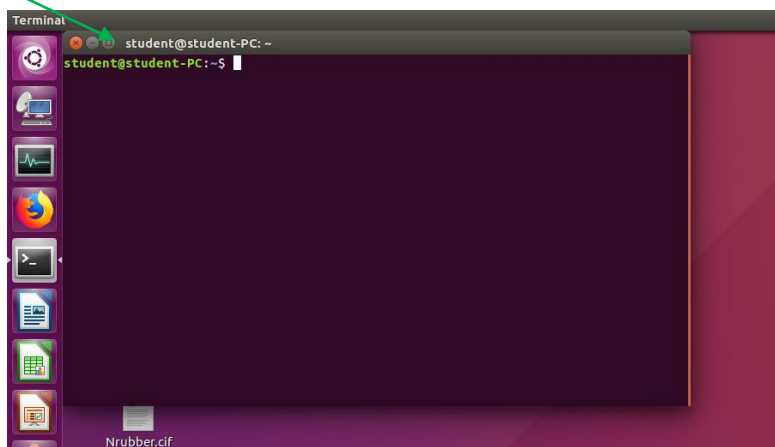
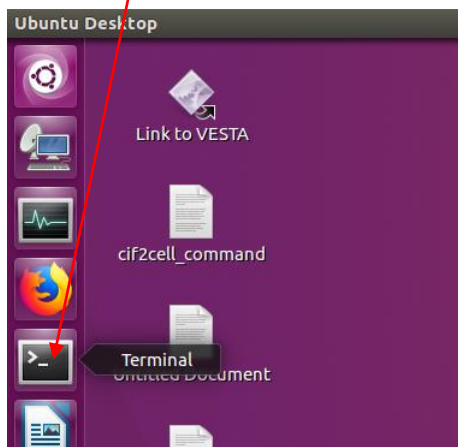


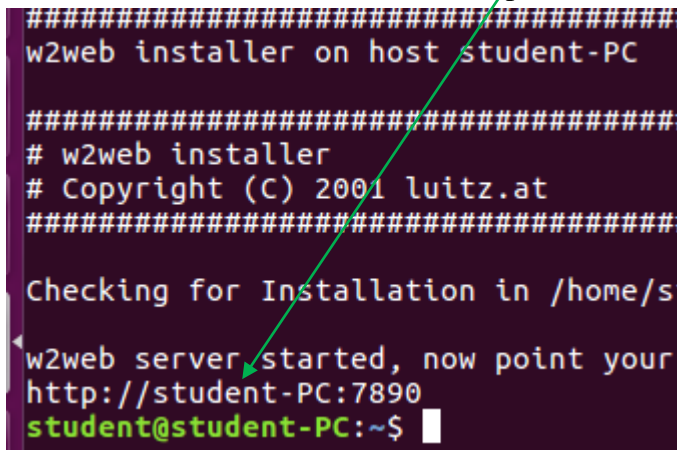
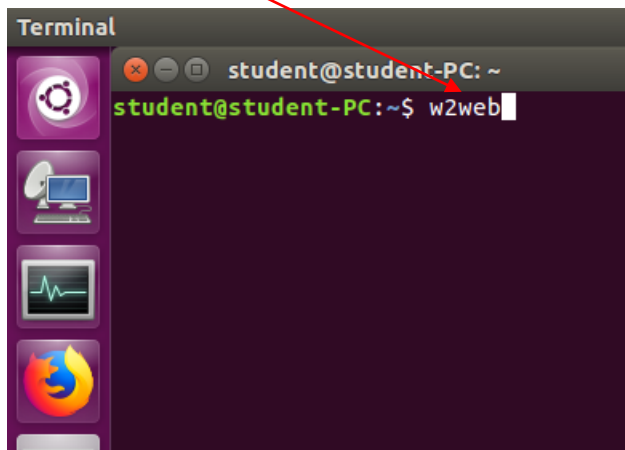
はじめての第一原理計算 (実習) WIEN2k 操作マニュアル

■ GUI(w2web)の起動

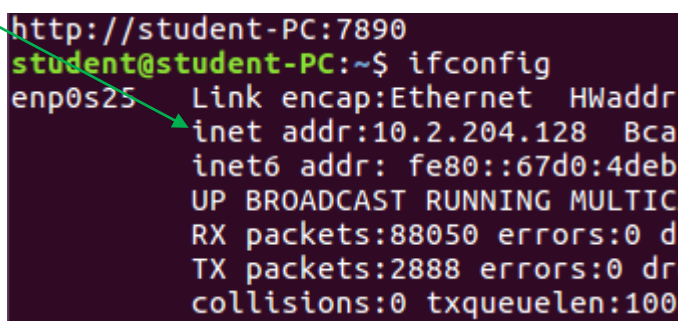
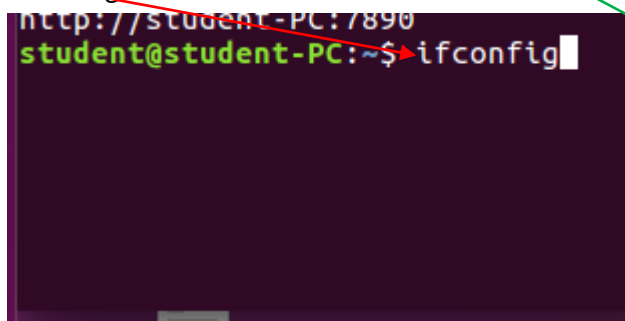
1. Terminal をクリック > Terminal のウィンドウが開く



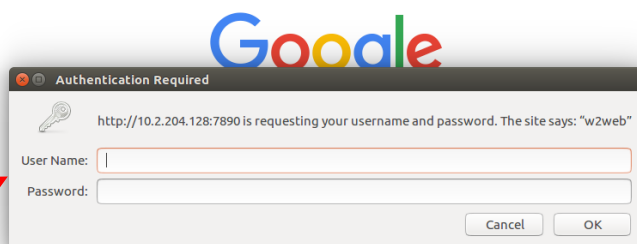
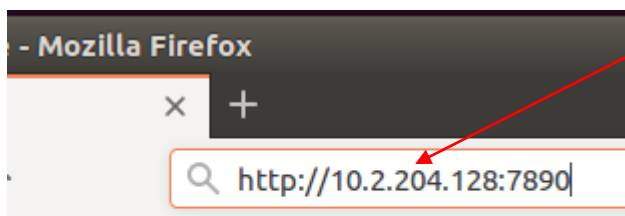
2. Terminal上で w2web と入力して Enter を押す > GUI(w2web)のURLが表示される (httpのある行)



3. ifconfig と入力して Enter を押す > IPアドレス (inet addr) の情報が得られる



4. Firefox や Safariなどを開いて、GUI(w2web)のURLの//から:までをIPアドレスに変えて入力

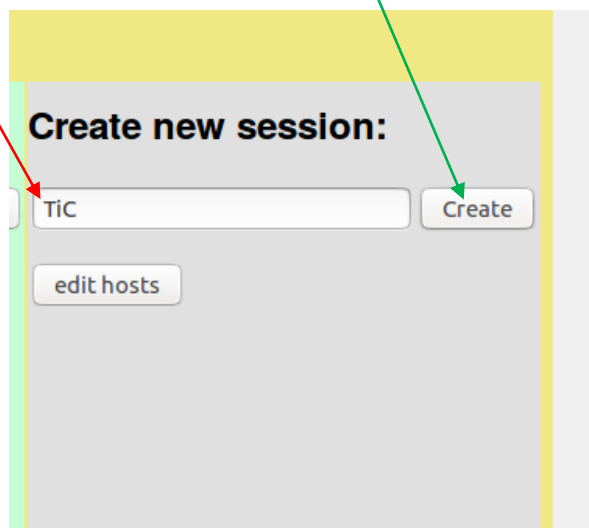
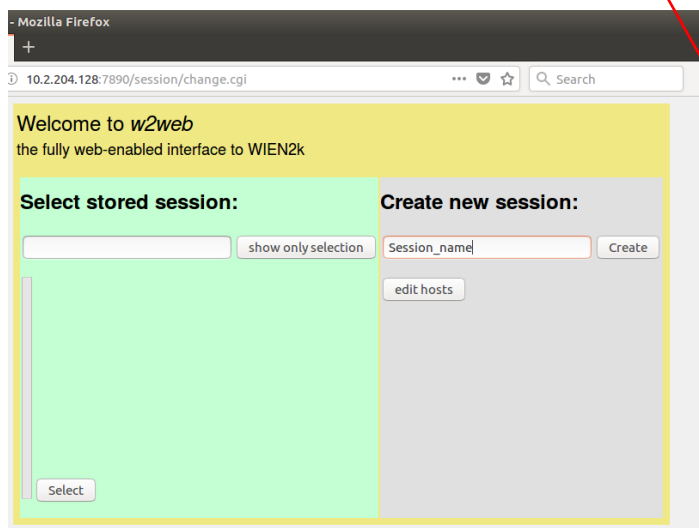


