

## WIEN2k TiC Example

Ubuntu 24.04.1 LTS

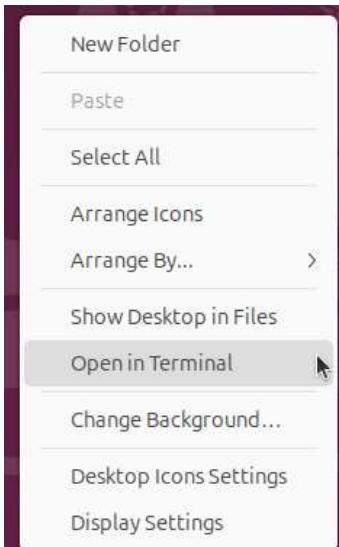
WIEN2k\_24.1 (Release 1/8/2024)

gfortran 13.3.0

WIEN2k patches [1]: SearchZ.patch, angle.patch, atom\_read.patch, x\_lapw.patch

[1] <https://github.com/gsabo/WIEN2k-Patches/tree/master/24.1>Open a terminal and start w2web

1. Right-click on the Linux desktop, and click on “Open in Terminal”:



2. Type w2web, and press enter to start w2web:

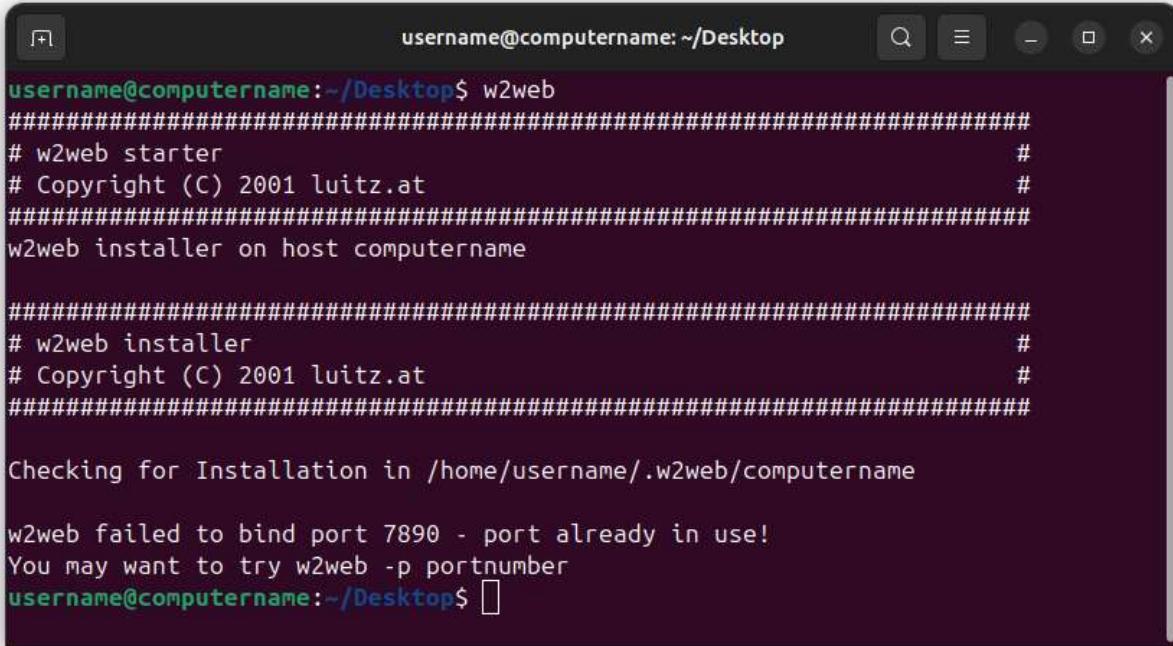
```
username@computername: ~/Desktop$ w2web
#####
# w2web starter
# Copyright (C) 2001 luitz.at
#####
w2web installer on host computername

#####
# w2web installer
# Copyright (C) 2001 luitz.at
#####

Checking for Installation in /home/username/.w2web/computername

w2web server started, now point your web browser to
http://localhost:7890
username@computername: ~/Desktop$ 
```

If your w2web is already started, you will get:



```
username@computername:~/Desktop$ w2web
#####
# w2web starter
# Copyright (C) 2001 luitz.at
#####
w2web installer on host computername

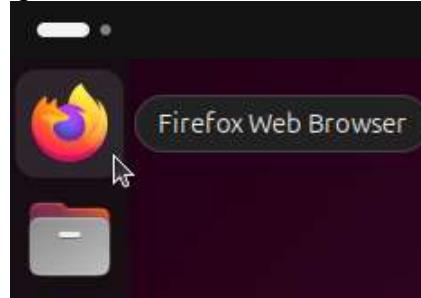
#####
# w2web installer
# Copyright (C) 2001 luitz.at
#####

Checking for Installation in /home/username/.w2web/computername

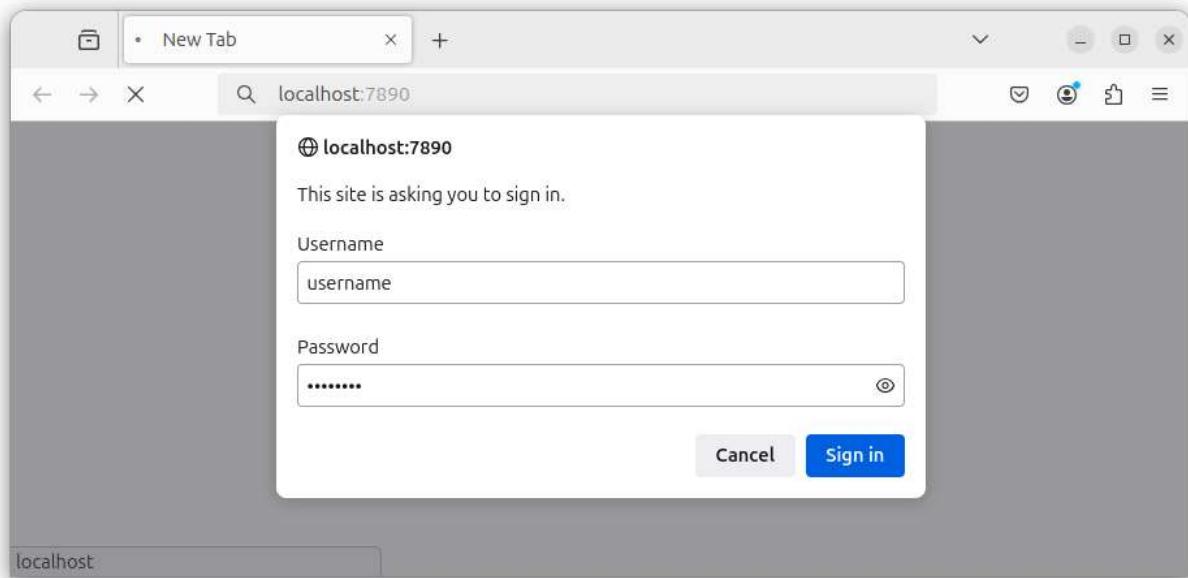
w2web failed to bind port 7890 - port already in use!
You may want to try w2web -p portnumber
username@computername:~/Desktop$ 
```

Open Firefox and login to w2web

3. Click on the Firefox icon to open Firefox:

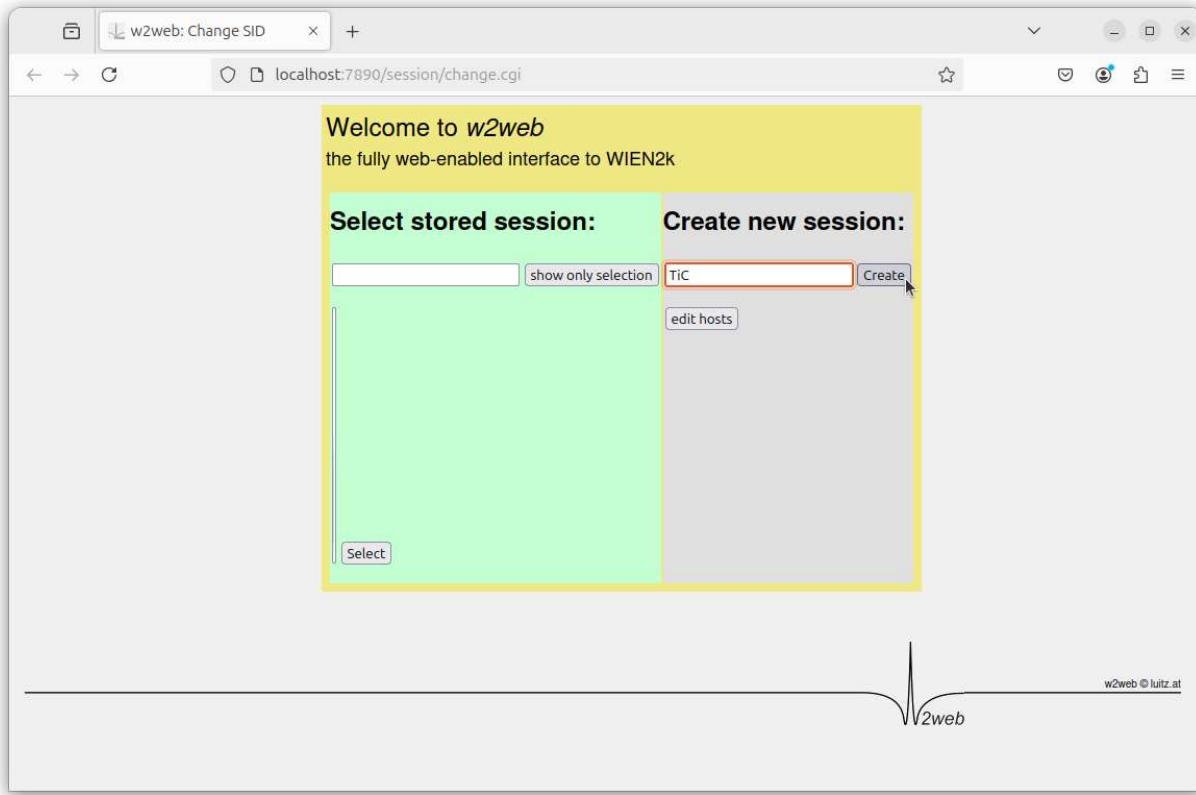


4. Enter url <http://localhost:7890>, type your w2web username and password, then click “Sign in” to login to w2web:

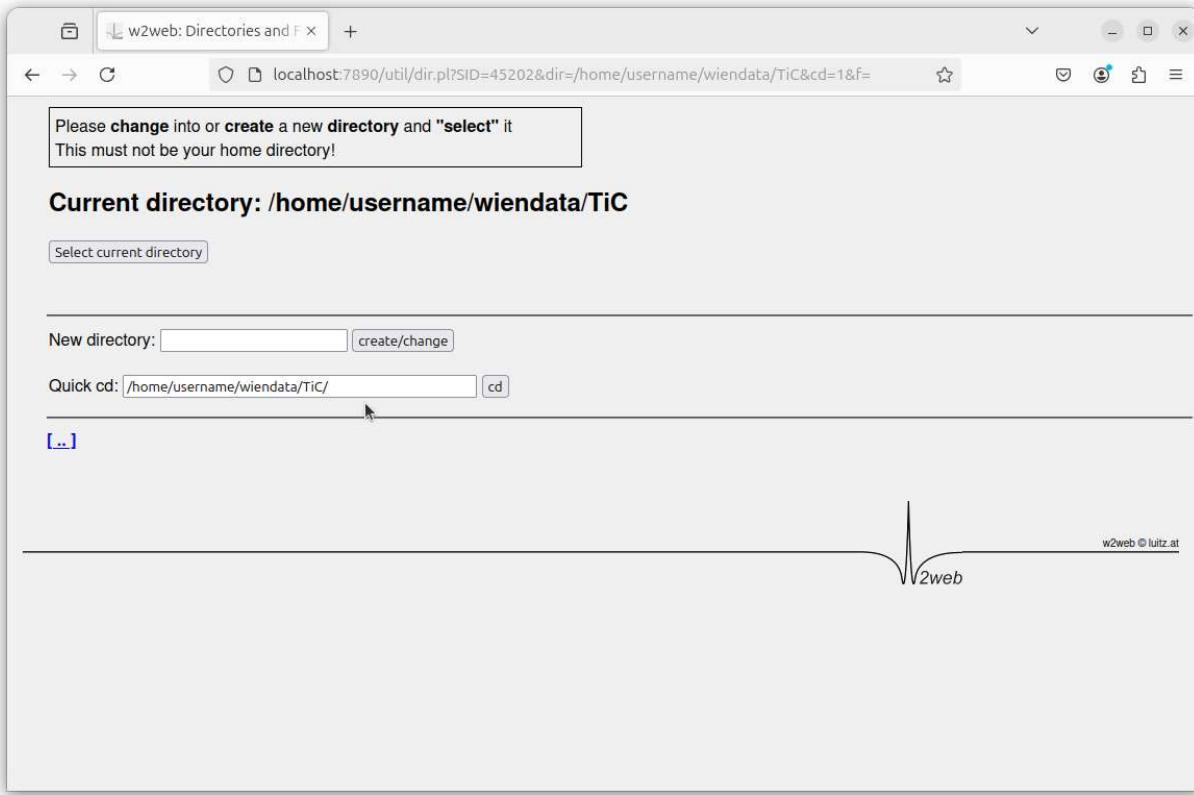


Create a new session (calculation)

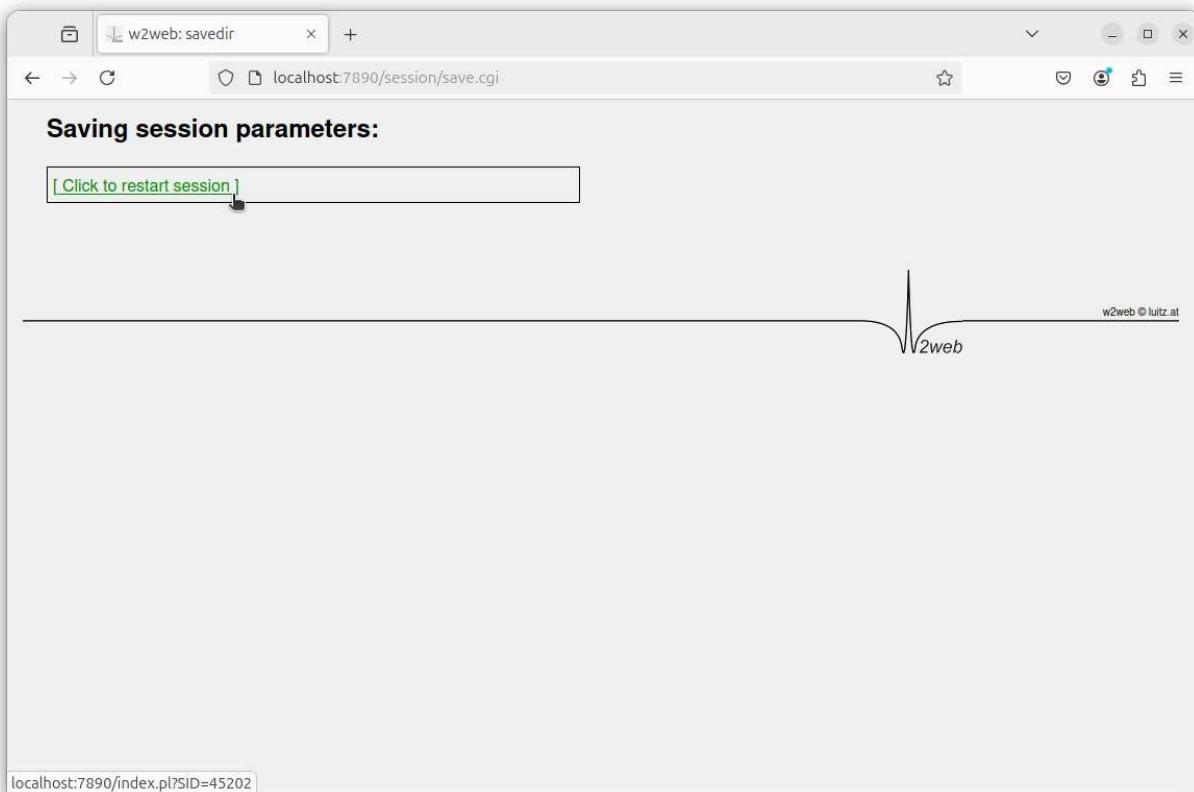
5. Enter “TiC” in the “Create new session:” box and then click the “Create” button:



