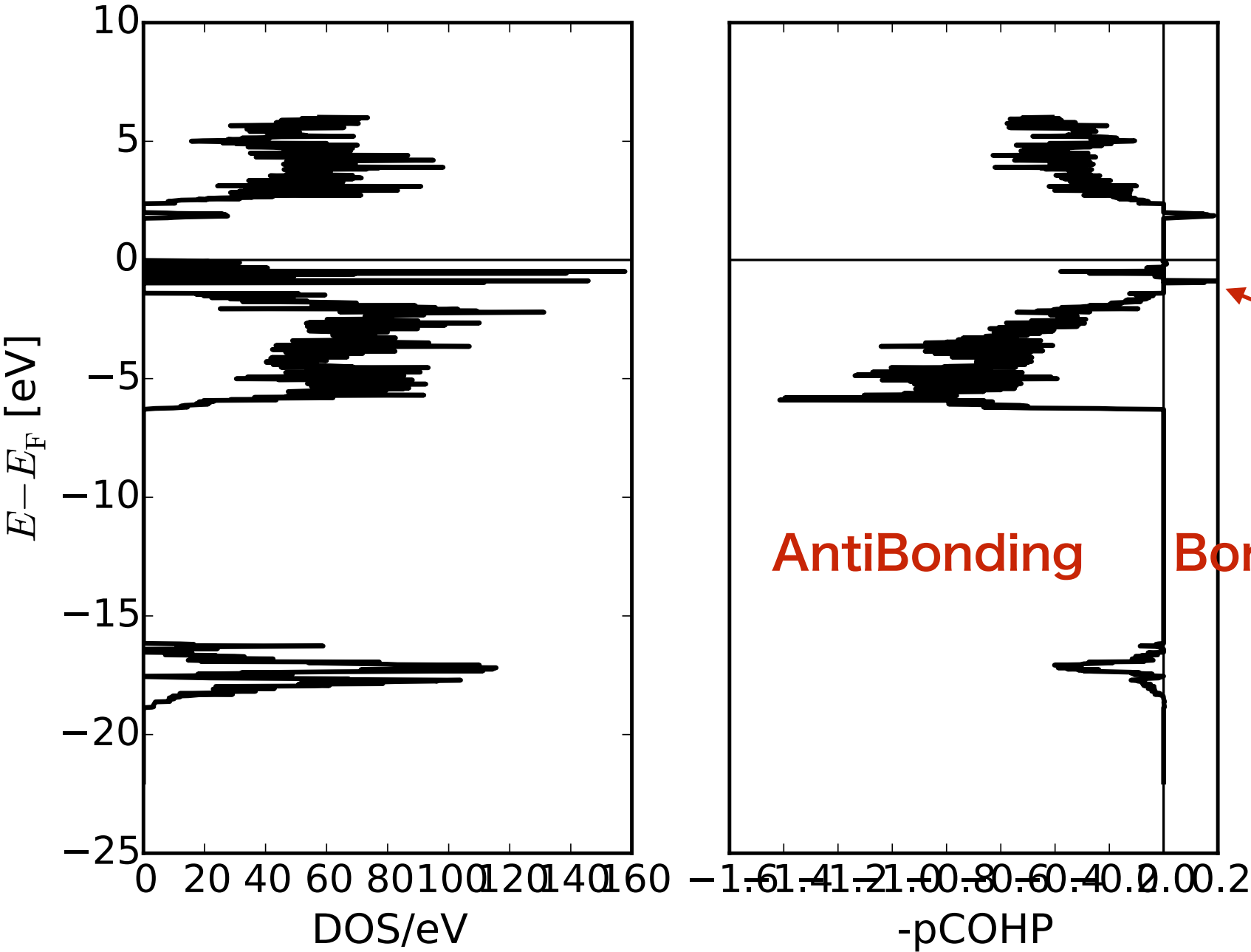
[lobsterin](#) で指定した軌道の計算の確認でもある

拙作: VplotCOHP_tate.py
COHP 解析をざっくりとする

NSW=50, ad_on_68 (044(70))

???

ちょっと意味不明
AntiBonding がValence
の下からある



Pd-O
Bonding ?