5. WIEN2kのUser NameとPasswordを聞かれるので入力

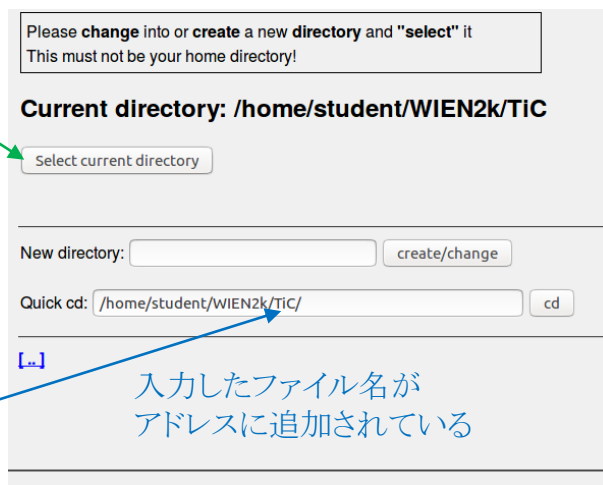
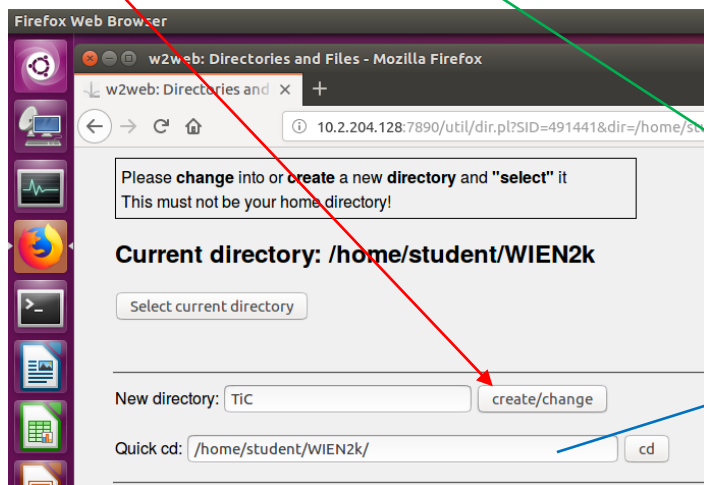
※ Linux PCに電源を入れたときに一度だけ行えばよい。上記の4以降は他のPCからでも行える

■ GUI(w2web)の操作 -1- (作業場所(フォルダ)の作成)

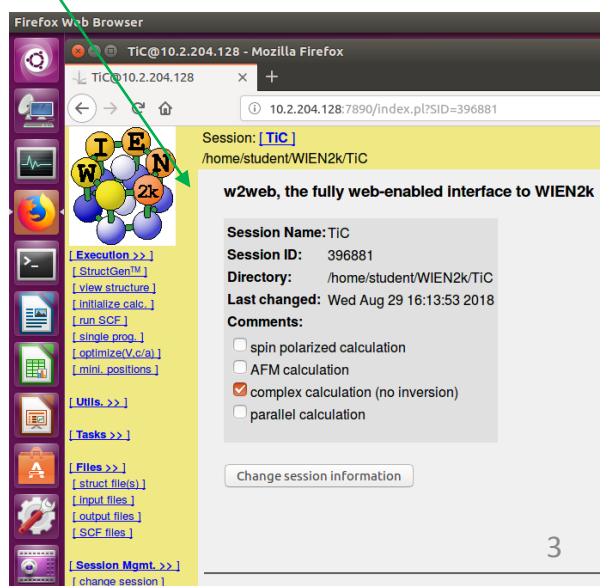
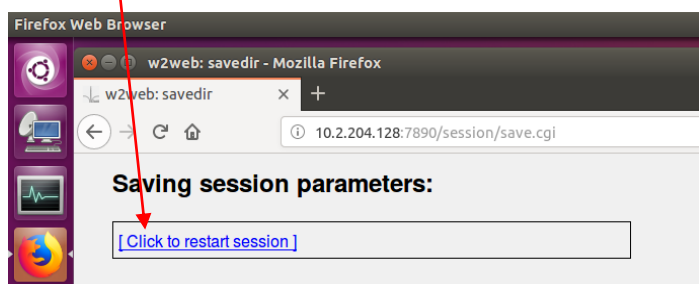
1. GUI(w2web)の画面 > Create new sessionの下に好きなファイル名を入力 > Create をクリック



2. create/change をクリック > Select current directory をクリック

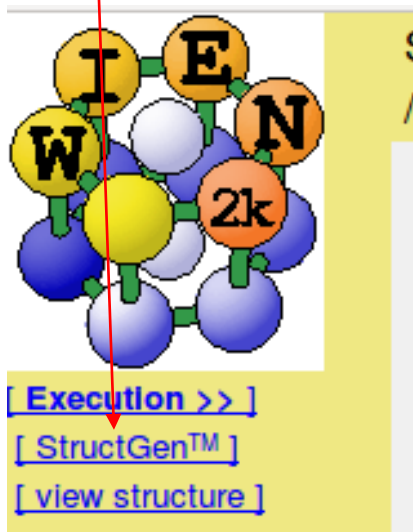


3. Click to restart session をクリック > 計算条件を入力する画面が得られる



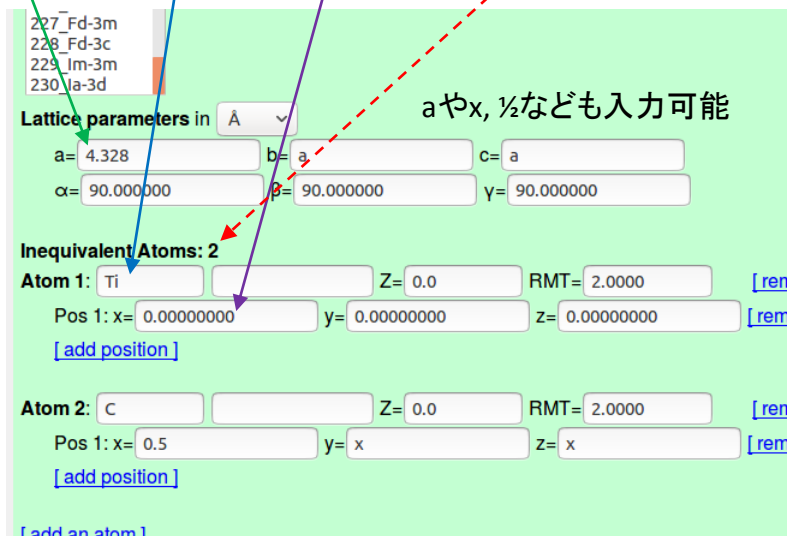
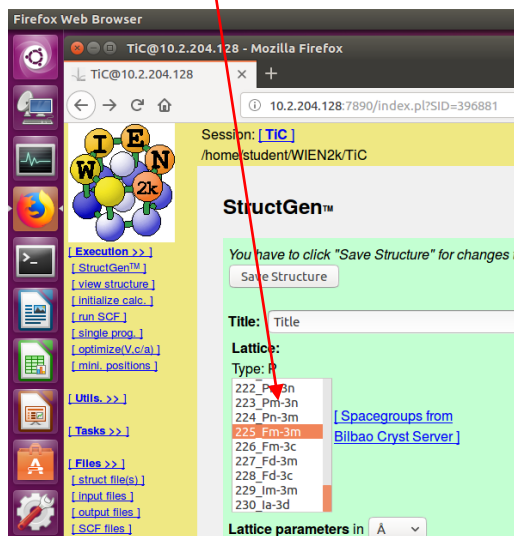
■ GUI(w2web)の操作 -2- (結晶構造の入力)