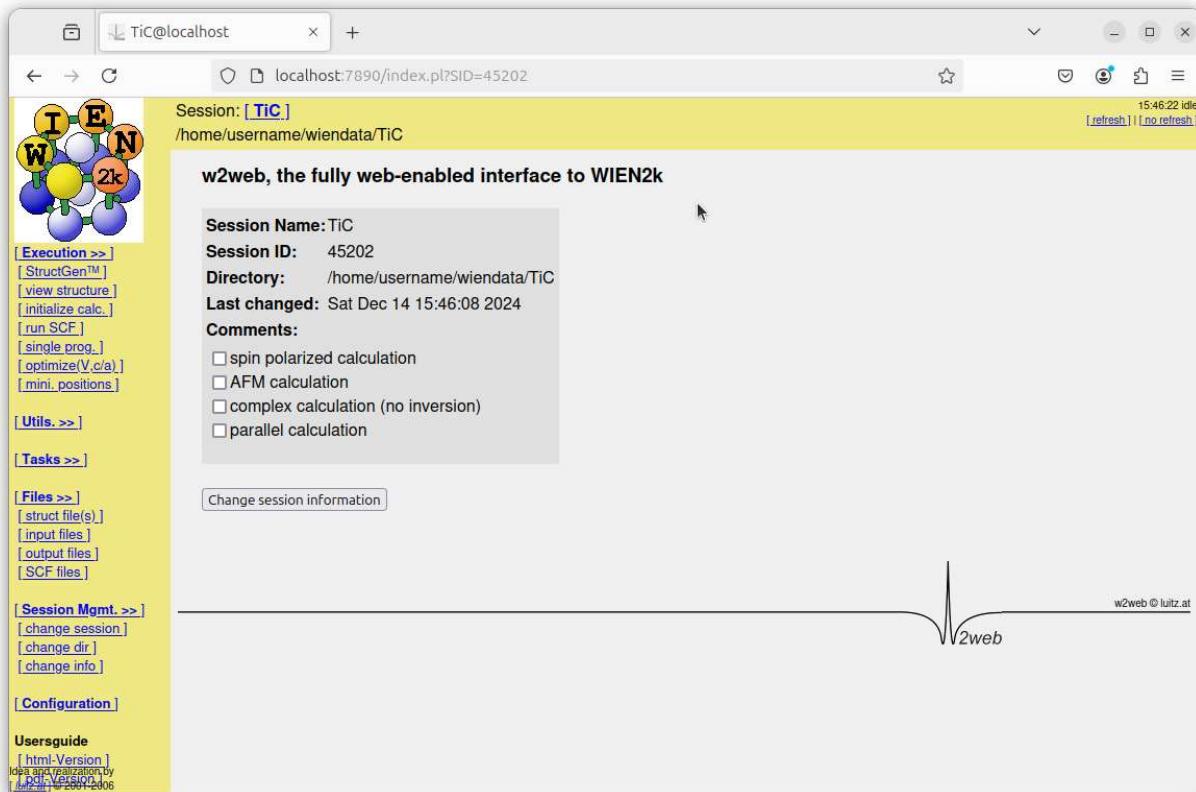
6. The “New directory” box will contain “TiC”, click the “create/change” button
7. The directory “TiC” is created and “TiC” will appear in the “Quick cd.” box:



8. Click on the “Select current directory” button
9. Click on the “Click to restart session” link:



10. The following window should appear:



### Create the TiC structure for calculation

11. In the left menu, click on StructGen™ under Execution
12. The “Number of atoms” is 2, click the “Generate template” button:

The screenshot shows the StructGen™ interface on a web browser. The title bar says "TiC@localhost". The main content area has a yellow header bar with "Session: [ TiC ]" and the path "/home/username/wiendata/TiC". Below this is a "StructGen™" section with a molecular model of TiC and the text "You do not have a TiC.struct file yet.". A box contains the instruction "You can create it using STRUCTGEN. Please specify the number of independent atoms of your initial structure!" followed by a "Number of atoms: [ 2 ]" input field and a "Generate template" button. Below this is an "Alternatively:" section with instructions for cif2struct and xyz2struct conversion. At the bottom, there's a note about uploading files. The left sidebar has a navigation menu with sections like "Execution >>", "Files >>", "Session Mgmt. >>", "Configuration", and "Usersguide".

13. Type “TiC” in the “Title” box
14. Select “F” for the Lattice
15. Type 4.328 for a, b, and c for the Lattice parameters.  
Note: Angstrom should be selected for the units and the angles  $\alpha$ ,  $\beta$ , and  $\gamma$  are 90 degrees by default.
16. Type “Ti” in the first box next to “Atom 1:”  
Note: By default, x = 0, y = 0, and z = 0, Z = 0, and RMT = 2
17. Type “C” in the first box next to “Atom 2:”  
Note: By default, Z = 0 and RMT = 2
18. Type 0.5 for x, y, and z

19. The settings should appear as:

The screenshot shows the TiC@localhost software interface. On the left is a sidebar with various buttons like 'Execution >>', 'StructGen™', 'view structure', etc. The main area has a yellow header bar with 'Session: [TiC.]' and the path '/home/username/wiendata/TiC'. Below this is a green panel containing the following information:

- Title:** TiC
- Lattice:**
  - Type: P
  - P
  - F
  - B
  - CXY
  - CYZ
  - CXZ
  - R
  - H
  - 1\_P1
- Lattice parameters in A**

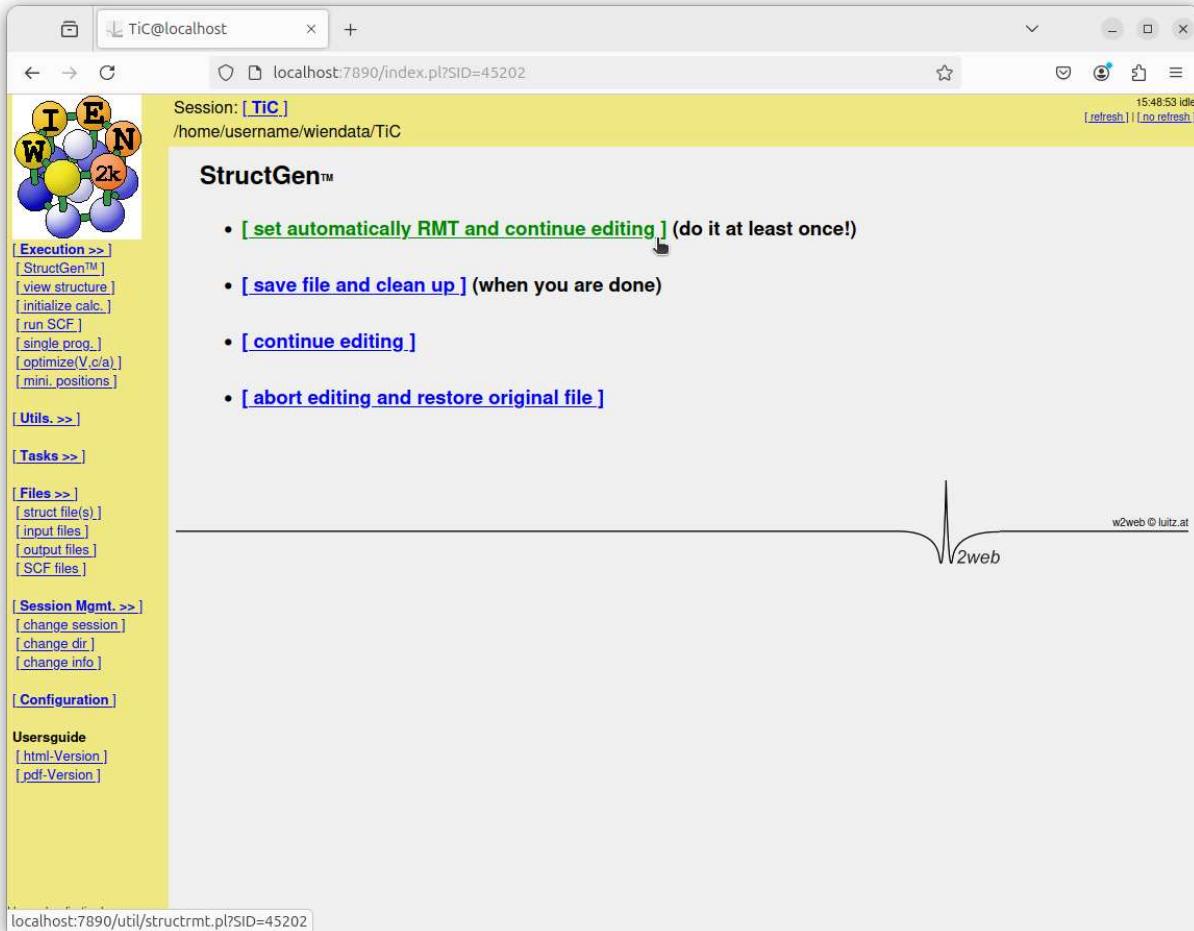
a= 4.328	b= 4.328	c= 4.328
α= 90.000000	β= 90.000000	γ= 90.000000

- Inequivalent Atoms: 2**
- Atom 1:** Ti, Z= 0.000, RMT= 2.0000
  - [remove atom]
  - Pos 1: x= 0.0000000 y= 0.0000000 z= 0.0000000 [remove] [split]
  - [add position]
- Atom 2:** c, Z= 0.000, RMT= 2.0000
  - [remove atom]
  - Pos 1: x= 0.5 y= 0.5 z= 0.5 [remove] [split]
  - [add position]
- Number of symmetry operations: generate**
- You have to click "Save Structure" for changes to take effect!**
- Save Structure** button

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20. Click the “Save Structure” button

21. Click the “set automatically RMT and continue editing” link:



22. Type 3 in the “Reduce RMTs by” box:

Session: [TiC.]  
/home/username/wiendata/TiC

15:48:53 idle  
[refresh] | [no refresh]

**Automatic determination of RMTs**

Please specify the desired RMT reduction compared to almost touching spheres.  
Typically use:

- for a single calculation: 0 %
- for force minimization: 1-5 %
- for volume effects you may need even larger reductions.

Reduce RMTs by  % using  new or  old scheme

**do it**

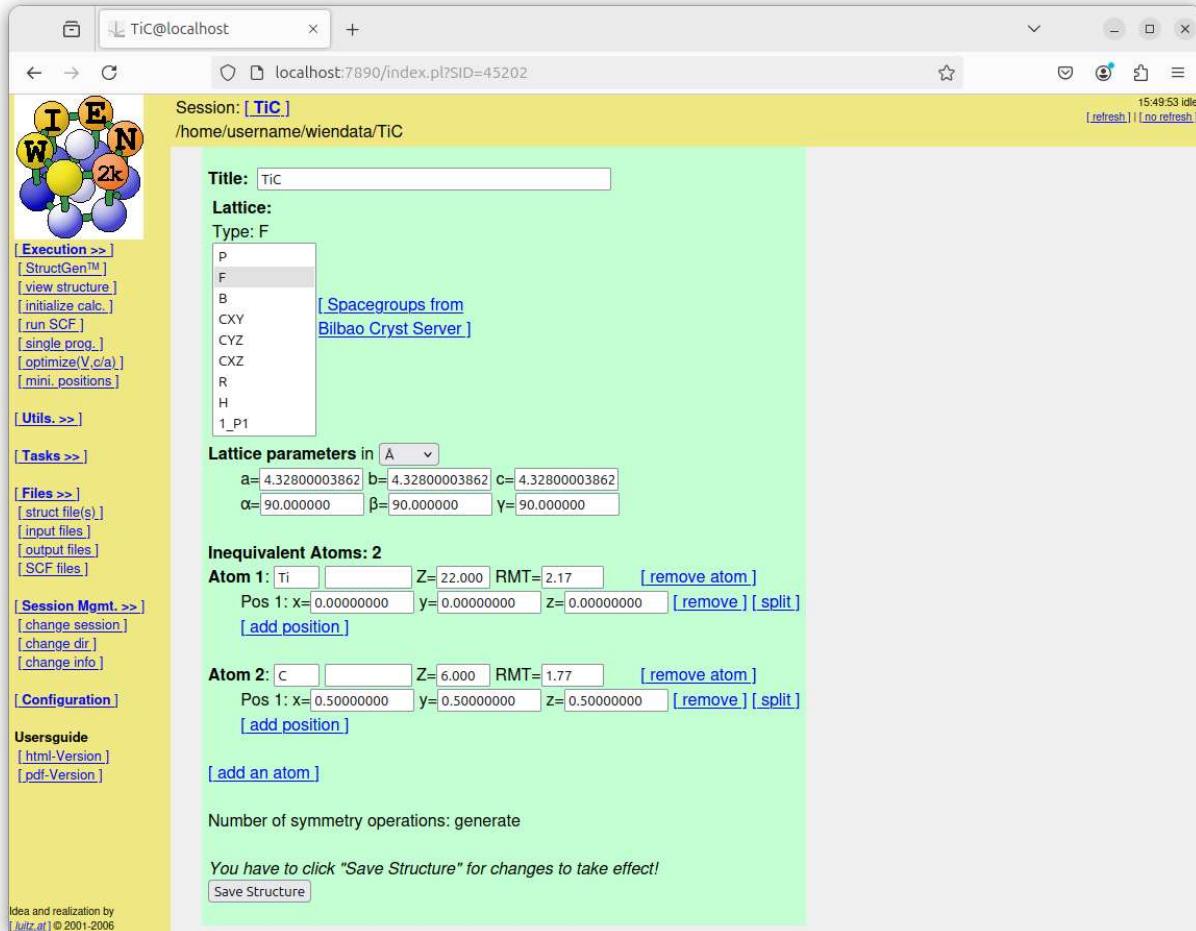
**Alternatively** you can specify the sphere radii explicitly by element using a syntax like: Fe:2.0,C:1.77,...  
Note: It is your responsibility that RMTs will not lead to overlapping spheres.  
Specify a comma separated list of **name:radius** as indicated above:

**do it**

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23. Click the “do it” button, the software adjusts the Zs and RMTs:



Usually, these RMTs set by the program are used. However, they are manually adjusted as follows in order to match the quickstart tutorial in the WIEN2k usersguide:

24. Type 2.0 in the “RMT” box for Atom 1
25. Type 1.9 in the “RMT” box for Atom 2
26. Click the “Save Structure” button

27. Click the “save file and clean up” link:

The screenshot shows a web-based application window titled "StructGen™". The URL is "localhost:7890/index.pl?SID=45202". The session name is "TiC". The main area displays the following information:

- Title:** TiC
- Lattice:** F
- Type:** F
- Lattice parameters in A:**
  - a = 4.32800003862
  - b = 4.32800003862
  - c = 4.32800003862
  - $\alpha = 90.000000$
  - $\beta = 90.000000$
  - $\gamma = 90.000000$
- Inequivalent Atoms: 2**
  - Atom 1:** Ti (highlighted), Z = 22.000, RMT = 2.0000  
Pos 1: x = 0.00000000, y = 0.00000000, z = 0.00000000
  - Atom 2:** C, Z = 6.000, RMT = 1.9000  
Pos 1: x = 0.50000000, y = 0.50000000, z = 0.50000000
- Number of symmetry operations:** generate
- View only mode --> [edit STRUCT file ]**

The left sidebar contains a navigation menu with the following items:

- [Execution >>]
  - [StructGen™]
  - [view structure]
  - [initialize calc.]
  - [run SCF]
  - [single prog.]
  - [optimize(V,c/a)]
  - [mini. positions]
- [Utils. >>]
- [Tasks >>]
- [Files >>]
  - [struct file(s)]
  - [input files]
  - [output files]
  - [SCF files]
- [Session Mgmt. >>]
  - [change session]
  - [change dir.]
  - [change info]
- [Configuration]
- Usersguide**
  - [html-Version]
  - [pdf-Version]

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## Initialize the calculation

28. In the left menu, click on “initialize calc.” under Execution
29. In general, click on buttons highlighted in red. We will go through each step, starting with clicking on the “x nn” button:

The screenshot shows the WIEN2k web interface for session 'TiC'. The main title is 'Initialize WIEN2k calculation'. Under 'Fast mode (recommended)', it says: 'This is in general the **recommended** way of initialization (**except for antiferromagnets, supercells and slabs with unclear symmetry**).'. It specifies the 'precision level' (0-3; 0n-3n for non-metals, default=1), 'RMT reduction by X % (default: RMT not changed)', 'VXC option (13=PBE, 5=LDA, 11=WC, 19=PBESol) [default=13]', 'energy separation between core/valence (default: -6.0 Ry)', 'RKMAX (3.0 - 10.0, be careful, this may influence the cputime by ORDERS of magnitude) [[Click here for more info](#)]', 'use TEMP (extrapolated to 0K) with smearing by X Ry (default: TETRA)', 'use TEMPS (finite T) with smearing by X Ry (default: TETRA)', 'use X k-points in full BZ (be careful, this may influence the cputime by ORDERS of magnitude; [[Click here for more info](#)])', and 'do not run dstart (after a first scf calculation in order to create higher precision inputs)'. A 'CHECK BATCH VALUES' button is at the bottom. Below this, under 'Individual mode (phase 1)', it says: 'For **antiferromagnets, self-generated structures, supercells and surfaces** we recommend to run at least the first steps (until instgen) manually and accept the recommendations of the symmetry programs.' A red box highlights the 'x nn' button, which is part of a group of buttons: 'check TiC.in1\_st set RKmax (usually 5.0-9.0). [[Click here for more info](#)]', 'view outputnn', 'x sgroup', 'view outputsgroup', 'x symmetry', 'check TiC.in2\_st set Fermi-method and GMAX', 'Prepare input files', 'view TiC.outputtd and cp TiC.in0\_std TiC.in0 check if gmax>gmin', and 'Perform spin-polarized calc.?'. A 'No' button is at the bottom right.

30. By default 2 should be given in the box, click the “Execute!” button:

The screenshot shows a web browser window titled "TiC@localhost" with the URL "localhost:7890/index.pl?SID=45202". The page displays a molecular structure with atoms labeled T, E, N, W, and 2k. A message at the top right says "NN needs input". Below the structure, there is a text input field containing the value "2" and a button labeled "Execute!". To the right of the input field, there is a small plot showing a single peak with the label "2web". On the left side of the page, there is a sidebar with various menu options under categories like "Execution >>", "StructGen™", "View structure", etc. At the bottom left, there is a note: "Idea and realization by [Jutz.at](#) © 2001-2006".

31. Click the “initlapw” button:

The screenshot shows a web-based graphical user interface for a molecular simulation program. On the left, there is a 3D ball-and-stick model of a molecule with atoms labeled T, E, N, W, and 2k. Below the model is a vertical sidebar with various menu options. The main area displays a command-line session with the following text:

```

Session: [TiC]
/home/username/wiendata/TiC
Commandline: x nn
Program input is: "2"

specify nn-bondlength factor: (usually=2) [and optionally dlimit, dstmax (about 1.d-5, 20)]
dfac,DSTMAX: 2.0000000000000000 20.0000000000000000
iix,iiy,iiz      5      5      5 40.893689999999992      40.89368999999992

    ATOM 1 Ti          ATOM 2 C
RMT( 1)=2.00000 AND RMT( 2)=1.90000
SUMS TO 3.90000 LT. NN-DIST= 4.08937

    ATOM 2 C          ATOM 1 Ti
RMT( 2)=1.90000 AND RMT( 1)=2.00000
SUMS TO 3.90000 LT. NN-DIST= 4.08937
STOP NN ENDS
0.001u 0.001s 0:00.00 0.0%   0+0k 0+32io 0pf+0w

Continue with


```

The 'initlapw' button is highlighted with a mouse cursor. The top right corner of the window shows the time as 15:51:54 idle and refresh/no refresh buttons. The bottom right corner has a logo for 'w2web'.

32. Click the “view outputnn” button  
 33. Click the “initlapw without saving” button:

Session: **TiC**  
 /home/username/wiendata/TiC

File: /home/username/wiendata/TiC.outputnn

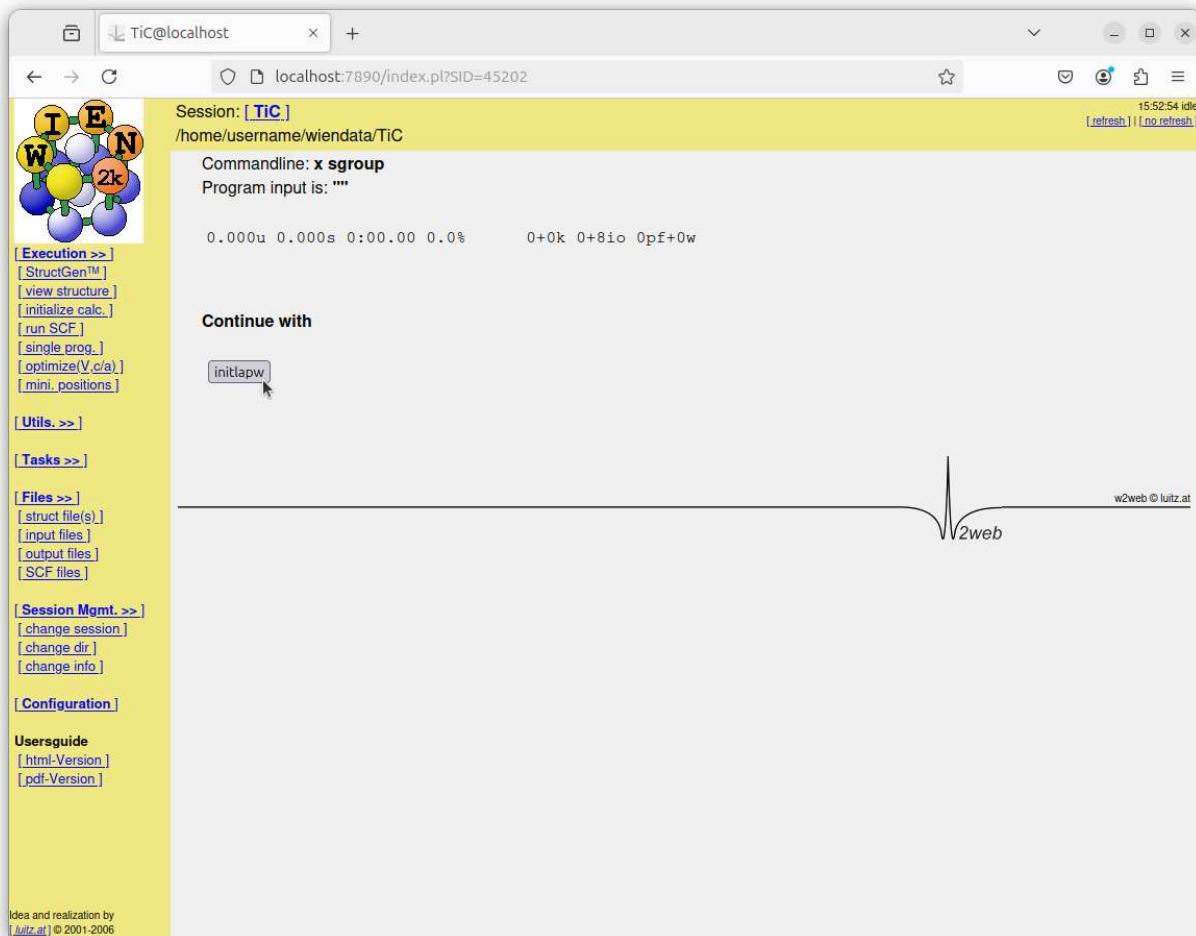
**initlapw without saving** **Save and initlapw** Download this file:

```

TiC
F          2
RELA
  8.178738  8.178738  8.178738  90.000000  90.000000  90.000000
  -1        0.00000000  0.00000000  0.00000000
               1
Ti      NPT= 781 R0=0.00005000 RMT= 2.0000 Z: 22.0
               1.00000000  0.00000000  0.00000000
               0.00000000  1.00000000  0.00000000
               0.00000000  0.00000000  1.00000000
               2        0.50000000  0.50000000  0.50000000
               1
C       NPT= 781 R0=0.00010000 RMT= 1.9000 Z: 6.0
               0.00000000  0.00000000  0.00000000
               0.00000000  0.00000000  0.00000000
               0.00000000  0.00000000  0.00000000
Bravais Matrix:
  0.000000    0.500000    0.500000
  0.500000    0.000000    0.500000
  0.500000    0.500000    0.000000
  
```

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34. Click the “x sgroup” button
35. Click the “initlapw” button:



36. Click the “view outputsgroup” button
37. Click the “initlapw without saving” button:

The screenshot shows a web browser window titled "TiC@localhost" at "localhost:7890/index.pl?SID=45202". The session name is "TiC". The left sidebar contains a molecular model of TiC and various navigation links like "StructGen™", "Execution >>", "File >>", "Session Mgmt. >>", "Configuration", and "Usersguide". The main content area displays session details and output files. A yellow bar at the top says "Session: [TiC] /home/username/wiendata/TiC". Below it, a "File:" section shows the path "/home/username/wiendata/TiC.TiC.outputsgroup". It contains three buttons: "initlapw without saving" (highlighted with a red box), "Save and initlapw", and "Download this file: ". The text area below lists Bravais lattice parameters and decomposition of basis vectors.

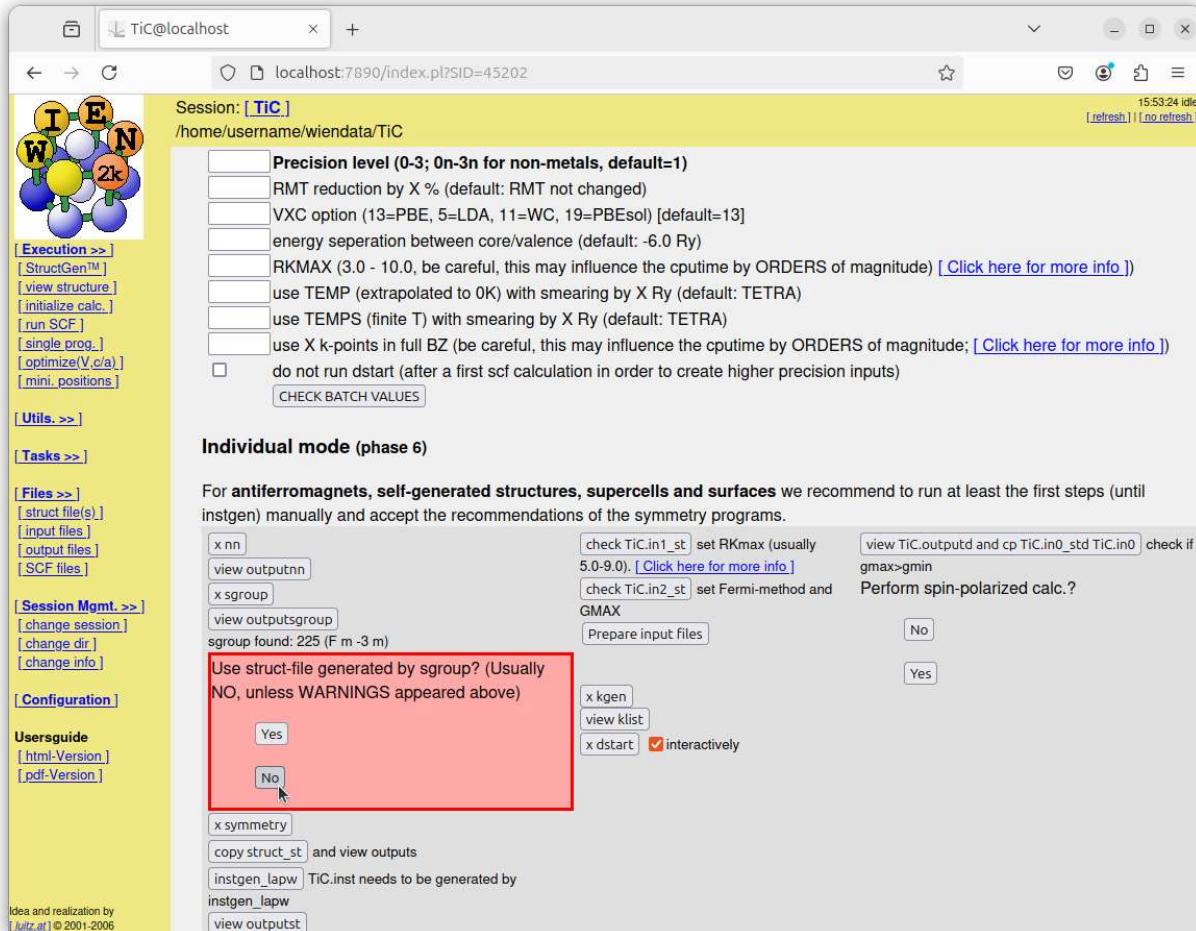
```
a          b          c
8.17873800  8.17873800  8.17873800
alpha       beta        gamma
90.00000000  90.00000000  90.00000000

===== Decomposition of new basis vectors over input basis =====
0.000000  1.000000  0.000000 <---- 1
0.000000  0.000000  1.000000 <---- 2
1.000000  0.000000  0.000000 <---- 3

==== Number of atoms in cell (only atoms of primitive cell): 2
==== Atom positions (only atoms of primitive cell):

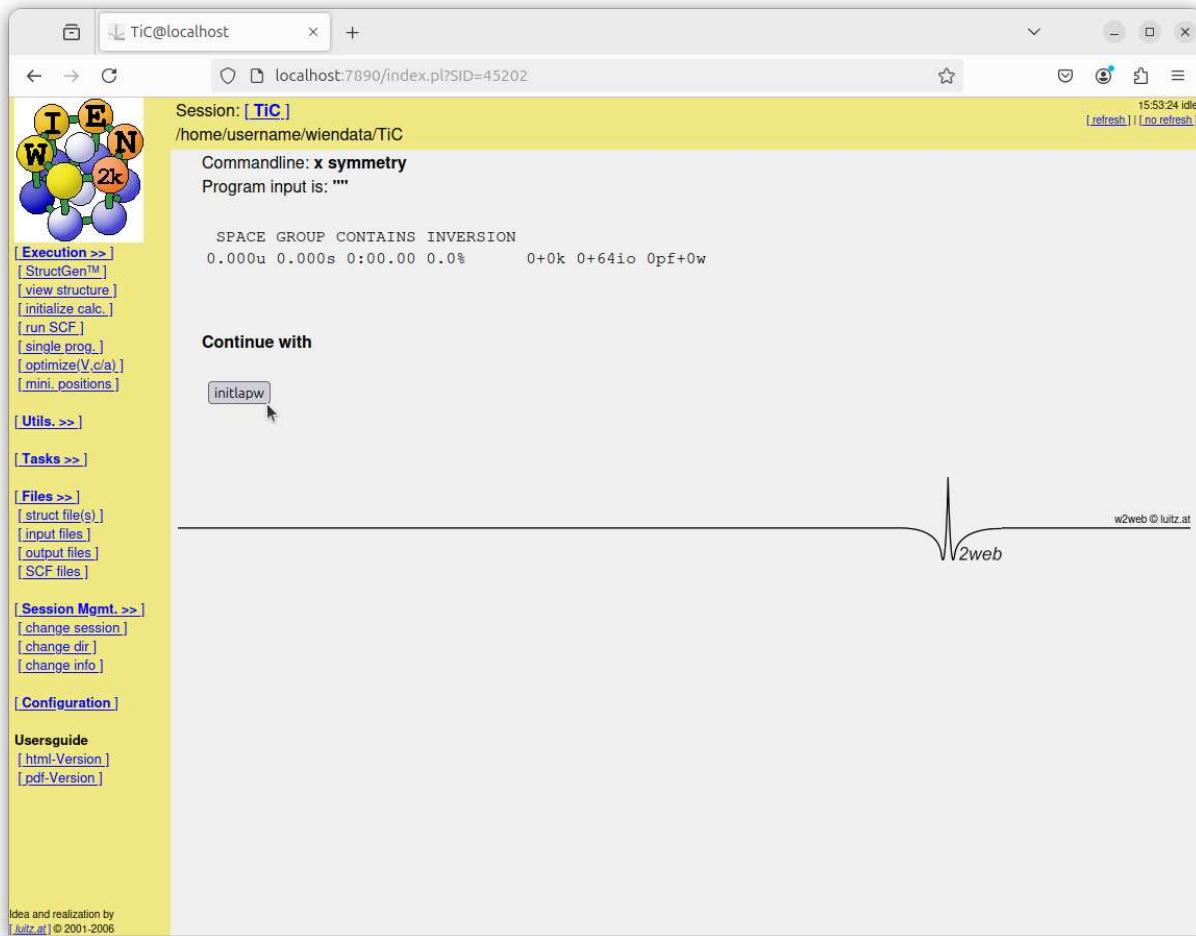
0.00000000  0.00000000  0.00000000
Ti
0.50000000  0.00000000  0.00000000
```