この計算、ほんとか？
間違った計算??

擬ポテンシャルのチョイスに注意

period	group												group					
	IA	IIA											IIIA	IVA	VA	VIA	VIIA	VIIIA
1	1 1.036 2.1 H Hydrogen																	2 4.00 He Helium
2	3 6.94 1.0 Li Lithium	4 9.01 1.5 Be Beryllium											5 10.81 2.0 B Boron	6 12.01 2.5 C Carbon	7 14.007 3.0 N Nitrogen	8 15.999 3.5 O Oxygen	9 18.998 4.0 F Fluorine	10 20.18 Ne Neon
3	11 22.99 0.9 Na Sodium	12 24.31 1.2 Mg Magnesium	group										13 26.98 1.5 Al Aluminum	14 28.09 1.8 Si Silicon	15 30.97 2.1 P Phosphorus	16 32.06 2.5 S Sulfur	17 35.45 3.0 Cl Chlorine	18 39.95 Ar Argon
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5	37 85.47 0.8 Rb Rubidium	38 87.62 1.0 Sr Strontium	39 88.91 1.3 Y Yttrium	40 91.22 1.4 Zr Zirconium	41 92.91 1.6 Nb Niobium	42 95.94 1.8 Mo Molybdenum	43 [97] Tc Technetium	44 101.07 2.2 Ru Ruthenium	45 102.91 2.2 Rh Rhodium	46 106.87 2.2 Pd Palladium	47 107.87 1.9 Ag Silver	48 112.41 1.7 Cd Cadmium	49 114.82 1.7 In Indium	50 118.69 1.8 Sn Tin	51 121.75 1.9 Sb Antimony	52 127.60 2.1 Te Tellurium	53 126.90 2.5 I Iodine	54 131.30 Xe Xenon
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additional
basis functions



refitted
basis functions



unchanged
basis functions



no PAW-PBE
pseudo potentials

Lanthanides	58 140.12 1.1 Ce Cerium	59 140.91 1.1 Pr Praseodymium	60 144.24 1.1 Nd Neodymium	61 [145] Pm Promethium	62 150.35 1.2 Sm Samarium	63 151.95 1.2 Eu Europium	64 157.95 1.2 Gd Gadolinium	65 158.92 1.2 Tb Terbium	66 162.50 1.2 Dy Dysprosium	67 164.93 1.2 Ho Holmium	68 167.26 1.2 Er Erbium	69 168.93 1.2 Tm Thulium	70 173.04 1.2 Yb Ytterbium	71 174.97 1.2 Lu Lutetium
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Actinides	90 232.04 Th Thorium	91 231.04 Pa Protactinium	92 238.03 U Uranium	93 237.05 Np Neptunium	94 [244] Pu Plutonium	95 [243] Am Americium	96 [247] Cm Curium	97 [247] Bk Berkelium	98 [251] Cf Californium	99 [254] Es Einsteinium	100 [257] Fm Fermium	101 [258] Md Mendelevium	102 [259] No Nobelium	103 [260] Lr Lawrencium
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拙作: VP スクリプト

擬ポテンシャルのチェック

NUMBER OF ATOMS= 3

NUMBER OF LISTS= 3

PAW_PBE **Pd_pv** 28Jan2005 EMAX= 250.925 (EMAX*1.3=326.203) **VRHFIN= 4p5s4d** ZVAL= 16.000

PAW_PBE **Zr_sv** 04Jan2005 EMAX= 229.898 (EMAX*1.3=298.867) **VRHFIN= 4s4p5s4d** ZVAL= 12.000

PAW_PBE O 08Apr2002 EMAX= 400.000 (EMAX*1.3=520) VRHFIN= s2p4 ZVAL= 6.000

lobsterin のサンプル

! You can also specify the basis functions per element manually, e.g.:

! basisfunctions Ga 4s 4p

! basisfunctions Sr 5s 4s 4p ! Sr_sv potential

Pd_{pv} 4p6, 4d10, 5s0 ZVAL=16

Zr_{sv} 4s2,4p6, 4d2, 5s2 ZVAL=12



lobsterin のサンプル

```
basisfunctions Pd 4p 5s 4d    ! Pd_pv  
basisfunctions Zr 4s 4p 5s 4d ! Zr_sv
```

！ ！ ！ 基底関数の修正が必要 ！ ！

計算中に出た様々な問題の検証

計算テスト中に出た謎のエラー

lobster

WARNING: If this value deviates too much from zero, please contact the author.