4. StructGen™ をクリック > 原子数を入力し、Generate template をクリック

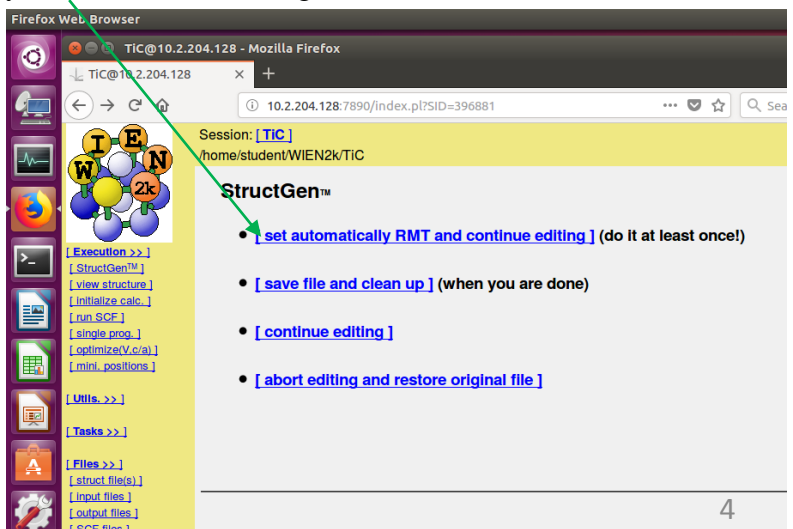
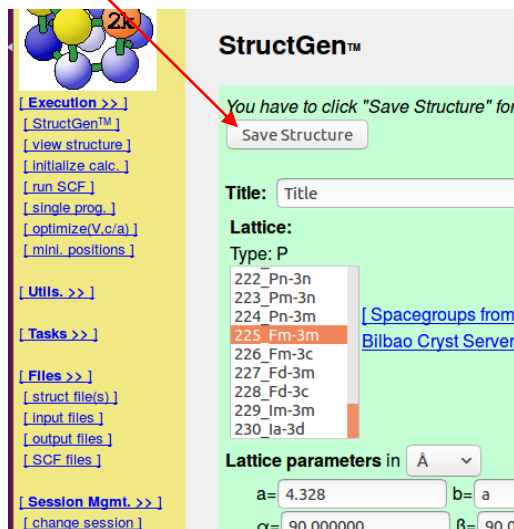


原子の数は、空間群を考慮したときに必要になる原子数。ハンドブックやcifに記載されている最小の原子数でよい

5. Lattice の下の欄から空間群を選択 > 格子定数、元素記号、原子座標を入力

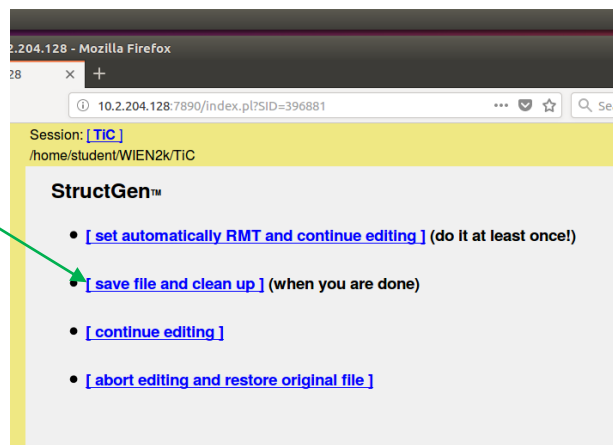
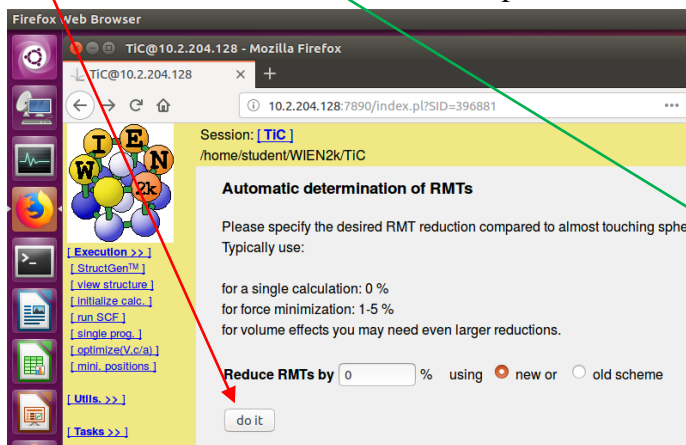


6. Save structure をクリック > set automatically RMT continue editing をクリック

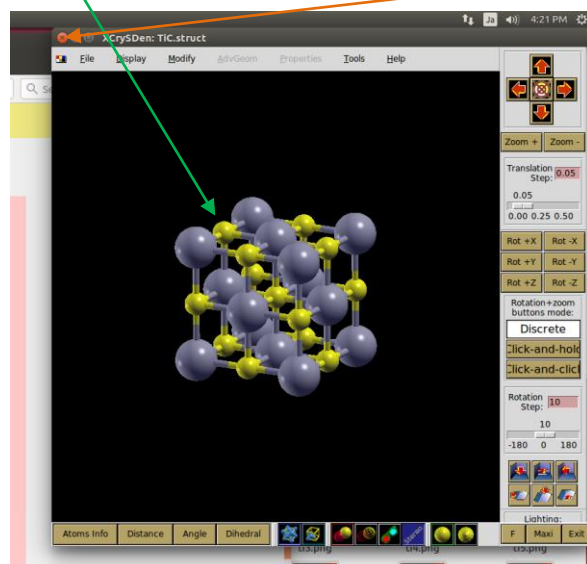
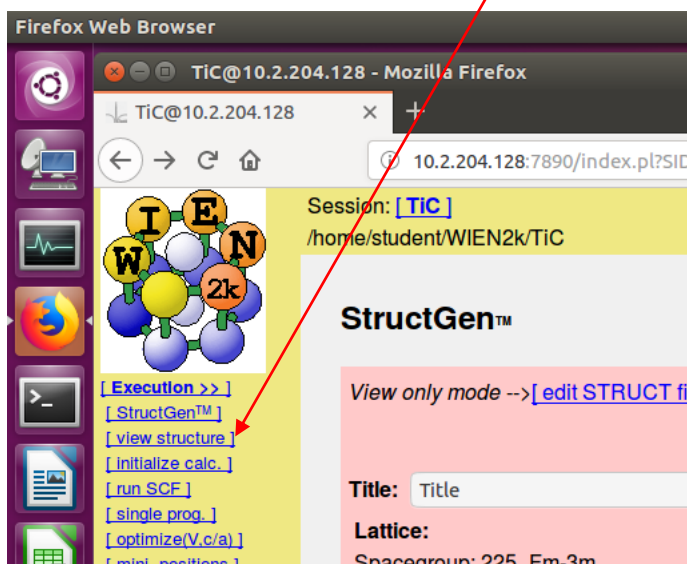


■ GUI(w2web)の操作 -3- (結晶構造の入力)

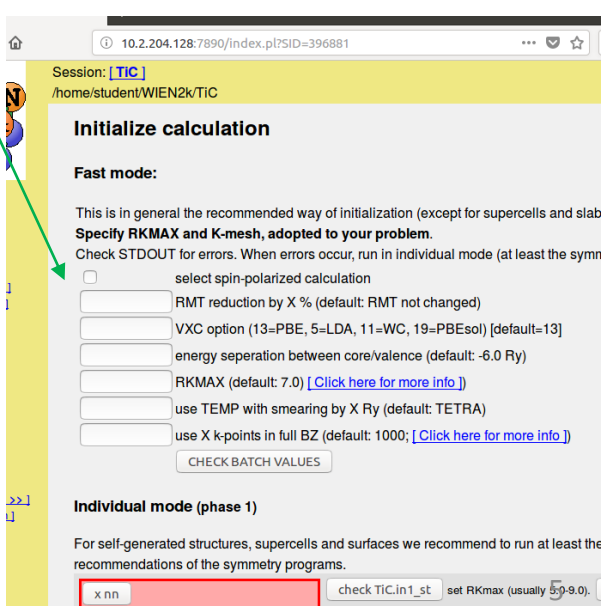
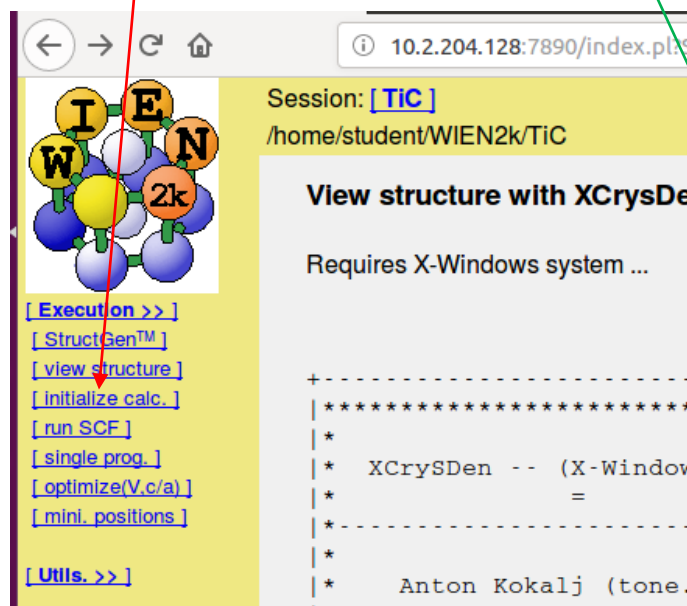
7. Do it をクリック > save file and clean up をクリック