38. Click the “No” button to “Use struct-file generated by sgroup”:

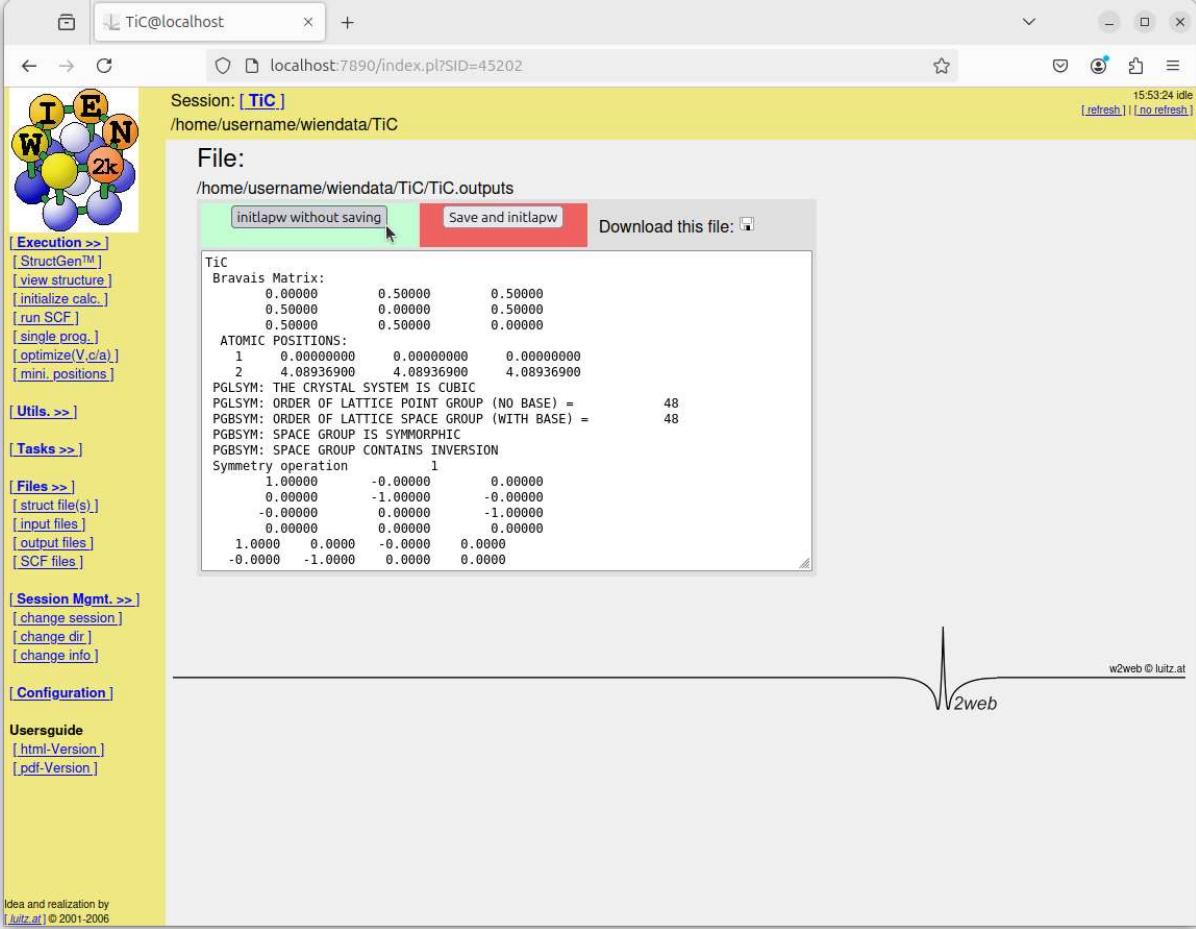


39. Click the “x symmetry” button

40. Click the “initlapw” button:



41. Click the “copy struct\_st” button  
 42. Click the “initlapw without saving” button:



The screenshot shows a web browser window titled "TiC@localhost" with the URL "localhost:7890/index.pl?SID=45202". The page displays session information for "Session: [TiC] /home/username/wiendata/TiC". On the left, there's a molecular model of TiC and a sidebar with various navigation links. The main content area shows the following text:

```

Session: [TiC]
/home/username/wiendata/TiC

File:
/home/username/wiendata/TiC.outputs

[initlapw without saving] [Save and initlapw] Download this file: [ ]
```

**TiC**

Bravais Matrix:

0.00000	0.50000	0.50000
0.50000	0.00000	0.50000
0.50000	0.50000	0.00000

ATOMIC POSITIONS:

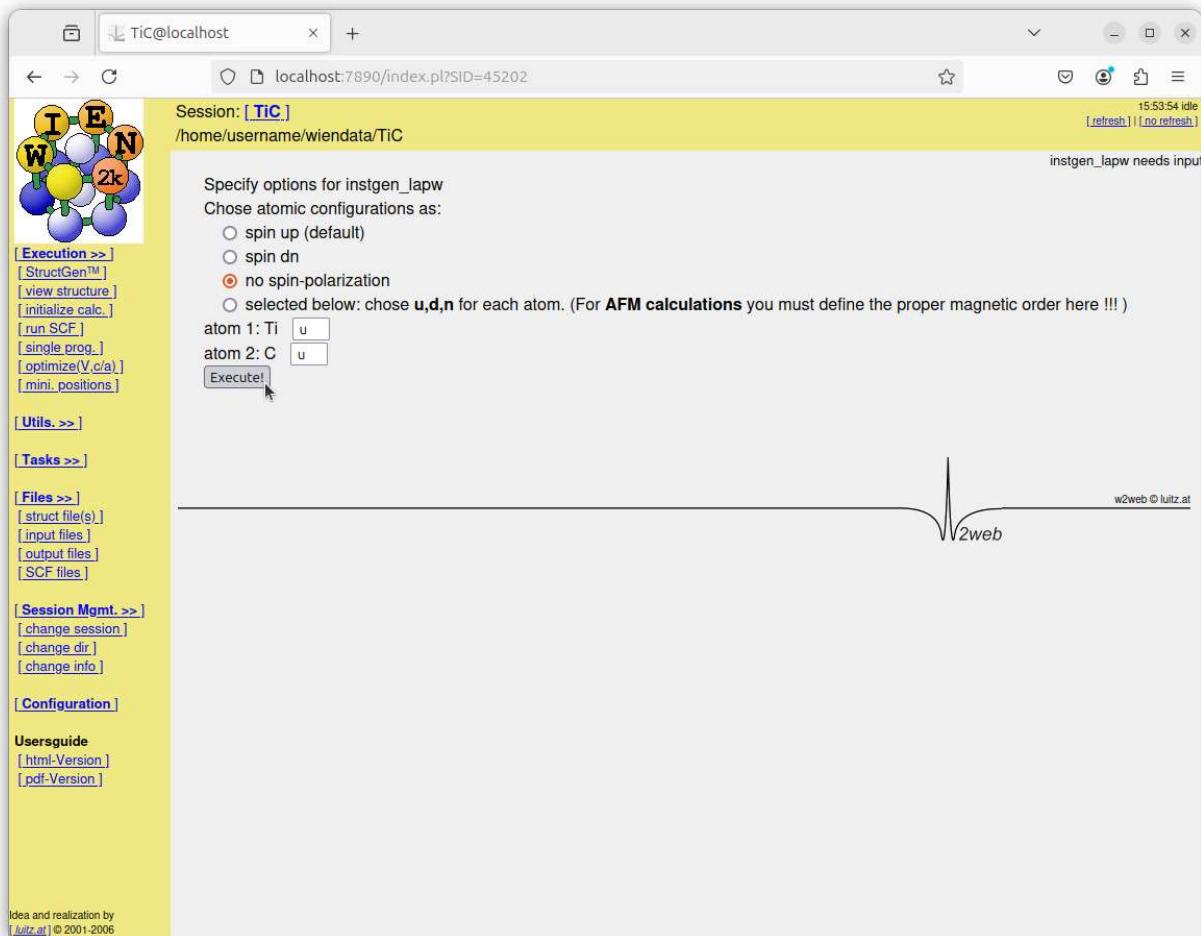
1	0.0000000	0.0000000	0.0000000
2	4.08936900	4.08936900	4.08936900

PGLSYM: THE CRYSTAL SYSTEM IS CUBIC  
 PGLSYM: ORDER OF LATTICE POINT GROUP (NO BASE) = 48  
 PGBSYM: ORDER OF LATTICE SPACE GROUP (WITH BASE) = 48  
 PGBSYM: SPACE GROUP IS SYMMORPHIC  
 PGBSYM: SPACE GROUP CONTAINS INVERSION  
 Symmetry operation 1

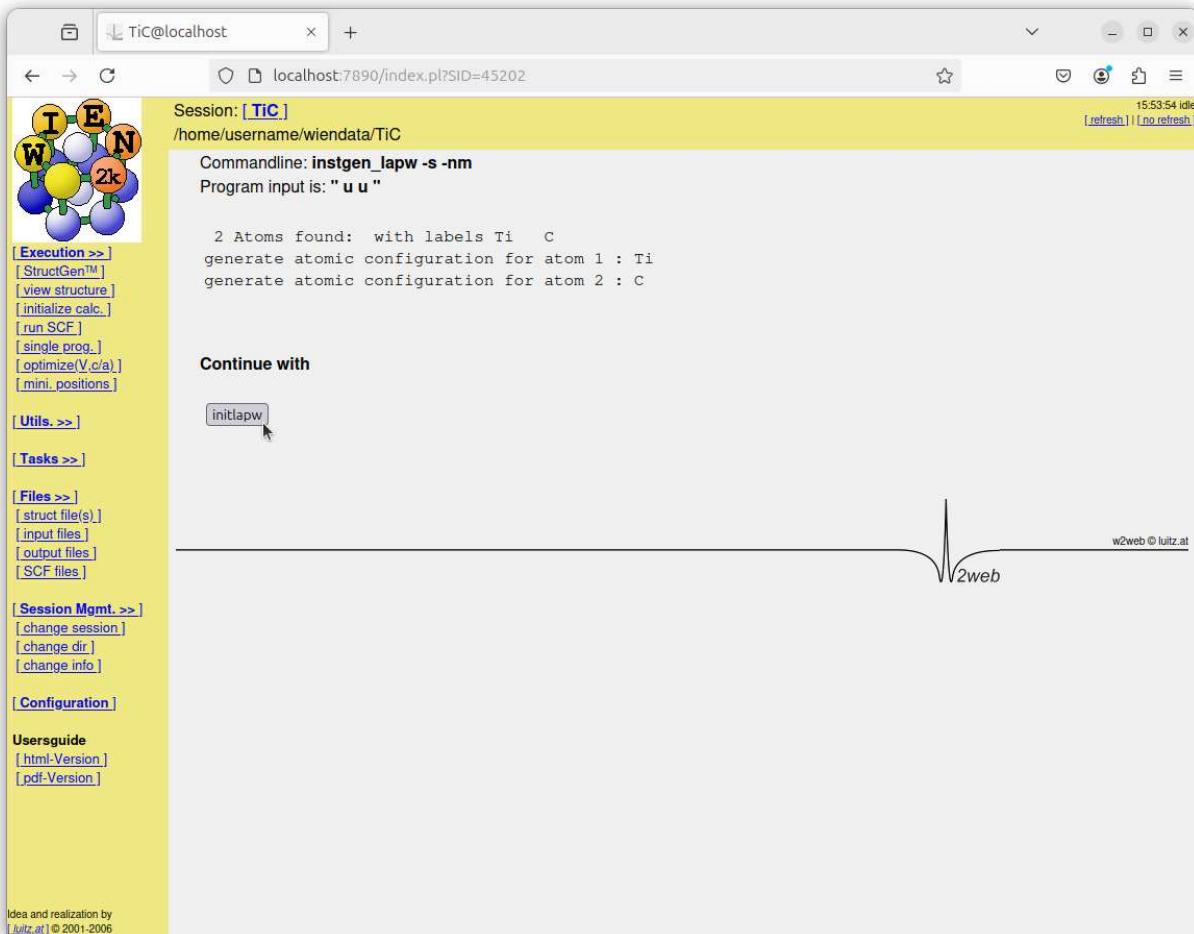
1.00000	-0.00000	0.00000
0.00000	-1.00000	-0.00000
-0.00000	0.00000	-1.00000
0.00000	0.00000	0.00000
1.00000	0.00000	-0.00000
-0.00000	-1.00000	0.00000

w2web © luitz.at

43. Click the “instgen\_lapw” button
44. Select “no spin-polarization” and then click the “Execute!” button:



45. Click the “initlapw” button:



46. Click the “x lstart” button

47. By default, -6.0 is in the box and PBE-GGA is selected, click the “Execute!” button:

The screenshot shows a web browser window titled "TiC@localhost" at "localhost:7890/index.pl?SID=45202". The session is named "TiC" and is located at "/home/username/wiendata/TiC". The status bar indicates "15:54:24 idle" and "LSTART needs input". On the left, there's a sidebar with various links for execution, utilities, tasks, files, session management, and configuration. The main content area displays a molecular model of TiC with atoms labeled I, E, N, W, and 2x. It includes a dropdown for "Select Exchange Correlation Potential" set to "PBE-GGA (Perdew-Burke-Ernzerhof 96)". Below it, there's a section for "ENERGY to separate core and valence states" with a field containing "-6.0" and a note about charge localization. A large "Execute!" button is highlighted with a cursor. The bottom right corner features a logo for "w2web © iuiz.at".