WARNING: PAW bands of k-point 0.111111 -0.222222 0.4

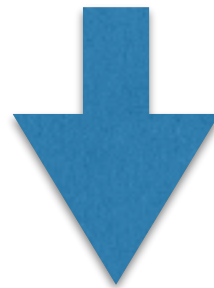
WARNING: only fulfill orthonormality with an accuracy of 9.99318e-05

WARNING: If this value deviates too much from zero, please contact the author.

WARNING: PAW bands of k-point 0.222222 -0.222222 0.4

WARNING: only fulfill orthonormality with an accuracy of 0.000104171

WARNING: If this value deviates too much from zero, please contact the author.



小さいunit-cell で LREAL が True の時に起きることが判明

記憶によれば、昔のVASPだと小さいセルだと

LREAL = Auto

としていると自動で False になったはずだが・・・

チェックしてみると、なぜか Auto で計算すると、

LREAL が True になっている

明示的に

LREAL = .False.

とすれば OK

現バージョン(2015.08.27 or 5.3.5) では LREAL は

Auto or A

projection done in real space,
fully automatic optimization of projection operators
no user interference required

注意)

Real Space にプロジェクションする

もっと単純なテスト
Pd-foil (FCC-Pd)

擬ポテンシャル: Pd

cohstartenergy -22

cohpendenergy 6

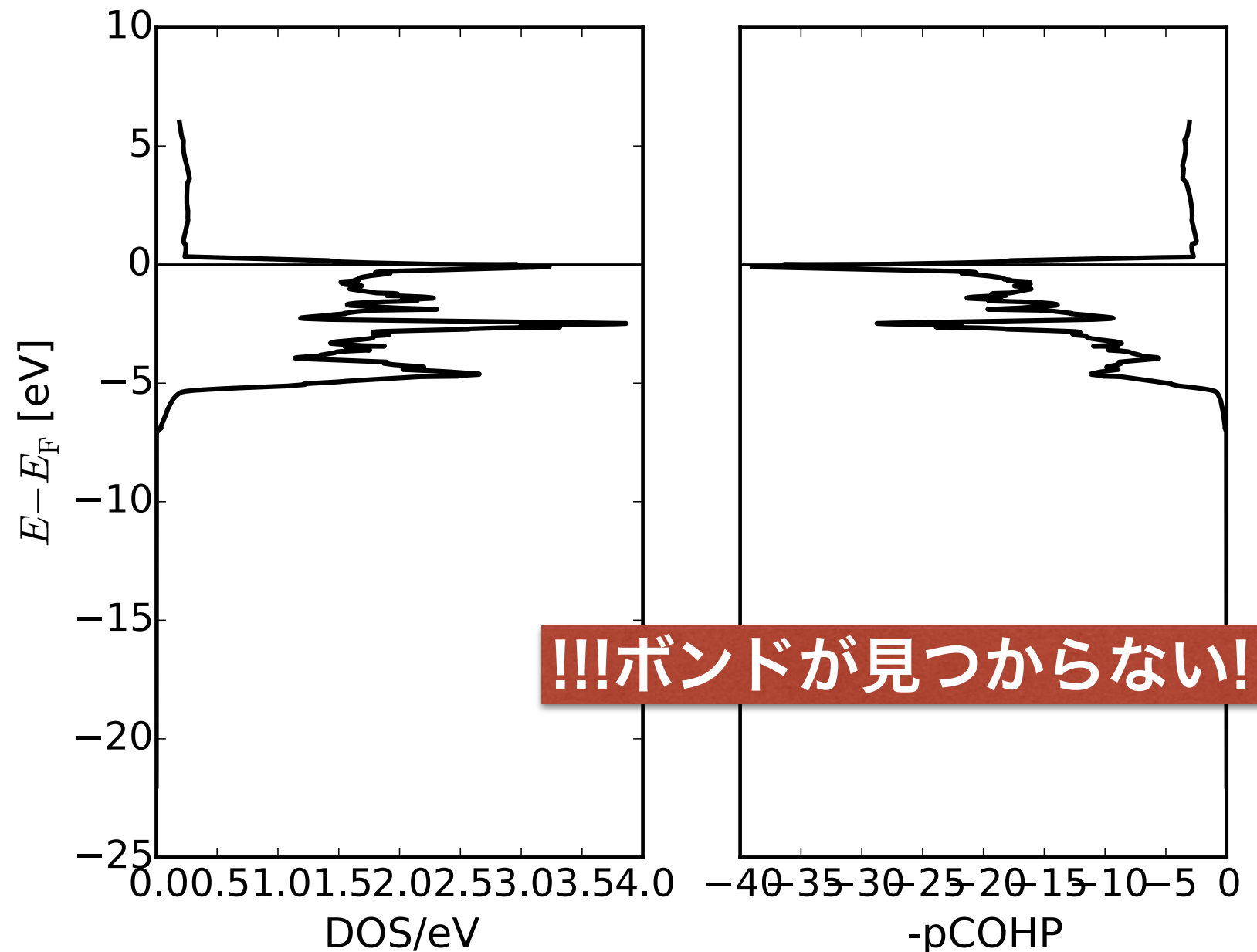
includeOrbitals spd

cohpbetween atom 1 atom 1

K: 12 12 12 gamma

Tetrahedron Method

**FCC の基本並進ベクトルで
FCC構造を作成**



Pd (Bunge) 4s 4p_y 4p_z 4p_x 4d_xy 4d_yz 4d_z^2 4d_xz 4d_x^2-y^2

NUMBER OF ATOMS= 1

NUMBER OF LISTS= 3

PAW_PBE Pd 04Jan2005 EMAX= 250.925 (EMAX*1.3=326.203) **VRHFIN= s1 ZVAL= 10.000**

Pd でボンディングバンドが見つからない！！

ログをよく見ると

WARNING: You did not specify any COHP pairs in the lobsterin file. As default
WARNING: I will try to find any pairs between 1.0 and 3.0 Å distance,
WARNING: but that might be wrong. If you want pCOHPs or pCOOPs, change the lobsterin!
found 0 interactions.

COHP ペアが見つからない (ボンドが見つからない)

FCC の基本並進ベクトルで
FCC構造を作成

FCC Pd $a=3.89$ (obs)