8. ピンク色の画面が得られる > view structure をクリック > 結晶構造が表示される > 確認後×で閉じる



9. Initialize calc. をクリック > 計算条件を入力する画面が表示される



■ GUI(w2web)の操作 -4- (計算条件の設定)

10. k点数=1000/(計算する系の体積/23.29)を入力 > CHECK BATCH VALUES

Fast mode:

This is in general the recommended way of initialization (except for supercells). **Specify RKMAX and K-mesh, adopted to your problem.** Check STDOUT for errors. When errors occur, run in individual mode (at least)

☐ select spin-polarized calculation

RMT reduction by X % (default: RMT not changed)

VXC option (13=PBE, 5=LDA, 11=WC, 19=PBEsol) [default=

energy separation between core/valence (default: -6) Ry

RKMAX (default: 7.0) [\[Click here for more info\]](#)

use TEMP with smearing by X Ry (default: TETRA)

288 use X k-points in full BZ (default: 1000; [\[Click here for mo](#)

23.29 = 2.856^3 = BCC Feの体積

水素を含んだ有機化合物は
デフォルトの7.0では
精度が高過ぎて時間がかかるので
RKMAXに4を入力する

11. RUN BATCH INITIALISATION をクリック > View STDOUT をクリック

Fast mode:

This is in general the recommended way of initialization (except for supercells). **Specify RKMAX and K-mesh, adopted to your problem.** Check STDOUT for errors. When errors occur, run in individual mode (at least)

☐ select spin-polarized calculation

RMT reduction by X % (default: RMT not changed)

VXC option (13=PBE, 5=LDA, 11=WC, 19=PBEsol) [default=

energy separation between core/valence (default: -6) Ry

RKMAX (default: 7.0) [\[Click here for more info\]](#)

use TEMP with smearing by X Ry (default: TETRA)

288 use X k-points in full BZ (default: 1000; [\[Click here for mo](#)

Your input seems to be ok and you can start

Session: [\[TIC\]](#)
/home/student/WIEN2k/TiC

Commandline: `init_lapw -bw -numk 288`
Program input is: ""

`cd /home/student/WIEN2k/TiC; echo '' | in`

[\[View STDOUT \]](#) to monitor the progress of this command

Execute another command line:

Type of execution: interactively

12. reload in reverse order をクリック > init_lapw finished ok で計算の準備が整う

Show STDOUT

```

next is setrmt
next is nn
specify nn-bondlength factor: (usually=2) [and optic
1.d-5, 20]]
DSTMAX: 20.00000000000000
iix,iyy,iiz 5 5 5 40
40.8936900000000 40.8936900000000

ATOM 1 Ti ATOM 2 C
RMT( 1)=2.24000 AND RMT( 2)=1.83000
SUMS TO 4.07000 LT. NN-DIST= 4.08937

ATOM 2 C ATOM 1 Ti
RMT( 2)=1.83000 AND RMT( 1)=2.24000
SUMS TO 4.07000 LT. NN-DIST= 4.08937
NN ENDS
0.0u 0.0s 0:00.00 0.0% 0+0k 0+32io 0pf+0w
next is sgroup
> sgroup (16:26:40) 0.0u 0.0s 0:00.00 0.0% 0+0
Names of point group: m-3m 4/m -3 2/m Oh
Names of point group: m-3m 4/m -3 2/m Oh
Number and name of space group: 225 (F m -3 m)
next is symmetry
> symmetry (16:26:40) 0.0u 0.0s 0:00.00 0.0% 0+0

```

Show STDOUT

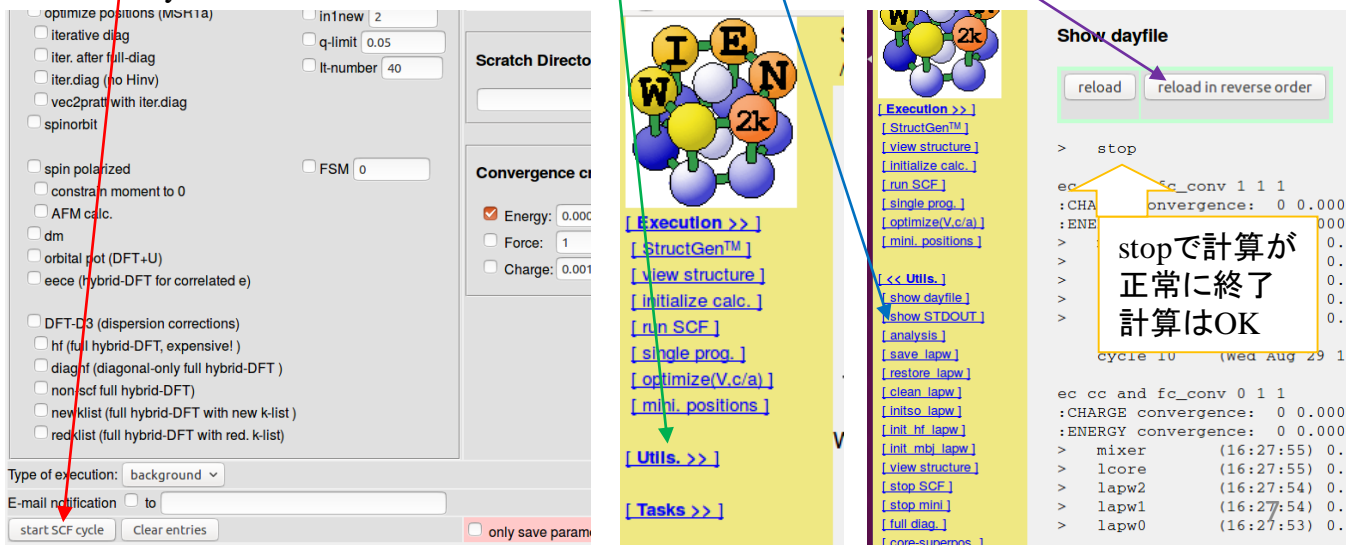
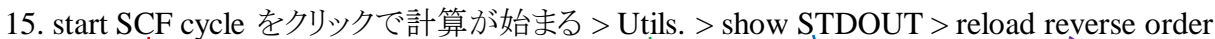
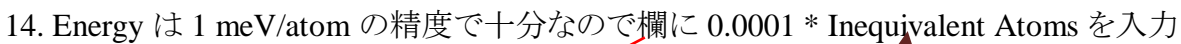
```

init_lapw finished ok
----> new TiC.in0 generated
1.0u 0.0s 0:01.83 56.2% 0+0k 19966+378io 51pf+0w
DSTART ENDS
> dstart -p (16:26:41) running dstart in single mode
next is dstart
KGEN ENDS
16 k-points generated, ndiv= 6
length of reciprocal lattice vectors: 1.331 1.331
NUMBER OF K-POINTS IN WHOLE CELL: 0 allows to specify
next is kgen
inputfiles prepared
> inputfiles prepared (16:26:41)
LSTART ENDS
2P -0.447703 -0.264914 1.00 0.00 0.6195
2P* -0.448366 -0.265504 1.00 0.00 0.6200

```

上から下まで
errorの表示なければok

13. Run SCFを入力 > 計算を実行させる画面が表示される



■ GUI(w2web)の操作 -6- (DOSの計算)

1. Tasks > DOS をクリック

The left screenshot shows the 'Tasks' menu with 'DOS' highlighted. The right screenshot shows the 'DOS' calculation options, including 'x lapw2 -qtl' and 'x tetra'.