## 48. Click the “initlapw” button:

The screenshot shows the TiC@localhost web interface. On the left, there's a sidebar with various buttons like 'Execution >>', 'StructGen™', 'view structure', etc. The main area displays command-line input and output. The output shows atomic configurations for Ti and C atoms, followed by a STOP LSTART ENDS message.

```

Session: [TiC]
/home/username/wiendata/TiC
Commandline: x Istart
Program input is: "13-6.0"

SELECT XC POT:
recommended: PBE [(13) GGA of Perdew-Burke-Ernzerhof 96]
LDA [(5)]
WC [(11) GGA of Wu-Cohen 2006]
PBESOL [(19) GGA of Perdew et al. 2008]

SELECT ENERGY to separate core and valence states:
recommended: -6.0 Ry (check how much core charge leaks out of MT-sphere)
ALTERNATIVELY: specify charge localization (between 0.97 and 1.0) to select core state

Atomic configuration for atom: Ti      Z= 22.00
    E-up (Ry)      E-dn (Ry)   Occupancy   q/sphere   core-state
  1S   -357.793778   -357.793778  1.00  1.00   1.0000  T
  2S   -39.452643   -39.452643  1.00  1.00   1.0000  T
  2P*  -32.924289   -32.924289  1.00  1.00   1.0000  T
  2P   -32.500026   -32.500026  2.00  2.00   1.0000  T
  3S   -4.601202   -4.601202  1.00  1.00   0.9831  F
  3P*  -2.886588   -2.886588  1.00  1.00   0.9622  F
  3P   -2.838251   -2.838251  2.00  2.00   0.9604  F
  3D*  -0.314106   -0.314106  1.00  1.00   0.7387  F
  4S   -0.328107   -0.328107  1.00  1.00   0.0910  F

Atomic configuration for atom: C      Z= 6.00
    E-up (Ry)      E-dn (Ry)   Occupancy   q/sphere   core-state
  1S   -20.092503   -20.092503  1.00  1.00   1.0000  T
  2S   -1.010581   -1.010581  1.00  1.00   0.7309  F
  2P*  -0.388826   -0.388826  0.50  0.50   0.6271  F
  2P   -0.388183   -0.388183  0.50  0.50   0.6266  F

STOP LSTART ENDS
0.045u 0.004s 0:00.05 80.0%      0+0k 128+984io 0pf+0w

```

**Continue with**

**initlapw**

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49. Click the “view outputst” button
50. Click the “initlapw without saving” button:

The screenshot shows a web browser window for the TiC@localhost application. The title bar reads "TiC@localhost" and the address bar shows "localhost:7890/index.pl?SID=45202". The main content area displays a molecular structure with atoms labeled I, E, N, W, and 2x. Below the structure, there is a sidebar with various links such as "Execution >>", "StructGen™", "view structure", "initialize calc.", "run SCF", "single prog.", "optimize(V,c/a)", "mini. positions", "Utils. >>", "Tasks >>", "Files >>", "Session Mgmt. >>", and "Configuration". The main panel shows session details: "Session: [TiC]", "File: /home/username/wiendata/TiC/TiC.outputst", and three buttons: "initlapw without saving" (highlighted in green), "Save and initlapw" (red), and "Download this file: ". The output text area contains the following data:

```
Ti          RHFS
NUMBER OF ITERATIONS 350
PRECISION OF ENERGIES 5.00E-07
WAVEFUNCTION 1.00E-06
POTENTIAL 1.00E-06
INTEGRATION WITH 971 POINTS STARTING AT 0.0011/22 AND INCREMENT 0.0136
ORBITAL    OCCUPATION    TRIAL ENERGIES
1S        1.000      -1.2100000E+02
1S        1.000      -1.2100000E+02
```

At the bottom right of the main panel, there is a "w2web" logo with a stylized wave graphic.

51. Click the “check TiC.in1\_st” button
52. Change “emax” in the file from 1.5 to 2.0
53. Click the “Save and initlapw” button:

The screenshot shows a web-based graphical user interface for a computational chemistry application. On the left, there's a sidebar with various menu items like 'Execution >>', 'StructGen™', 'view structure', etc. The main area features a 3D ball-and-stick model of a molecule with atoms labeled T, E, N, W, and 2k. Below the model is a code editor window titled 'File: /home/username/wiendata/TIC/TIC.in1\_st'. The code contains several lines of parameters and vectors. A red rectangular box highlights the 'Save and initlapw' button, which is located just above the code editor. The status bar at the bottom right indicates 'w2web © lutz.at'.

```

Session: [TIC]
/home/username/wiendata/TIC/TIC.in1_st

File:
/home/username/wiendata/TIC/TIC.in1_st

initlapw without saving Save and initlapw Download this file: □

WEEFIL EE= 0.50000 (WEEFIL, WEPRI, ENFIL, SUPWF)
7.00   10   4 ELPAPXG BL 64 (R-MT*K-MAX,MAX L IN WF,V-NMT,LIB)
0.30   5   0 (GLOBAL E-PARAMETER WITH n OTHER CHOICES, global APW/LAPW)
0   0.30   0.0000 CONT 1
0   -4.30   0.0001 STOP 1
1   0.30   0.0000 CONT 1
1   -2.54   0.0010 CONT 1
2   0.30   0.0010 CONT 1
0.30   3   0 (GLOBAL E-PARAMETER WITH n OTHER CHOICES, global APW/LAPW)
0   0.30   0.0000 CONT 1
0   -0.71   0.0010 CONT 1
1   0.30   0.0000 CONT 1
K-VECTORS FROM UNIT:4 -9.0      2.0    emin / de (emax=Ef+de) / nband

```

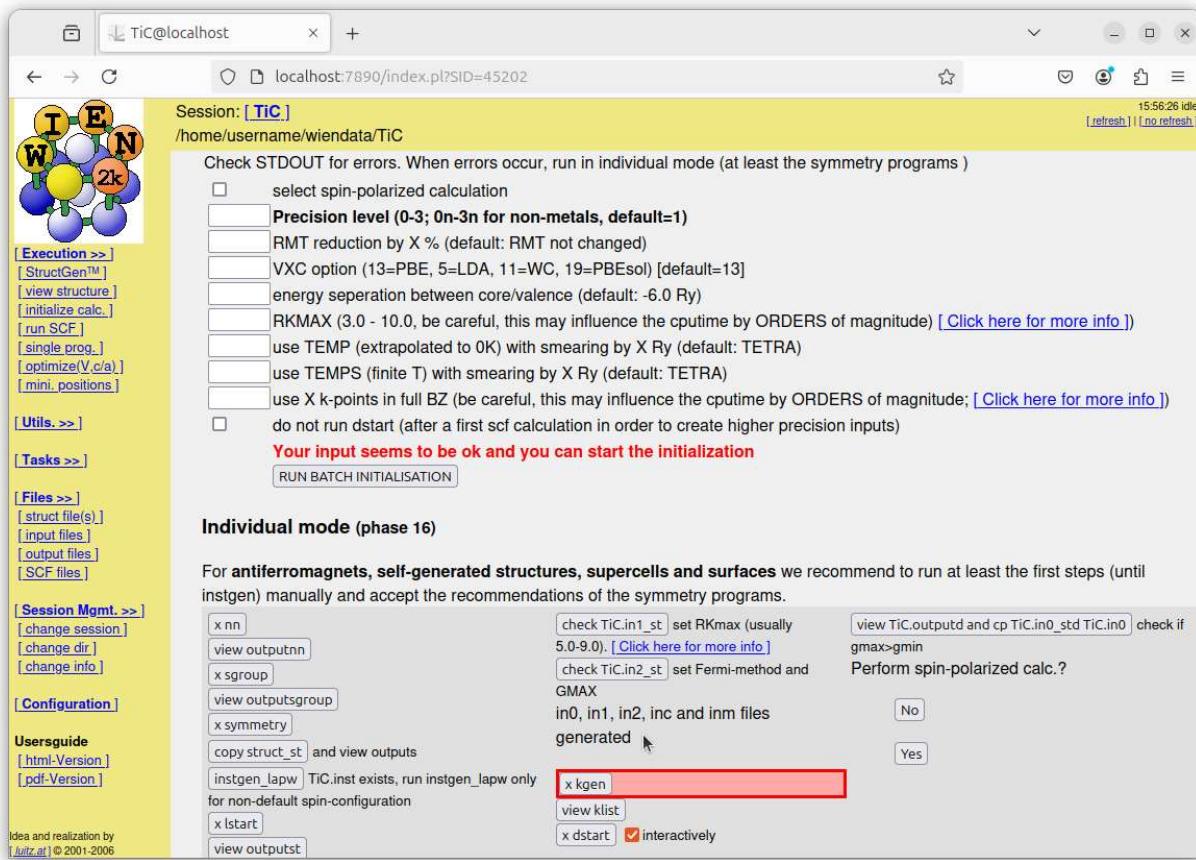
54. Click the “check TiC.in2\_st” button
55. Click the “initlapw without saving” button:

The screenshot shows a web browser window titled "TiC@localhost" at "localhost:7890/index.pl?SID=45202". The session name is "Session: [TiC] /home/username/wiendata/TiC". On the left, there's a sidebar with various links like "Execution >>", "File >>", "Session Mgmt. >>", "Configuration", and "Usersguide". The main content area displays a file named "TiC.in2\_st" with the following text:

```
TOT          (TOT,FOR,STR,STRF,QL,EG,FERMI)
-12.0      16.0   0.50 0.05 1  EMIN, NE, ESEPERMIN, ESEPER0, iqtlSAVE
TETRA      0.000   (GAUSS,ROOT,TEMP,TETRA,ALL           eval)
  0 0 4 0 4 4 6 0 6 4
  0 0 4 0 4 4 6 0 6 4
12.00      GMAX
NOFILE     FILE/NOFILE  write reciplist
```

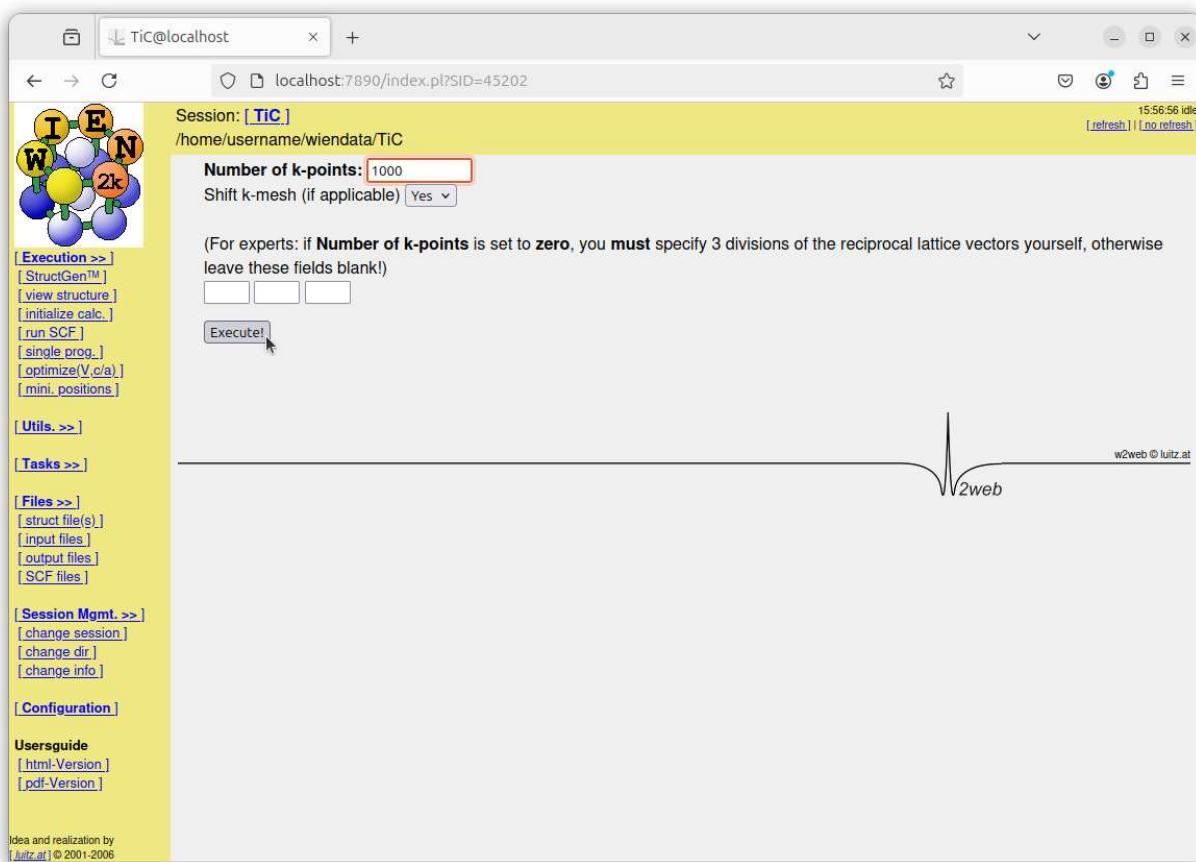
At the top of the file view, there are three buttons: "initlapw without saving" (highlighted in green), "Save and initlapw" (red), and "Download this file: □". The bottom right corner of the page has a "w2web" logo.

56. Click the “Prepare input files” button (message ‘in0, in1, in2, inc and inm files generated’ appears on screen):



57. Click the “x kgen” button

58. Type 1000 in the “Number of k-points” box, then click the “Execute!” button:



59. Click the “initlapw” button:

The screenshot shows a web-based graphical user interface for a computational chemistry program. On the left, there is a sidebar with a molecular structure visualization and several menu items:

- [Execution >>]
  - [StructGen™]
  - [view structure]
  - [initialize calc.]
  - [run SCF]
  - [single prog.]
  - [optimize(V,c/a)]
  - [mini\_positions]
- [Utils. >>]
- [Tasks >>]
- [Files >>]
  - [struct file(s)]
  - [input files]
  - [output files]
  - [SCF files]
- [Session Mgmt. >>]
  - [change session]
  - [change dir.]
  - [change info]
- [Configuration]
- Usersguide**
  - [html-Version.]
  - [pdf-Version.]