3.89

0.000000 0.500000 0.500000

0.500000 0.000000 0.500000

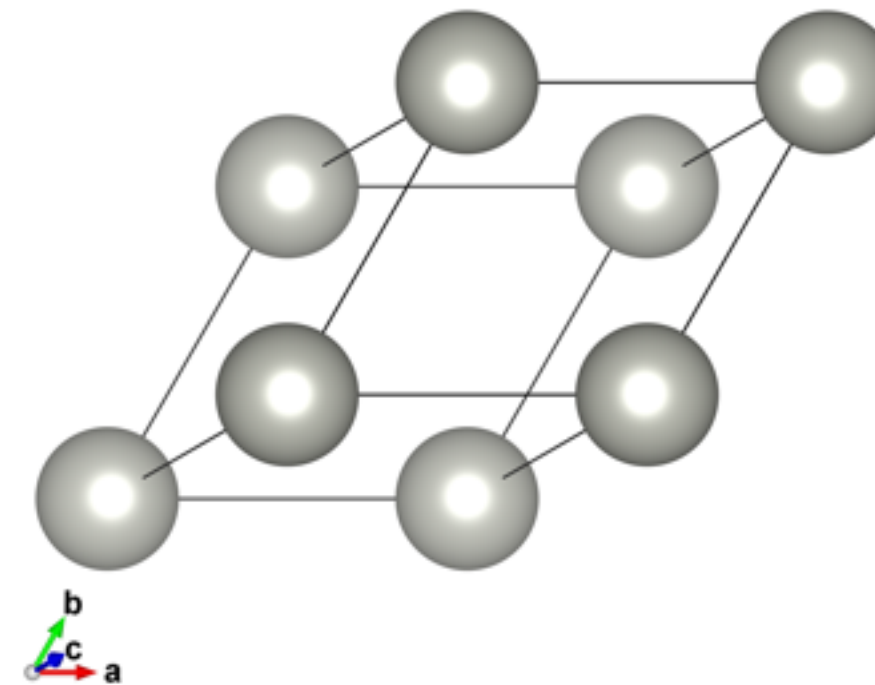
0.500000 0.500000 0.000000

Pd

1

Direct

0.000000 0.000000 0.000000



単位胞に一つの原子

on-site で結合の議論は出来ない・・・っぽい

SC の基本並進ベクトルで
FCC構造を作成

Pd P1 cubic (FCC)

3.89

1.000000 0.000000 0.000000

0.000000 1.000000 0.000000

0.000000 0.000000 1.000000

Pd

4

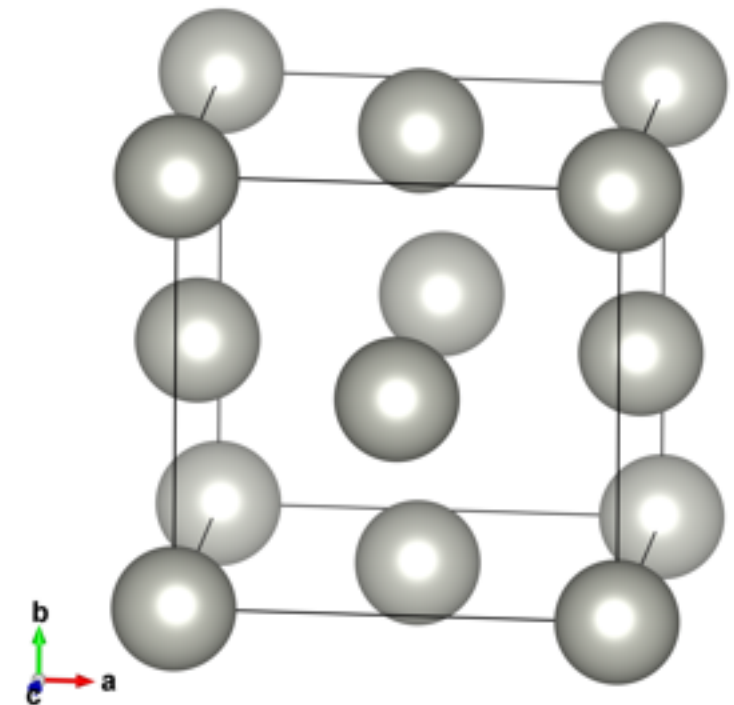
Direct !! (Direct or Cartesian)