Session: [TIC]
/home/student/WIEN2k/TIC

Show dayfile

reload reload in reverse order

> stop

ec cc and fc_conv 1 1 1
:CHARGE convergence: 0 0.0000
:ENERGY convergence: 1 0.0002

> mixer (16:27:56) 0.0
> lcore (16:27:56) 0.0
> lapw2 (16:27:56) 0.3
> lapw1 (16:27:56) 0.7
> lapw0 (16:27:55) 0.9

cycle 10 (Wed Aug 29 16:27:55)

ec cc and fc_conv 0 1 1
:CHARGE convergence: 0 0.0000
:ENERGY convergence: 0 0.0002

> mixer (16:27:55) 0.0
> lcore (16:27:55) 0.0
> lapw2 (16:27:54) 0.4
> lapw1 (16:27:54) 0.8
> lapw0 (16:27:53) 0.9

cycle 9 (Wed Aug 29 16:27:53)

ec cc and fc_conv 0 1 1
:CHARGE convergence: 0 0.0000
:ENERGY convergence: 0 0.0002

> mixer (16:27:53) 0.0
> lcore (16:27:53) 0.0
> lapw2 (16:27:53) 0.3
> lapw1 (16:27:53) 0.7

Execution >>
[StructGen™]
[view structure]
[initialize calc.]
[run SCF]
[single prog.]
[optimize(v.c/a)]
[mini_positions]
[Utils. >>]
[El. Dens.]
[DOS]
[XSPEC]
[TELNES3]
[OPTIC]
[Bandstructure]

Session: [TIC]
/home/student/WIEN2k/TIC

Show dayfile

reload reload in reverse order

> stop

ec cc and fc_conv 1 1 1
:CHARGE convergence: 0 0.0000 .0097
:ENERGY convergence: 1 0.0002 .0000

> mixer (16:27:56) 0.0u 0.0s
> lcore (16:27:56) 0.0u 0.0s
> lapw2 (16:27:56) 0.3u 0.0s
> lapw1 (16:27:56) 0.7u 0.0s
> lapw0 (16:27:55) 0.9u 0.0s

cycle 10 (Wed Aug 29 16:27:55)

ec cc and fc_conv 0 1 1
:CHARGE convergence: 0 0.0000 .0236
:ENERGY convergence: 0 0.0002 .0004

> mixer (16:27:55) 0.0u 0.0s

2. 濃い灰色のところを下まで順番に表示されるボタンを押していけばよい (他のTasksも同様)

The screenshot shows the 'Density of states' calculation options. The 'Optional steps' section includes buttons for 'x kgen', 'x lapw1', and 'x qtl'. The 'Optional alternative to "x lapw2 -qtl" (f-states, SO-DOS, rotations)!' section includes buttons for 'x qtl' and 'x tetra'. The 'Necessary steps' section includes buttons for 'x lapw2 -qtl', 'x tetra', 'view TIC.output', and 'dosplot'. The 'The required input file TIC.int can be generated by:' section includes buttons for 'configure TIC.int', 'configure input-file for TETRA', and 'edit TIC.int'. The 'save_lapw -dos' button is at the bottom.

Session: [TIC]
/home/student/WIEN2k/TIC

Density of states

Optional steps:

edit TIC.in1 Edit TIC.in1 and specify a larger E-max (bottom of file)

x kgen Prepare a denser k-mesh

x lapw1 Create eigenvalues at denser k-mesh or higher E-max ☒ Interactively

Optional alternative to "x lapw2 -qtl" (f-states, SO-DOS, rotations) !

edit TIC.inq Edit input-file for QTL

x qtl Calculate partial charges with QTL program ☐ so ☒ Interactively

Necessary steps:

① x lapw2 -qtl Calculate partial charges ☐ so ☒ Interactively

The required input file TIC.int can be generated by:

configure TIC.int configure input-file for TETRA ② edit TIC.int Edit input-file for TETRA

③ x tetra Calculate partial DOS ☒ Interactively

④ view TIC.output Check output of TETRA

⑤ dosplot Plot DOS or download DOS ASCII-data files for plotting with your own plotting program

save_lapw -dos with name:

下記の3.から具体的に示していく

薄い灰色の範囲はオプションで
Versionが上がって追加された
計算に慣れたらトライしてみるとよい

②は左側よりも
右側のボタンの方が
入力が分かりやすい

3. x lapw2 -qtl をクリック > continue with DOS をクリック (表示されたボタンを押していけばよい)

The screenshot shows the 'Necessary steps' section of the 'Density of states' calculation options. The 'x lapw2 -qtl' button is highlighted. The 'x tetra' button is also highlighted. The 'view TIC.output' button is highlighted. The 'dosplot' button is highlighted. The 'save_lapw -dos' button is at the bottom.

Necessary steps:

x lapw2 -qtl Calculate partial charges ☐ so ☒ Interactively

The required input file TIC.int can be generated by:

configure TIC.int configure input-file for TETRA edit TIC.int

x tetra Calculate partial DOS ☒ Interactively

view TIC.output Check output of TETRA

dosplot Plot DOS or download DOS ASCII-data files for plotting with your own plotting program

save_lapw -dos with name:

The screenshot shows the 'Continue with' section of the 'Density of states' calculation options. The 'continue with DOS' button is highlighted.

/home/student/WIEN2k/TIC

Commandline: x lapw2 -qtl
Program input is: ""

LAPW2 END
0.1u 0.0s 0:00.05 300.0% 0+0k 0+1256io 0pf+0w

Continue with

continue with DOS

■ GUI(w2web)の操作 -7- (DOSの計算)

4. edit フォルダ名.int をクリック > 表示させる各原子の各軌道を入力する画面が開く

Necessary steps:

x lapw2 -qtl Calculate partial charges ☐ so ☒ interactively

The required input file TiC.int can be generated by

configure TiC.int configure input-file for TETRA **edit TiC.int** Edit

x tetra Calculate partial DOS ☒ interactively

view TiC.output Check output of TETRA

dosplot Plot DOS or download DOS ASCII-data files for plotting v

save_lapw -dos with name:

5. 表示させた条件を書き入れる

表示させる軌道は左から1, 2, 3, ... となっている

DOSを表示させる数

ATOMの番号
0は全体
最大+1はinterstitial

コメント(出力したときの名称)

表示させる軌道の番号。1はtotで全部(s+p+d+f)となる

6. Save and continue with DOS をクリックして書き換えを保存する

Session: **TIC**

/home/student/WIEN2k/TIC

File:

/home/student/WIEN2k/TIC/TiC.int

continue with DOS without saving **Save and continue with DOS** Download this

Header from TiC.qtl:

ATOM	COLUMN
ATOM 1: Ti:	tot, s, p, d, D-eg, D-t2g, f
ATOM 2: C:	tot, s, p, d, D-eg, D-t2g, f

Title

```

-0.50 0.002 1.500 0.003 # EMIN, DE, EMAX, Gauss-broadening(>de)
4 N 0.000 # NUMBER OF DOS-CASES below, G/L/B broadening (Ry)
0 1 total # atom, case=column in qtl-header, label
1 4 Ti d
2 3 C p
3 1 interstitial
SUM: 0 2 # NUMBER OF SUMMATIONS, max: 02 of summands
2 5 # this sums dos-cases 2+5 from the input above
    
```

■ GUI(w2web)の操作 -8- (DOSの計算)

7. x tetra をクリック > continue with DOS をクリック

Necessary steps:

x lapw2 -qtl Calculate partial charges ☐ so ☒

The required input file TiC.int ca

configure TiC.int configure input-file for TETRA

x tetra Calculate partial DOS ☒ interactively

view TiC.outputtt Check output of TETRA

dosplot Plot DOS or download DOS ASCII-da

save_lapw -dos with name:

Session: [TIC]
/home/student/WIEN2k/TIC

Commandline: x tetra
Program input is: ""

LEGAL END TETRA
0.0u 0.0s 0:00.01 0.0% 0+0k 2152+440io 10pf+0w

Continue with

continue with DOS

Execution >>>
[StructGen™]
[view structure]
[initialize calc.]
[run SCF]
[single prog.]
[optimize(V.c/a)]
[mini_positions]
Utils. >>>
[<< Tasks]
[El. Dens.]
[DOS]
[XSPEC]
[TELNES3]
[OPTIC]
[Bandstructure]

8. view ファイル名.output をクリック > Save and continue with DOS をクリック

Necessary steps:

x lapw2 -qtl Calculate partial charges ☐ so ☒

The required input file TiC.int ca

configure TiC.int configure input-file for TETRA

x tetra Calculate partial DOS ☒ interactively

view TiC.outputtt Check output of TETRA

dosplot Plot DOS or download DOS ASCII-da

save_lapw -dos with name:

Session: [TIC]
/home/student/WIEN2k/TIC

File:
/home/student/WIEN2k/TIC/TiC.outputtt

continue with DOS without saving Save and continue with DOS Download this file:

Title
IAV : 0
NPRINT : 1
4 CASES FOR DOS : ATOM L

title
LATTICE CONST.= 8.17878 8.17878 8.17878 FERMI ENERGY= -0.70902
134 <; NMAT <; 156 SPIN=1 NATO= 3
JATOM 1 MULT= 1 ISPLIT= 2 tot,0,1,2,D-eg,D-t2g,3
JATOM 2 MULT= 1 ISPLIT= 2 tot,0,1,2,D-eg,D-t2g,3
CASE 1: ATOM NUMBER 0 COLUMN READ 0 DOSTYPE=total-DOS
CASE 2: ATOM NUMBER 1 COLUMN READ 4 DOSTYPE= 1:d
CASE 3: ATOM NUMBER 2 COLUMN READ 3 DOSTYPE= 2:p
CASE 4: ATOM NUMBER 3 COLUMN READ 1 DOSTYPE= 3:666
We will add 0 DOS-cases together:
BAND LIMITS OF BAND 1 ARE -3.45081 -3.44350
BAND LIMITS OF BAND 2 ARE -1.72609 -1.68912
BAND LIMITS OF BAND 3 ARE -1.71189 -1.68912
BAND LIMITS OF BAND 4 ARE -1.70206 -1.68912

Execution >>>
[StructGen™]
[view structure]
[initialize calc.]
[run SCF]
[single prog.]
[optimize(V.c/a)]
[mini_positions]
Utils. >>>
[<< Tasks]
[El. Dens.]
[DOS]
[XSPEC]
[TELNES3]
[OPTIC]
[Bandstructure]

Files >>>
[struct.files]
[input.files]
[output.files]
[SCF.files]

9. dosplot をクリック > 表示する軌道を選択 > plot をクリック > DOSが得られる

Necessary steps:

x lapw2 -qtl Calculate partial charges ☐ so ☒

The required input file TiC.int ca

configure TiC.int configure input-file for TETRA

x tetra Calculate partial DOS ☒ interactively

view TiC.outputtt Check output of TETRA

dosplot Plot DOS or download DOS ASCII-da

save_lapw -dos with name:

Session: [TIC]
/home/student/WIEN2k/TIC

Density of states

We are in Dosplot mode:

Set ranges (optional):
xmin= xmax= ymin= ymax= **PLOT**

You can select from 4 DOS in TiC.int.
Please select up to 4 lines to plot.

no line ☐ ☐ ☐ ☐

line:1 (total DOS) of TIC ☒ ☐ ☐ ☐

line:2 (d) of atom Ti ☐ ☒ ☐ ☐

line:3 (p) of atom C ☐ ☐ ☒ ☐

line:4 (interstitial) of TIC ☐ ☐ ☐ ☒

Define for first line: Label= Linetype(0-9)= 1 Linewidth= 1

Define for second line: Label= Linetype(0-9)= 2 Linewidth= 2

Define for third line: Label= Linetype(0-9)= 3 Linewidth= 2

Define for fourth line: Label= Linetype(0-9)= 4 Linewidth= 2

Plot DOS in Color Labels= 24 pt

Execution >>>
[StructGen™]
[view structure]
[initialize calc.]
[run SCF]
[single prog.]
[optimize(V.c/a)]
[mini_positions]
Utils. >>>
[<< Tasks]
[El. Dens.]
[DOS]
[XSPEC]
[TELNES3]
[OPTIC]
[Bandstructure]

Files >>>
[struct.files]
[input.files]
[output.files]
[SCF.files]

■ GUI(w2web)の操作 -9- (バンド分散の計算)

1. Bandstructure をクリック > バンド分散用の画面が開く

Session: [TIC]
/home/student/WIEN2k/TIC

Show dayfile

reload reload in rev

> stop

ec cc and fc_conv :
:CHARGE convergence
:ENERGY convergence
> mixer (1)
> lcore (1)
> lapw2 (1)
> lapw1 (1)
> lapw0 (1)

cycle 10 (W

ec cc and fc_conv :
:CHARGE convergence
:ENERGY convergence
> mixer (1)

Band structure

Generate k-mesh using XCrysden (save klist as xcrysden.klist)

fcc create TIC.klist_band [Brillouinzones from Bilbao Cryst Server]

x lapw1-band Calculate Eigenvalues ☒ interactively

needed only for continuous lines in the plot (not for non-symmorphic spacegroups)!

x irrep Calculate irreducible representations ☐ so ☒ interactively

for band character plots only!

x lapw2-band-qtli Calculate partial charges ("qtli"-file) ☐ so ☒ interactively

edit TIC.insp Insert correct EF

x spaghetti Calculate bandstructure ☐ so ☒ interactively

plot bandstructure Plot bandstructure or download Xmgrace files for plotting with xmgrace

save_lapw -band with name:

2. 濃い灰色のところを下まで順番に表示されるボタンを押していけばよい (他のTasksも同様)

Generate k-mesh using XCrysden (save klist as xcrysden.klist)

fcc create TIC.klist_band [Brillouinzones from Bilbao Cryst Server]

② x lapw1-band Calculate Eigenvalues ☒ interactively

needed only for continuous lines in the plot (not for non-symmorphic spacegroups)!

x irrep Calculate irreducible representations ☐ so ☒ interactively

for band character plots only!

x lapw2-band-qtli Calculate partial charges ("qtli"-file) ☐ so ☒ interactively

③ edit TIC.insp Insert correct EF

④ x spaghetti Calculate bandstructure ☐ so ☒ interactively

⑤ plot bandstructure Plot bandstructure or download Xmgrace files for plotting with xmgrace

save_lapw -band with name:

DOSのときと同様に
基本的に表示されるボタンを押していく
③だけは入力が必要なので
下記の3.で具体的に示す

3. ③では0.XXXXのところに E_F (フェルミ準位)を書き入れる > Save continue with bandstructure

File:
/home/student/WIEN2k/TIC/TIC.insp

continue with bandstructure without saving Save and continue with bandstructure Download this

Header from TIC.qtl and possible FERMI energies:

ATOM 1: Ti: tot,s,p,d,D-eg,D-t2g,f
ATOM 2: C: tot,s,p,d,D-eg,D-t2g,f

/home/student/WIEN2k/TiC/TiC.scf: EF (TETRAH.M.)= 0.7090202053

Figure configuration
5.0 3.0
10.0 15.0
1.0 4
1.0 1
1.1 2 4
Data configuration
-14.0 8.0 2
1 0.0000
1 999
0 1 0.2

Fermi switch:
0...no line
1...solid line
2...dashed line
3...dotted line

Line switch:
0...dots

2) コピーする

1) 計算で得られた E_F が表示されている

File:
/home/student/WIEN2k/TIC/TIC.insp

continue with bandstructure without saving Save and continue with bandstructure Download this

Header from TIC.qtl and possible FERMI energies:

ATOM 1: Ti: tot,s,p,d,D-eg,D-t2g,f
ATOM 2: C: tot,s,p,d,D-eg,D-t2g,f

/home/student/WIEN2k/TiC/TiC.scf: EF (TETRAH.M.)= 0.7090202053

Figure configuration
5.0 3.0
10.0 15.0
1.0 4
1.0 1
1.1 2 4
Data configuration
-14.0 8.0 2
1 0.7090202053
1 999
0 1 0.2

Fermi switch:
0...no line
1...solid line
2...dashed line
3...dotted line

Line switch:
0...dots

3) ペーストする

■ 付録: cifファイルの読み取り

1. Files をクリック > new file をクリック > 好きな名称.cif と入力 > create をクリック

The screenshot shows the WIEN2k web interface. On the left, a sidebar menu has 'Files' highlighted. In the center, there's a logo with 'I E N' and 'W 2k'. On the right, the 'New file' dialog is open, showing 'filename' as 'pet4.cif' and a 'create' button. Arrows indicate the sequence: from 'Files' to 'new file', then to the filename input, and finally to the 'create' button.