Idea and realization by [luitz.at](#) © 2001-2006

The main content area displays session information and command-line output:

Session: [TiC.]  
/home/username/wiendata/TiC  
Commandline: x kgen  
Program input is: " 1000 1 "  
  
NUMBER OF K-POINTS IN WHOLE CELL: (0 for 3 divisions of K, -1 for delta-K)  
length of reciprocal lattice vectors (bohr^-1): 1.331 1.331 1.331  
47 k-points generated, ndiv= 10 10 10  
delta-K (bohr^-1): 0.1331 0.1331 0.1331  
STOP KGEN ENDS  
0.004u 0.002s 0:00.00 0.0% 0+0k 0+200io 0pf+0w

Continue with

**initlapw**

w2web © luitz.at

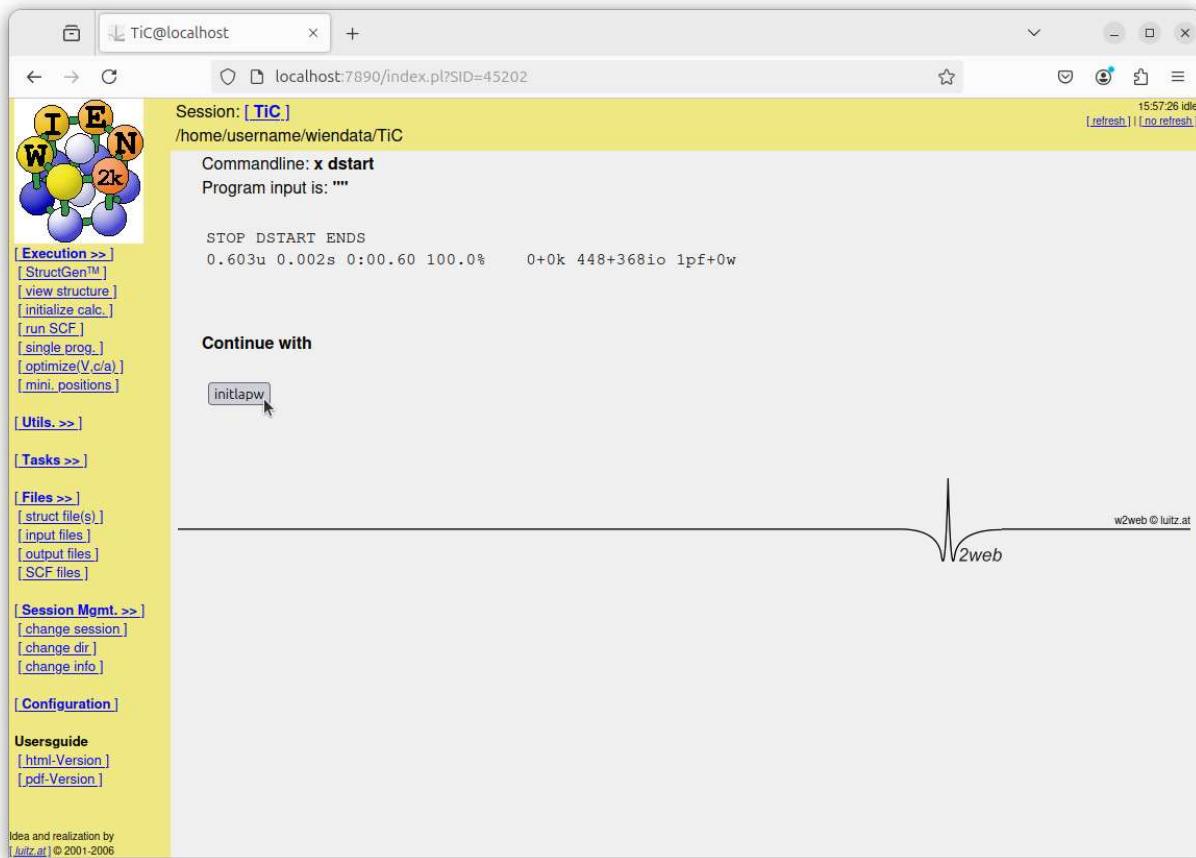
60. Click the “view klist” button

61. Click the “initlapw without saving” button:

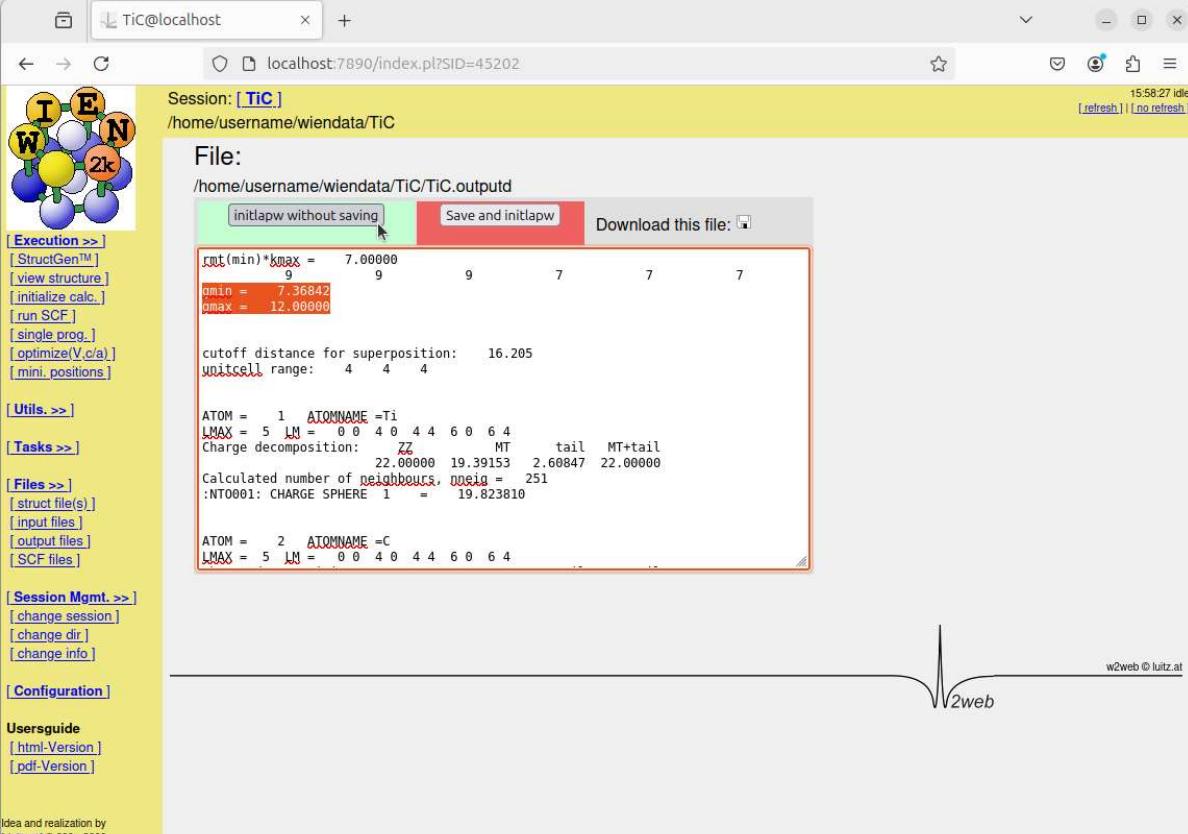
The screenshot shows a web browser window titled "TiC@localhost" with the URL "localhost:7890/index.pl?SID=45202". The page displays a session named "TiC" with the path "/home/username/wiendata/TiC". On the left, there is a molecular structure diagram and a sidebar with various menu options like "Execution >>", "Tasks >>", "Files >>", "Session Mgmt. >>", "Configuration", and "Usersguide". The main content area shows a table titled "File: /home/username/wiendata/TiC.TiC.klist". At the top of this table is a button labeled "initlapw without saving" which is highlighted with a red box. Below it are buttons for "Save and initlapw" and "Download this file:". The table itself contains numerical data. In the bottom right corner of the page, there is a logo for "w2web" with the text "w2web © luitz.at".

	1	0	0	0	10	1.0	-7.0	1.5	1000	k, d
1	2	1	1	-1	10	8.0				
2	3	2	2	-2	10	8.0				
3	4	3	3	-3	10	8.0				
4	5	4	4	-4	10	8.0				
5	6	5	5	-5	10	4.0				
6	7	2	0	0	10	6.0				
7	8	3	1	-1	10	24.0				
8	9	4	2	-2	10	24.0				
9	10	5	3	-3	10	24.0				
10	11	6	4	-4	10	24.0				
11	12	7	5	-5	10	24.0				
12	13	8	6	-6	10	24.0				
13	14	9	7	-7	10	24.0				
14	15	10	8	-8	10	12.0				
15	16	4	0	0	10	6.0				
16	17	5	1	-1	10	24.0				
17	18	6	2	-2	10	24.0				
18	19	7	3	-3	10	24.0				
19	20	8	4	-4	10	24.0				

62. Click the “x dstart” button (interactively checked by default)  
63. Click the “initlapw” button:



64. Click the “view TiC.outputd and cp TiC.in0\_std TiC.in0” button  
 65. Notice that the condition gmax > gmin is met and click the “initlapw without saving” button:



The screenshot shows a web browser window titled "TiC@localhost" at "localhost:7890/index.pl?SID=45202". The session name is "TiC" and the path is "/home/username/wiendata/TiC". On the left, there's a molecular model of a TiC structure with atoms labeled I, E, N, W, and 2x. A sidebar contains various execution, tasks, files, and session management buttons. The main content area displays a file named "TiC.outputd" with the following text:

```

File: /home/username/wiendata/TiC/TiC.outputd
[initlapw without saving] [Save and initlapw] [Download this file]

rcut(min)*kmax = 7.00000
9         9         9         7         7         7         7

gmin = 7.36842
gmax = 12.00000

cutoff distance for superposition: 16.205
unitcell range: 4 4 4

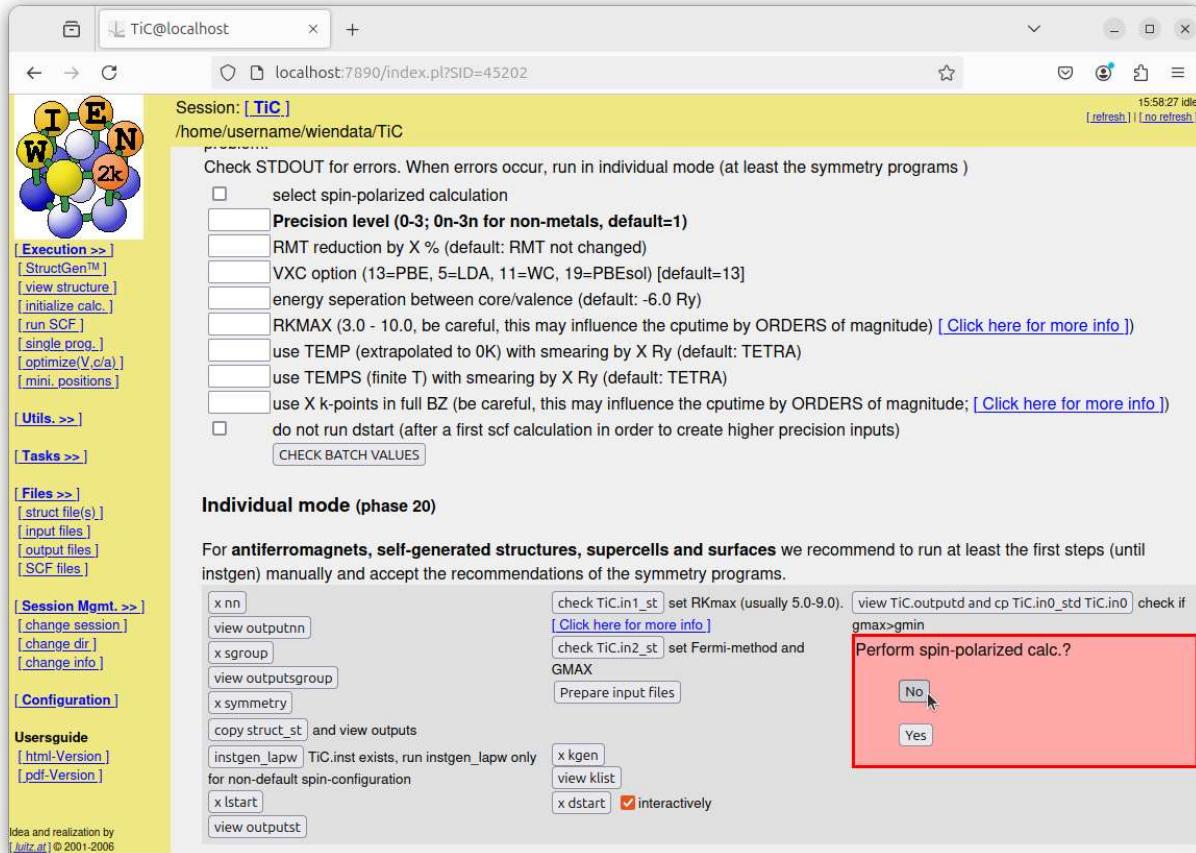
ATOM = 1 ATOMNAME =Ti
LMAX = 5 LM = 0 0 4 0 4 4 6 0 6 4
Charge decomposition: ZZ MT tail MT+tail
22.00000 19.39153 2.60847 22.00000
Calculated number of neighbours, nneg = 251
:NT0001: CHARGE SPHERE 1 = 19.823810

ATOM = 2 ATOMNAME =C
LMAX = 5 LM = 0 0 4 0 4 4 6 0 6 4

```

A red box highlights the "initlapw without saving" button. The bottom right corner of the window features a logo for "w2web" with the text "w2web © luitz.at".