0.000000 0.000000 0.000000

0.500000 0.500000 0.000000

0.500000 0.000000 0.500000

0.000000 0.500000 0.500000



解析にバンドが少ないときはこのエラーが出る

Pd (Bunge) 4s 4p_y 4p_z 4p_x 4d_xy 4d_yz 4d_z^2 4d_xz 4d_x^2-y^2

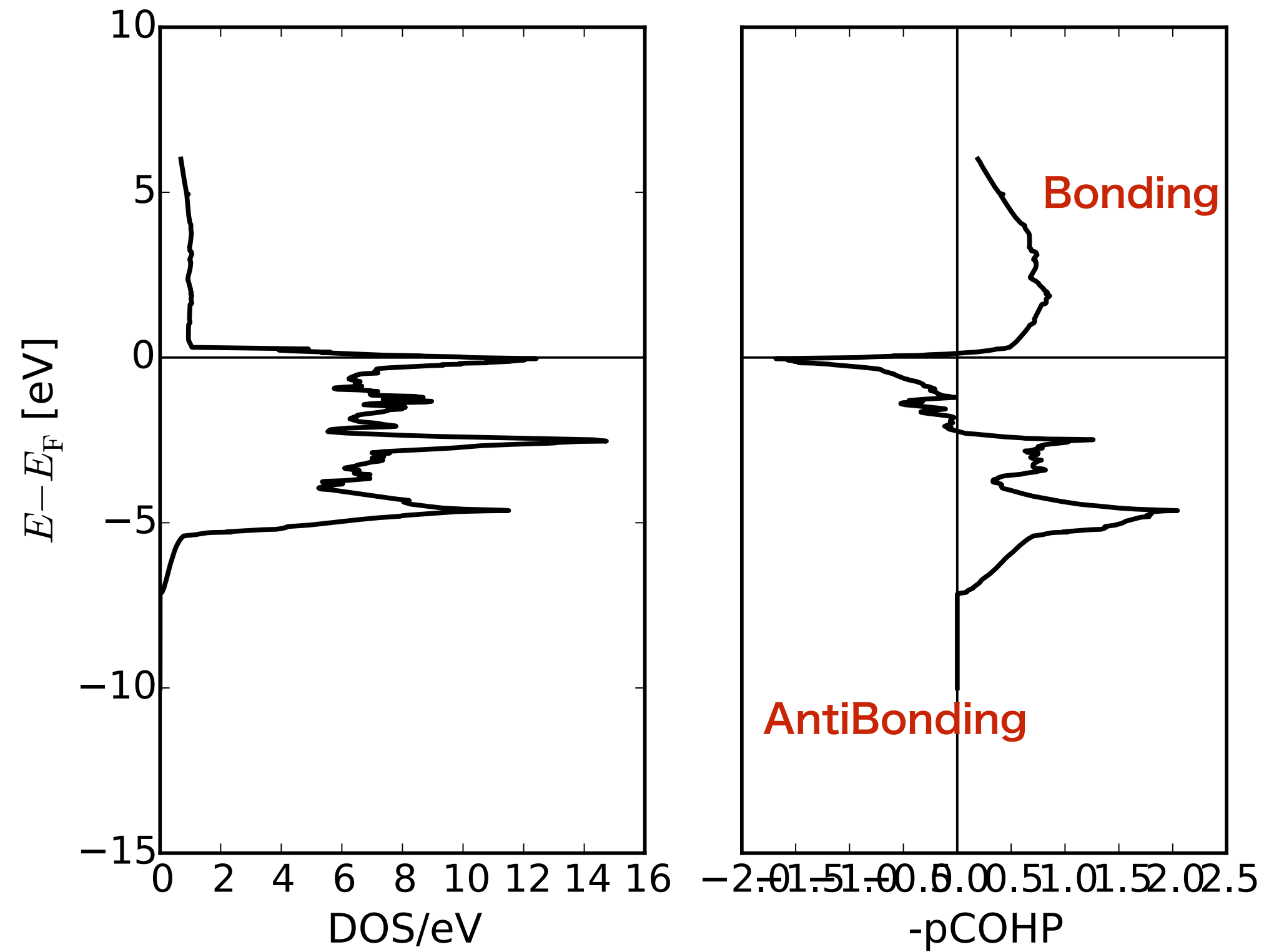
WARNING: You are employing too few bands in you PAW calculation. To reconstruct

WARNING: the Hamilton matrix in the local basis, you need to use at least

WARNING: **36 bands**. pCOHP analyses will be disabled. Please check the manual!

(指定したエネルギーの範囲の) 解析には
最低 38 のバンドが必要
—> NBANDS の修正

FCC Pd の COHP 解析



気になるログの出力

WARNING: You are using a symmetrized k-point grid. If you don't know what that means
WARNING: stop here and check the manual. Prepare a k-point grid that spans the whole
WARNING: Brillouin zone, restart your quantum-mechanical calculation and try again!