2. cifファイルを開いて中身をコピー＆ペースト > Save をクリック

The screenshot shows the 'cif' file content in a text area. The content includes crystallographic data such as 'CRYSTAL DATA', 'Data_VESTA_phase_1', and 'Chemical name: common'. A 'Save' button is visible at the bottom right of the text area. Arrows indicate the sequence: from the 'cif' file content to the 'Save' button.

cifファイル形式の変更によって
動作しないこともある

WIEN2k 14 では下記のように変更が必要

_space_group_name_H-M_alt
_space_group_IT_number
_space_group_symop_operation_xyz



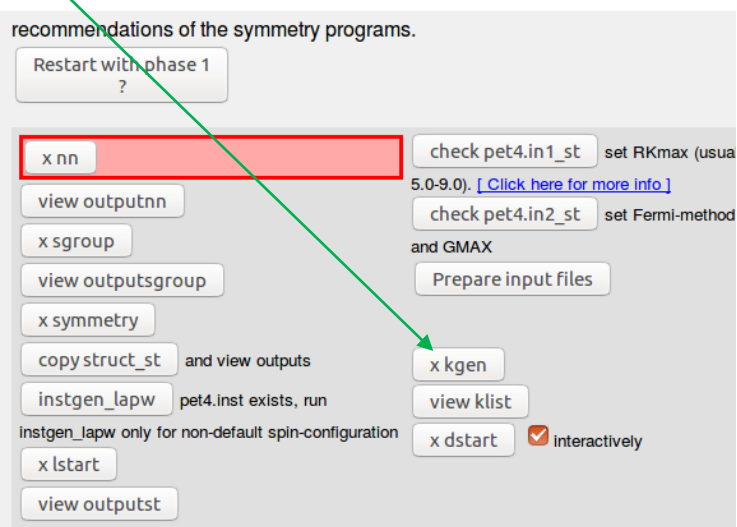
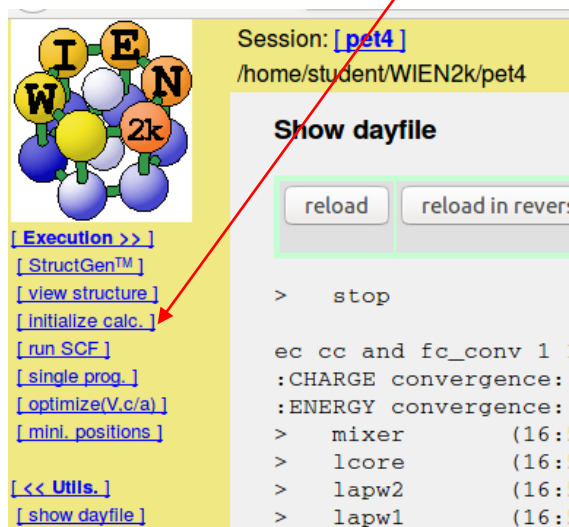
_symmetry_space_group_name_H-M
_symmetry_Int_Tables_number
_symmetry_equiv_pos_as_xyz

3. StructGen™をクリック > ファイル名.cif にチェックを入れる > Use selected CIF/TXT file をクリック

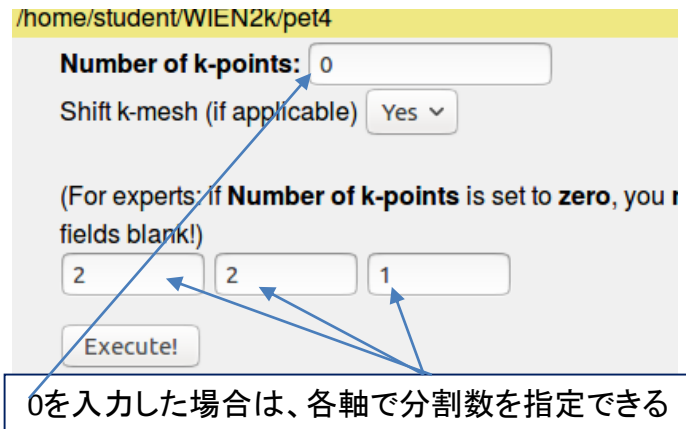
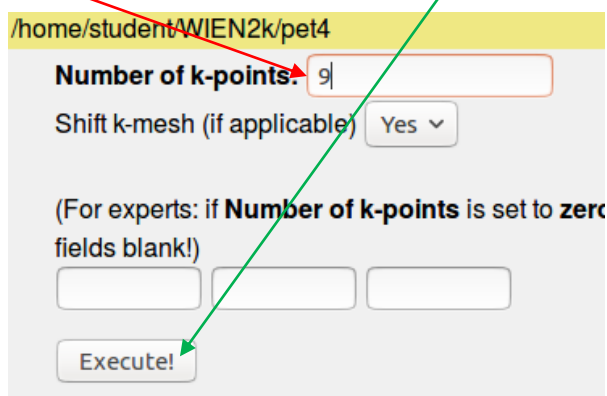
The screenshot shows the StructGen™ web interface. It has a sidebar menu with 'StructGen™' highlighted. The main content area shows a message: 'You do not have a pet4.struct file yet. You can create it using STRUCTGEN. Please specify the number of independent atoms of your initial structure!'. Below this, there's a 'Number of atoms: 2' input field and a 'Generate template' button. Further down, there's a section 'Alternatively:' with a checkbox 'Use cif2struct to convert a "cif" file: (e.g. from the inorganic crystal structure database)'. This checkbox is checked. Below it, there's a list of 'cif' files, with 'pet4.cif' selected. A 'Use selected CIF/TXT file' button is at the bottom. On the right, there's a 'Save Structure' button and a 'Title' input field. Below that, there's a 'Lattice' section with 'Spacegroup: 2_P1_1' and a list of atoms (F, B, CXY, CYZ, CXZ, H, 1_P1, 2_P1). There's also a 'Lattice parameters' section with input fields for 'a', 'b', 'c', 'α', 'β', and 'γ'. At the bottom, there's an 'Inequivalent Atoms: 11' section with input fields for 'Atom 1: O', 'Pos 1: x', 'y', 'z', 'RMT', and 'Pos 2: x', 'y', 'z'. Arrows indicate the sequence: from 'StructGen™' to the 'Use selected CIF/TXT file' button, then to the 'Save Structure' button, and finally to the 'Title' input field.

■ 付録: k点を増加させる方法

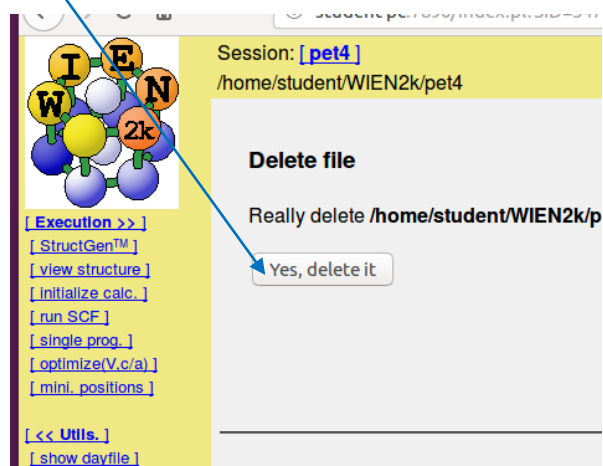
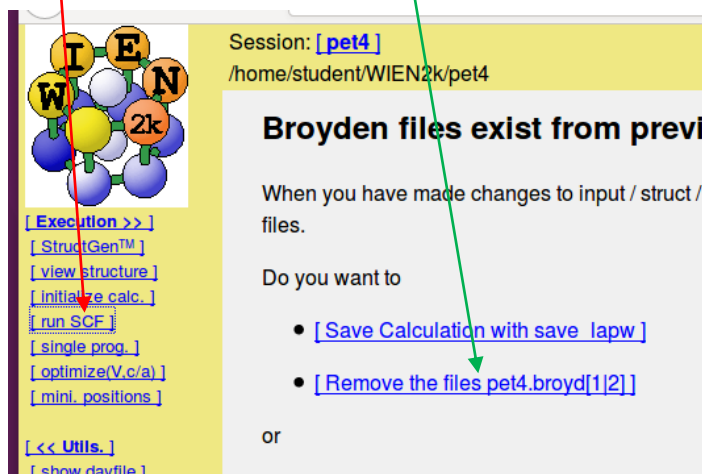
1. run SCF が終了後 > Initialize calc. をクリック > x kgen をクリック