**KPOINTS は symmetrize k-points を使っているので、
IBZ の中を全部Mesh切りしてないので注意せよ！**

WAVE は対称性なしで計算するか

KPOINTS ファイルを手動でゾーンすべてを分断すること

lobster のマニュアル

LOBSTER does not yet deal with **k**-point symmetry—in other words, your VASP `WAVECAR` must contain results for the *entire* mesh, not only the irreducible one usually given in the `IBZKPT` file. To get out of trouble, **you must switch off symmetry in the INCAR (`ISYM = -1`) completely.**

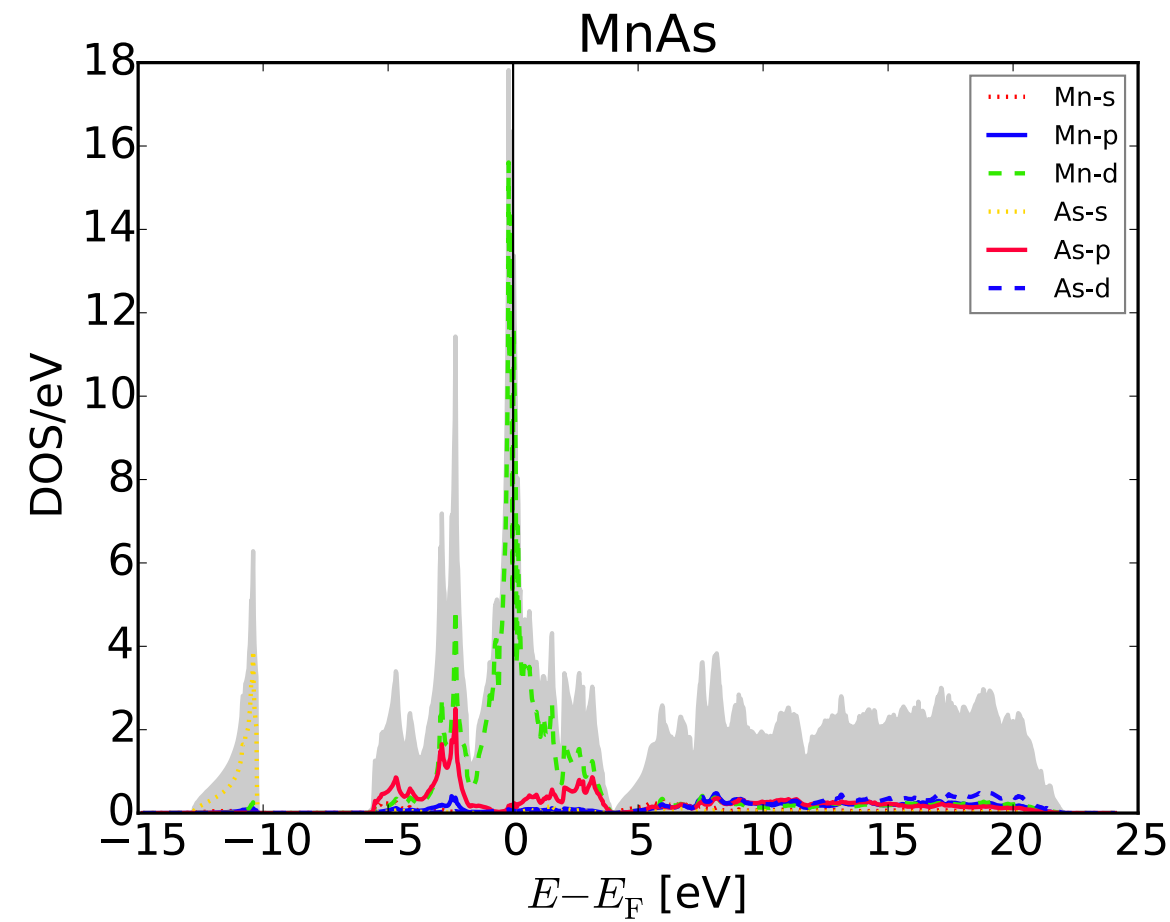
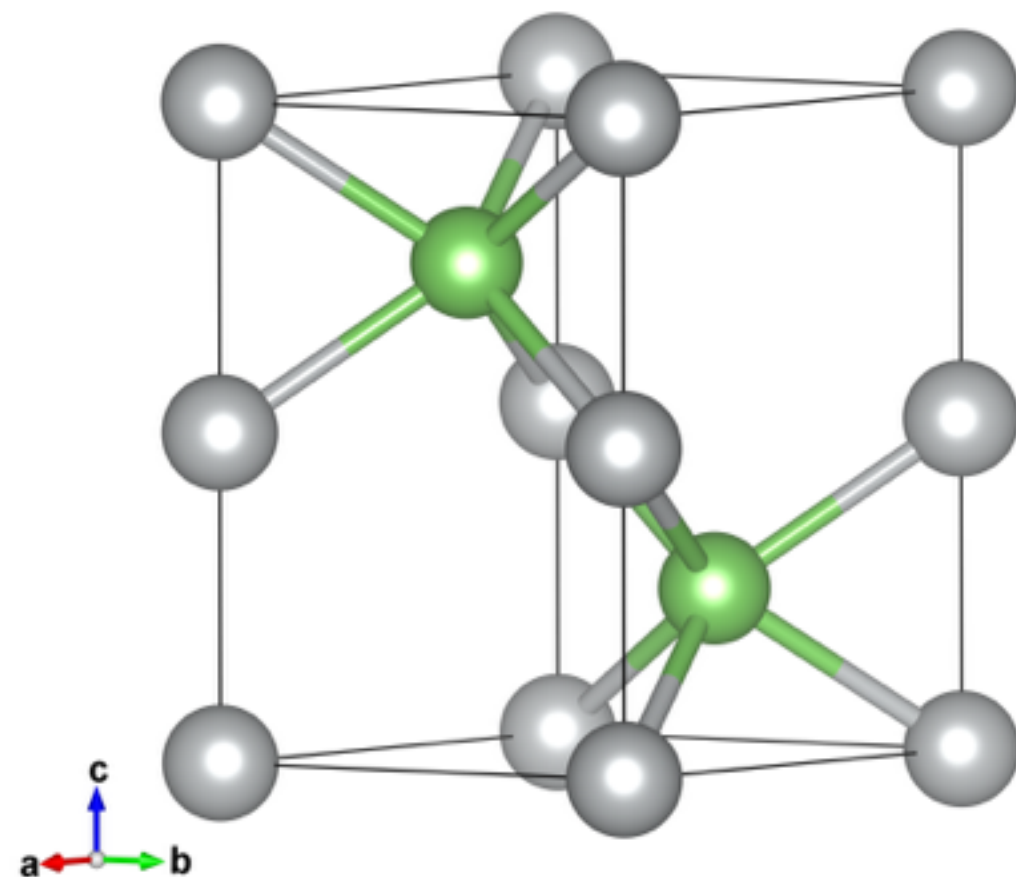
ISYM の変更に関する諸々のテスト

NiAs-type MnAs (a=3.71, c=5.69)

3.71		
0.500000	-0.8660254038	0.000000
0.500000	0.8660254038	0.000000
0.000000	0.000000	1.53369272

Ni As
2 2

Direct		
0.000000	0.000000	0.000000
0.000000	0.000000	0.500000
0.3333333333	0.6666666667	0.250000
0.6666666667	0.3333333333	0.750000



ISYM = 2

NKPTS = 270 (16x16x16 Gamma)

Total: 52.673 (sec)

```
DAV: 9  -0.265764577116E+02  0.18564E-01  -0.36152E-02 28988  0.158E+00  0.655E-01
DAV: 10  -0.265751401125E+02  0.13176E-02  -0.49996E-03 29172  0.376E-01  0.281E-01
DAV: 11  -0.265752688227E+02  -0.12871E-03  -0.14210E-04 18376  0.597E-02  0.987E-02
DAV: 12  -0.265752359435E+02  0.32879E-04  -0.66553E-05 12748  0.823E-02
1 F= -.26575236E+02 E0= -.26575236E+02 d E =0.000000E+00
```

ISYM = -1 (default)

K点の数16倍

NKPTS = 4096 (16x16x16 Gamma)

Total: 960.985 (sec)

```
DAV: 12  -0.265756815775E+02  0.34223E-03  -0.96579E-03449112  0.280E-01  0.545E-01
DAV: 13  -0.265752774340E+02  0.40414E-03  -0.44470E-03213624  0.148E-01  0.947E-02
DAV: 14  -0.265752708157E+02  0.66182E-05  -0.70597E-04199040  0.929E-02
1 F= -.26575271E+02 E0= -.26575271E+02 d E =0.000000E+00
```