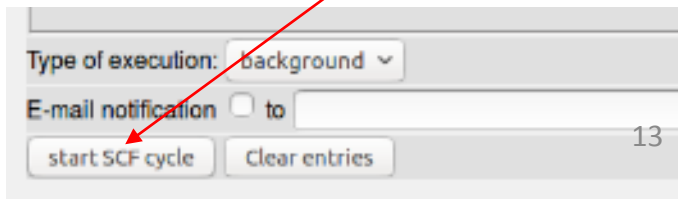
2. k点数を入力する > Execute! をクリック



3. run SCF をクリック > Remove the files ... をクリック > Yes, delete it をクリック

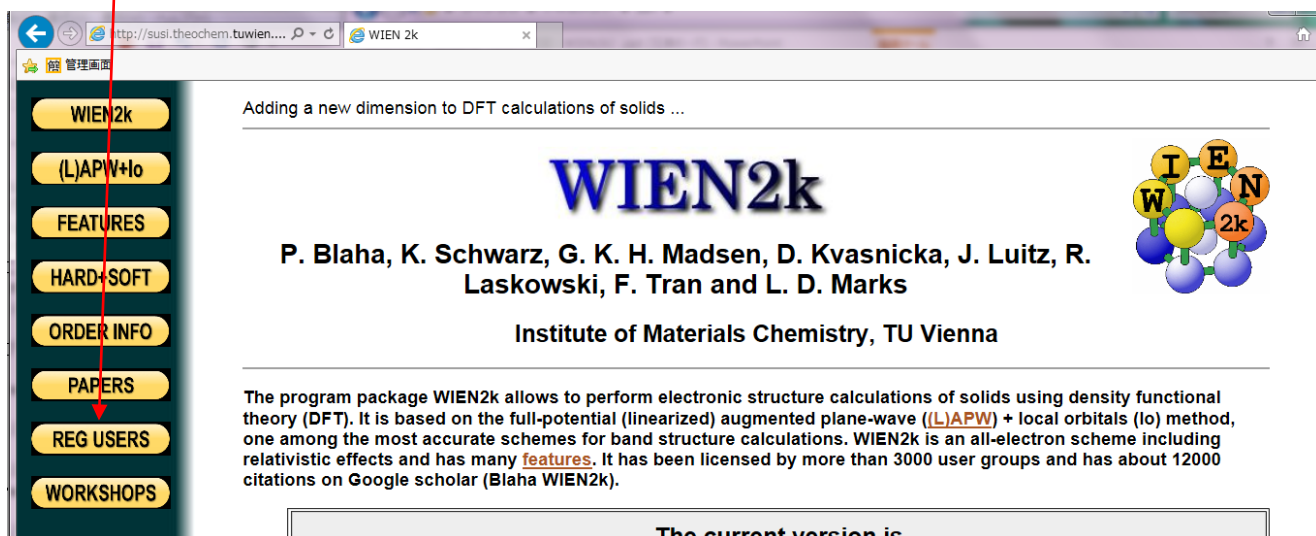


4. 再度 run SCF をクリックすれば SCF Cycle の画面が表示される > start SCF cycle をクリックで走る

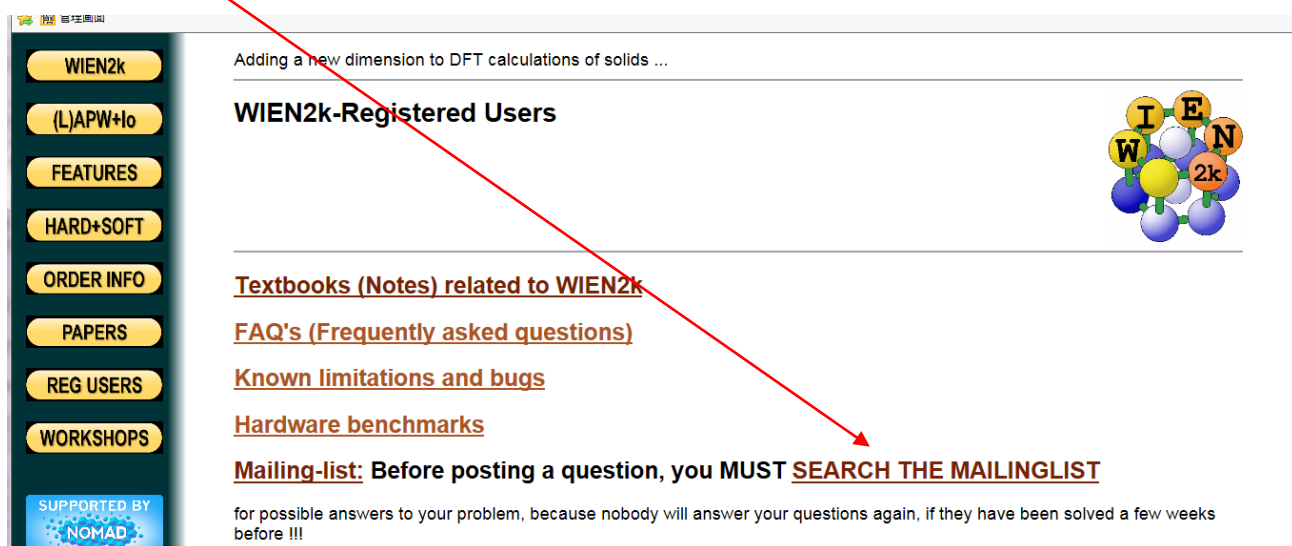


■ 付録：XPSスペクトルの計算についての情報の取得方法

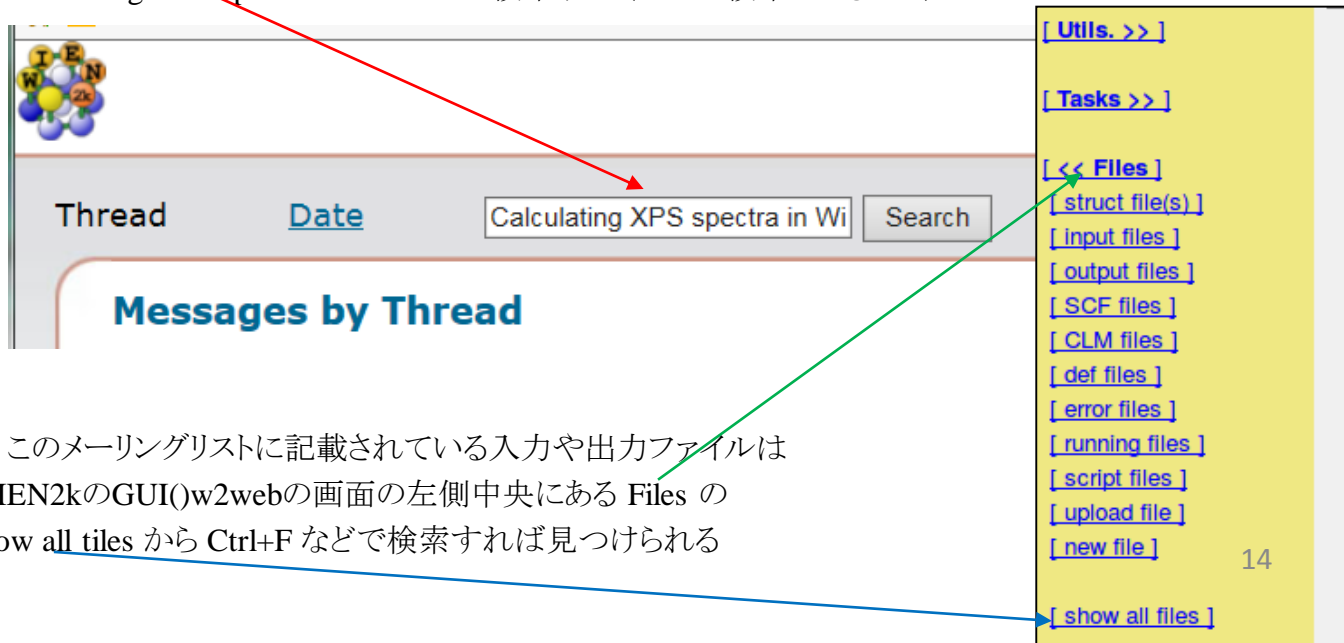
1. REG USERS をクリック



2. SEARCH THE MAILINGLIST をクリック



3. Calculating XPS spectra in Wien2k で検索する (XPSで検索してもよい)



※ このメーリングリストに記載されている入力や出力ファイルは
WIEN2kのGUI(w2web)の画面の左側中央にある Files の
show all tiles から Ctrl+F など検索すれば見つかる