66. Click the “No” button to “Perform spin-polarized calc.? ”:

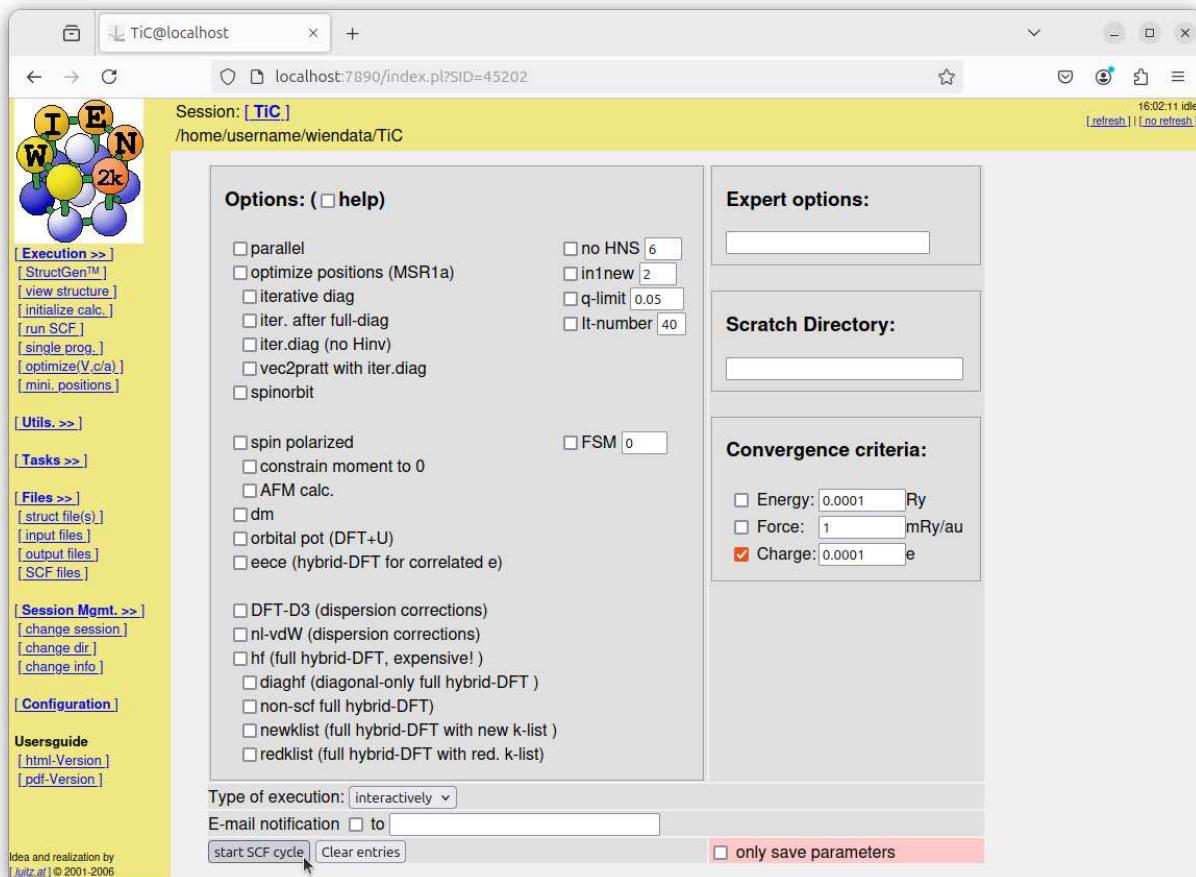


67. Click the “Continue with run SCF” link:

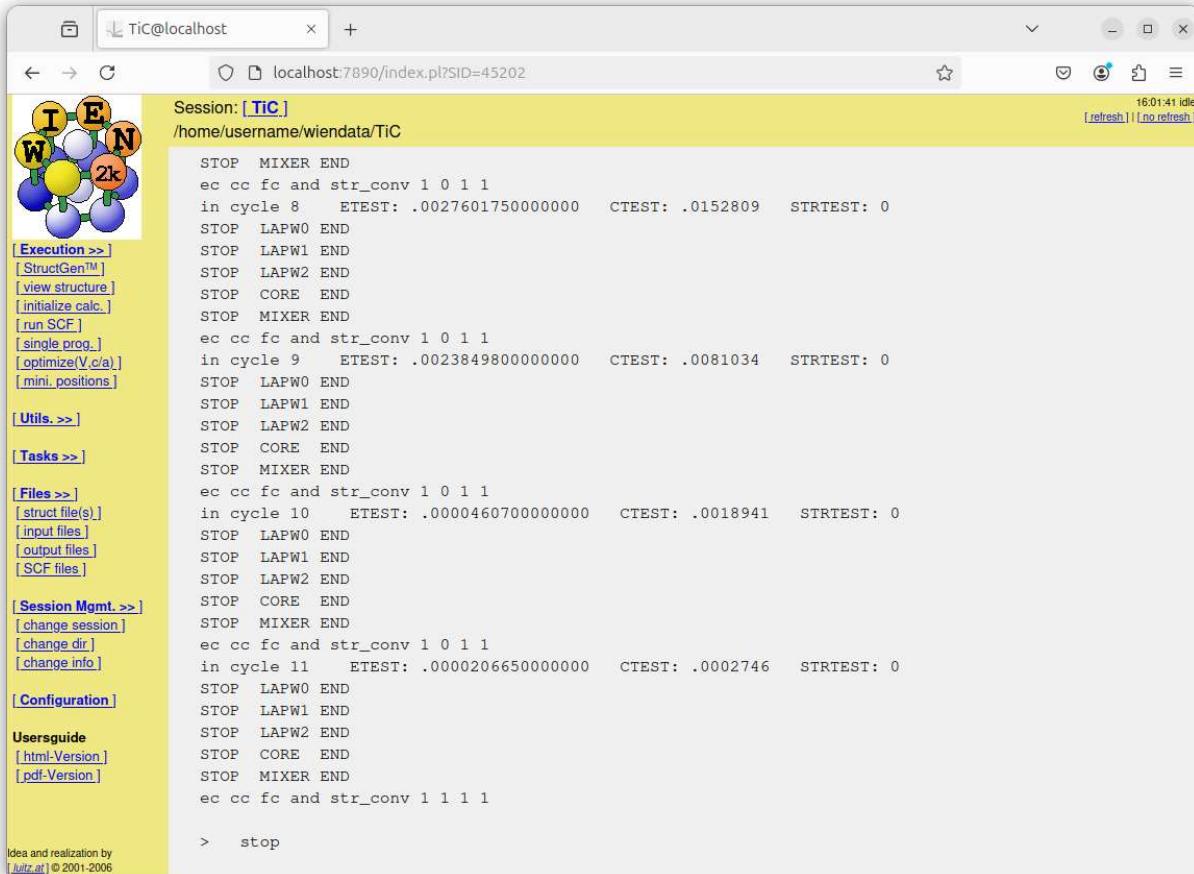
The screenshot shows a web browser window titled "TiC@localhost" at the URL "localhost:7890/index.pl?SID=45202". The page displays a session configuration for a TiC calculation. On the left, there is a sidebar with various navigation links under categories like "Execution >>", "Tasks >>", "Files >>", "Session Mgmt. >>", and "Configuration". The main content area shows session details such as energy separation, RKMAX, and TEMPS settings. A note about antiferromagnets and self-generated structures recommends manual steps until instgen. Below this, a section titled "Initialization done" contains a green button labeled "[ Continue with run SCF ]". The status bar at the bottom of the browser window shows the URL "localhost:7890/exec/scf.pl?SID=45202".

### Run the calculation

68. Uncheck the “Energy” box, check the “Charge” box, and type 0.0001 into the box next to it.  
 69. Select “interactively” for the “Type of execution”, then click the “start SCF cycle” to perform the calculation:



70. As shown, this calculation converges after 11 cycles:



The screenshot shows a web browser window titled "TiC@localhost" displaying the URL "localhost:7890/index.pl?SID=45202". The page content is a session log for a molecular calculation. On the left, there is a sidebar with various menu options such as "Execution >>", "StructGen™", "view structure", "initialize calc.", "run SCF", "single prog.", "optimize(V,c/a)", "mini. positions", "Utils. >>", "Tasks >>", "Files >>", "Session Mgmt. >>", "Configuration", and "Usersguide". Below these menus is a note: "Idea and realization by [fritz.at] © 2001-2006". The main area of the page displays the following text:

```

Session: [ TiC. ]
/home/username/wiendata/TiC
16:01:41 idle
[ refresh ] | [ no refresh ]

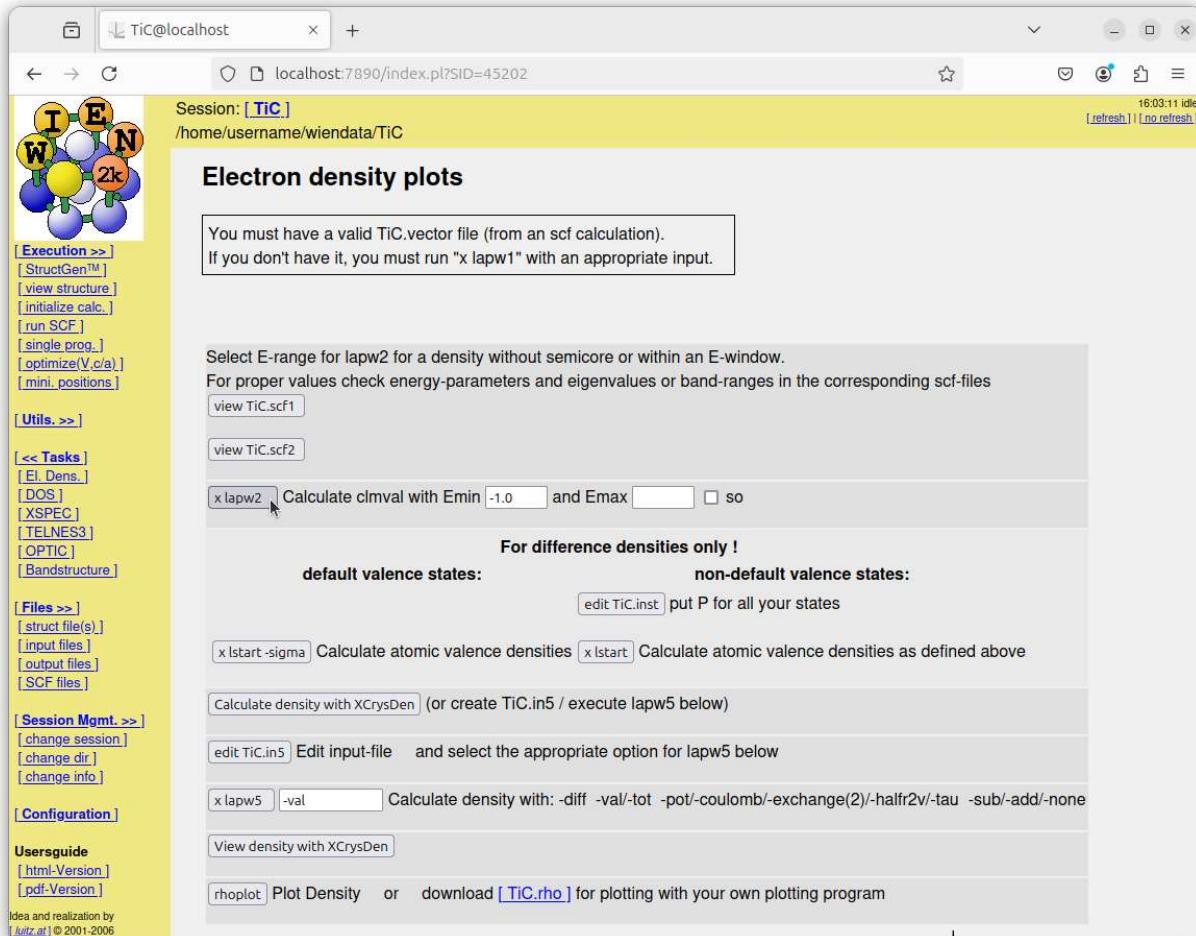
STOP MIXER END
ec cc fc and str_conv 1 0 1 1
in cycle 8      ETEST: .0027601750000000    CTEST: .0152809    STRTEST: 0
STOP LAPW0 END
STOP LAPW1 END
STOP LAPW2 END
STOP CORE END
STOP MIXER END
ec cc fc and str_conv 1 0 1 1
in cycle 9      ETEST: .0023849800000000    CTEST: .0081034    STRTEST: 0
STOP LAPW0 END
STOP LAPW1 END
STOP LAPW2 END
STOP CORE END
STOP MIXER END
ec cc fc and str_conv 1 0 1 1
in cycle 10     ETEST: .0000460700000000    CTEST: .0018941    STRTEST: 0
STOP LAPW0 END
STOP LAPW1 END
STOP LAPW2 END
STOP CORE END
STOP MIXER END
ec cc fc and str_conv 1 0 1 1
in cycle 11     ETEST: .0000206650000000    CTEST: .0002746    STRTEST: 0
STOP LAPW0 END
STOP LAPW1 END
STOP LAPW2 END
STOP CORE END
STOP MIXER END
ec cc fc and str_conv 1 1 1 1

> stop

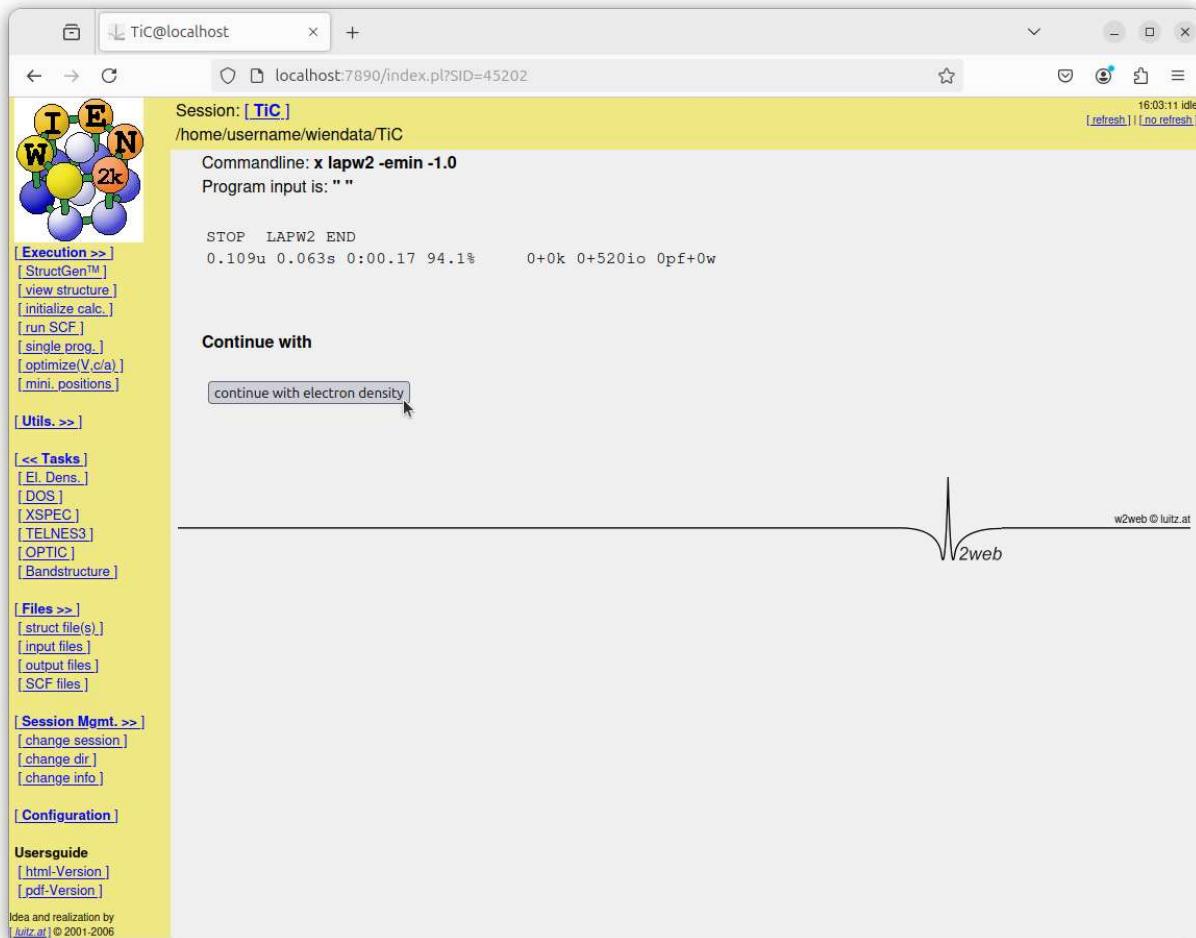
```

## Plot electron density

71. In the left menu, click “El. Dens.” under “Tasks”
72. Click the “x lapw2” button with Emin -1.0:



73. Click the “continue with electron density” button:



74. Click the “edit TiC.in5” button

75. Modify the file to look like the following (i.e., like the quickstart in the WIEN2k usersguide):

First three lines in TiC.in5 were changed to:

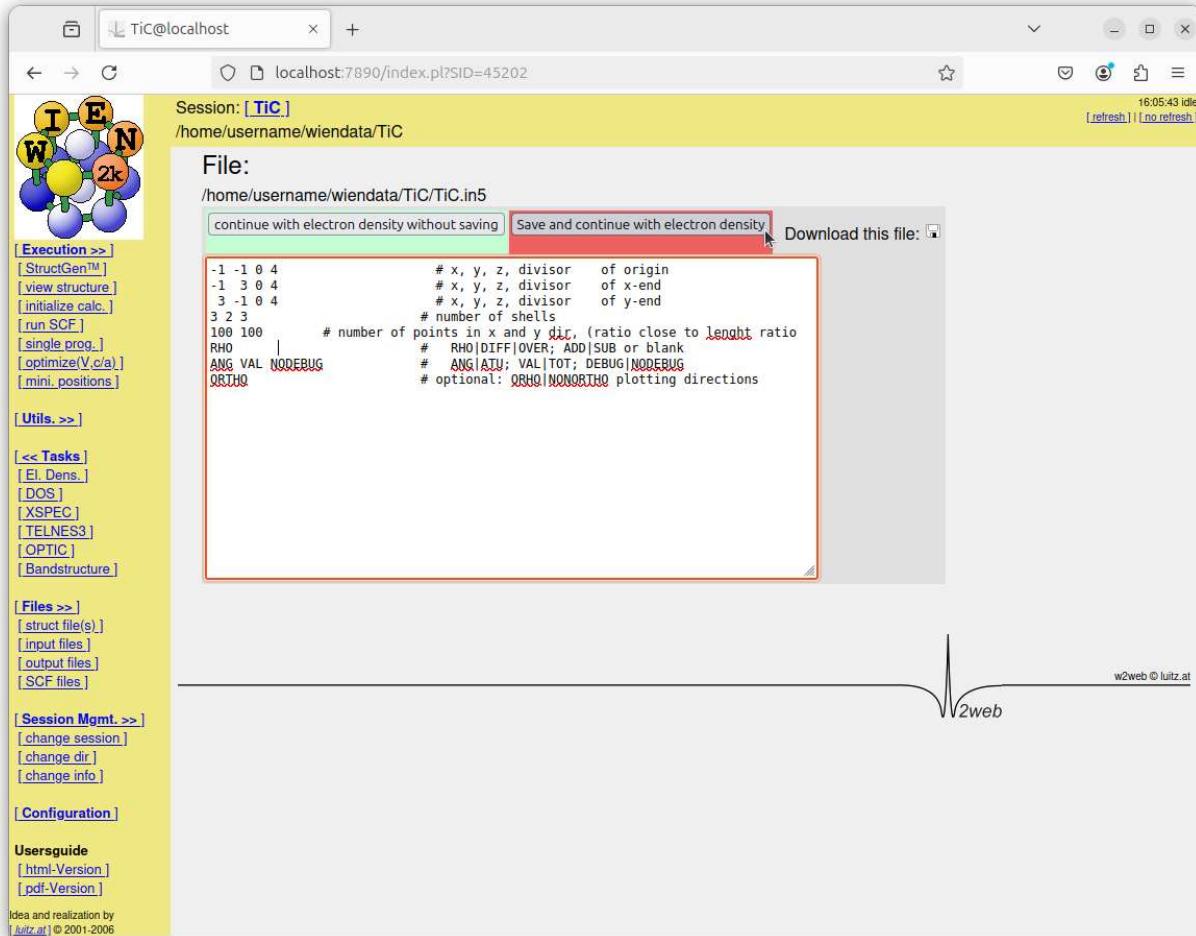
-1 -1 0 4 #origin of plot

-1 3 0 4 #x-end of plot

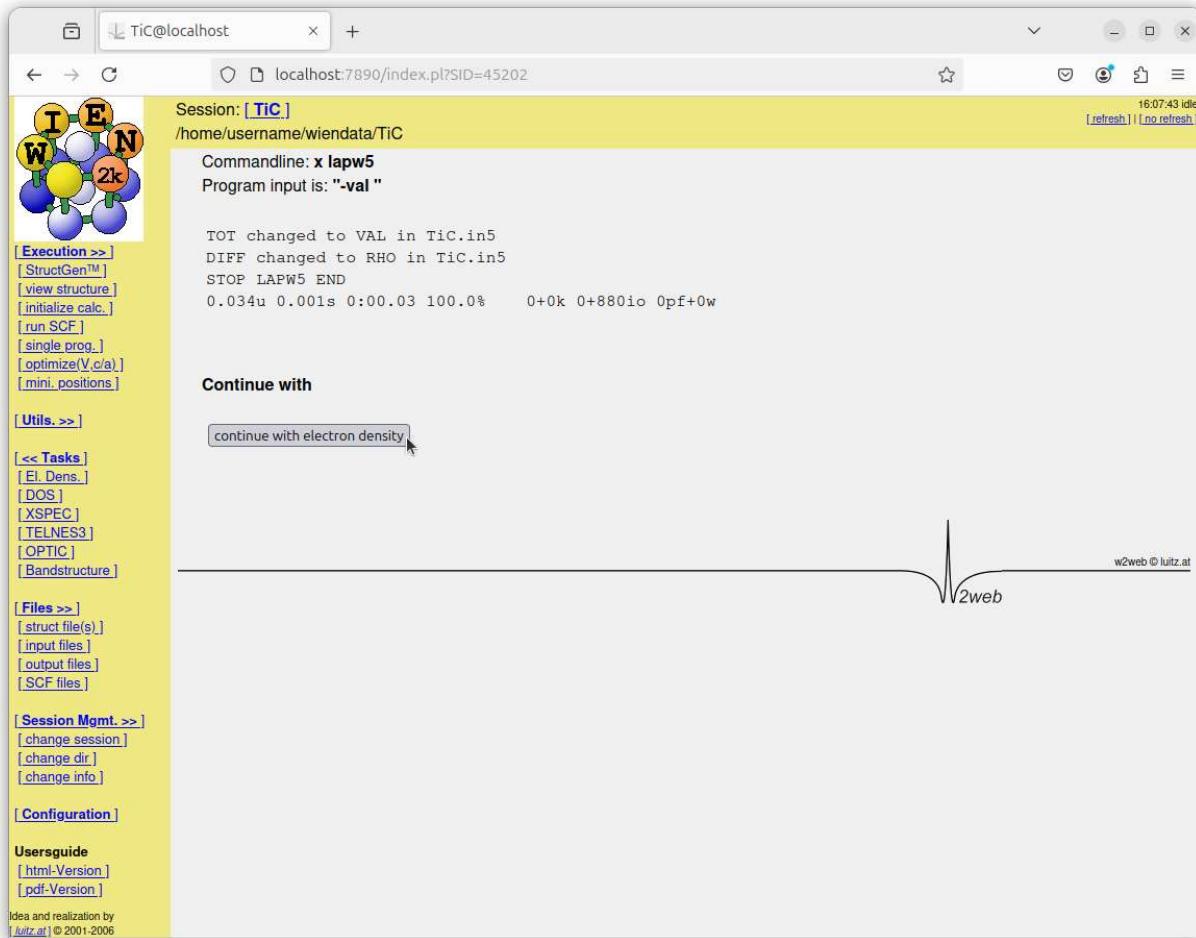
3 -1 0 4 #y-end of plot

ADD was removed

76. Click the “Save and continue with electron density” button

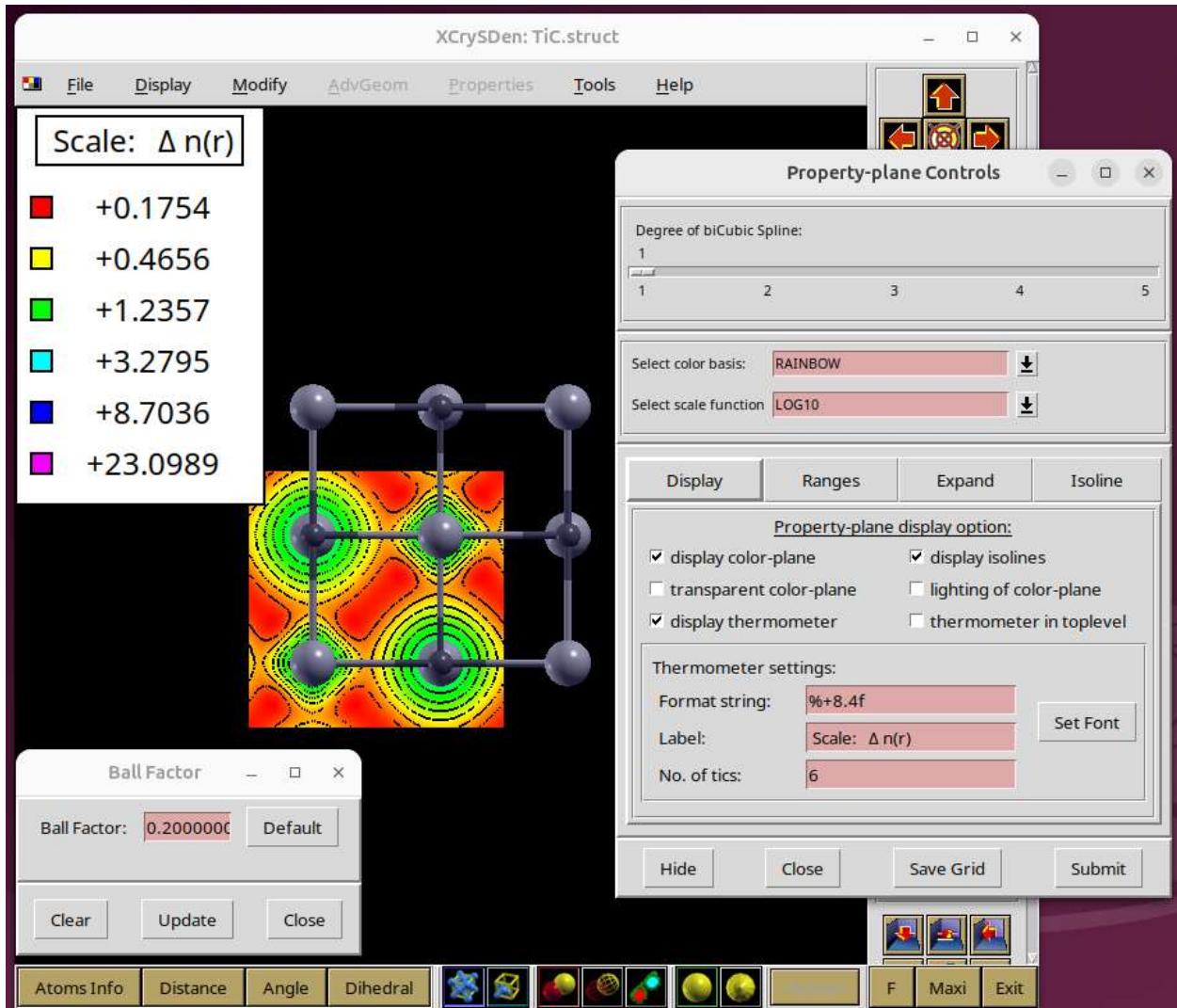


77. Click the “x lapw5” button  
 78. Click the “continue with electron density” button:



79. Click the “View density with XCrysDen” button  
 80. Select “RAINBOW” for “Select color basis”  
 81. Select “LOG10” for “Select scale function:”  
 82. Check “display thermometer”  
 83. Click the “Submit” button  
 84. Click “Modify”, then click “Ball Factor”  
 85. Change Factor to 0.2 and click the “Update” button  
 86. Can rotate the structure by left clicking in the black widow and then moving the mouse

87. The following results (compare to Figure 3.8 in the WIEN2k usersguide [2]):



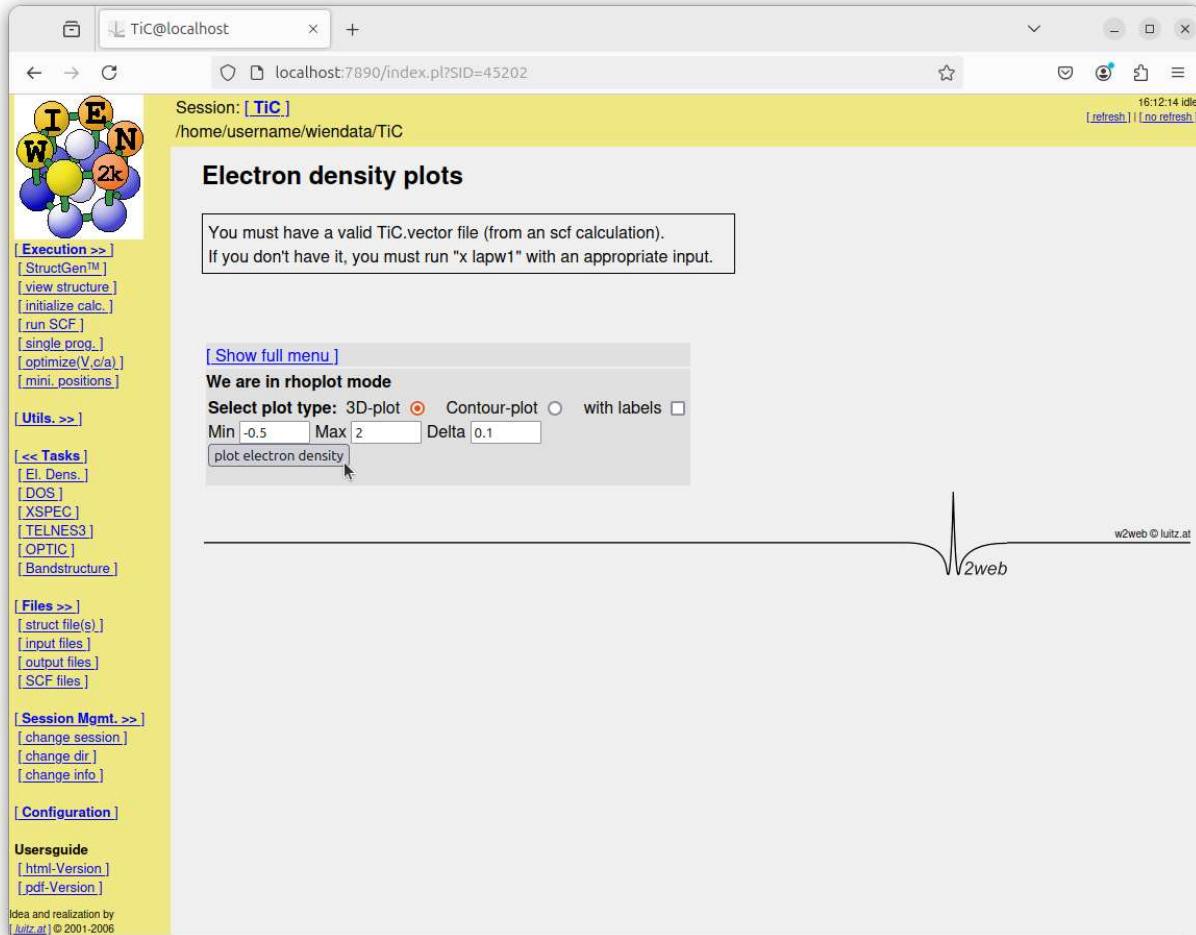
[2] [http://www.wien2k.at/reg\\_user/textbooks/usersguide.pdf](http://www.wien2k.at/reg_user/textbooks/usersguide.pdf)

88. Click the “x” in the top right corner to close XCrySDen

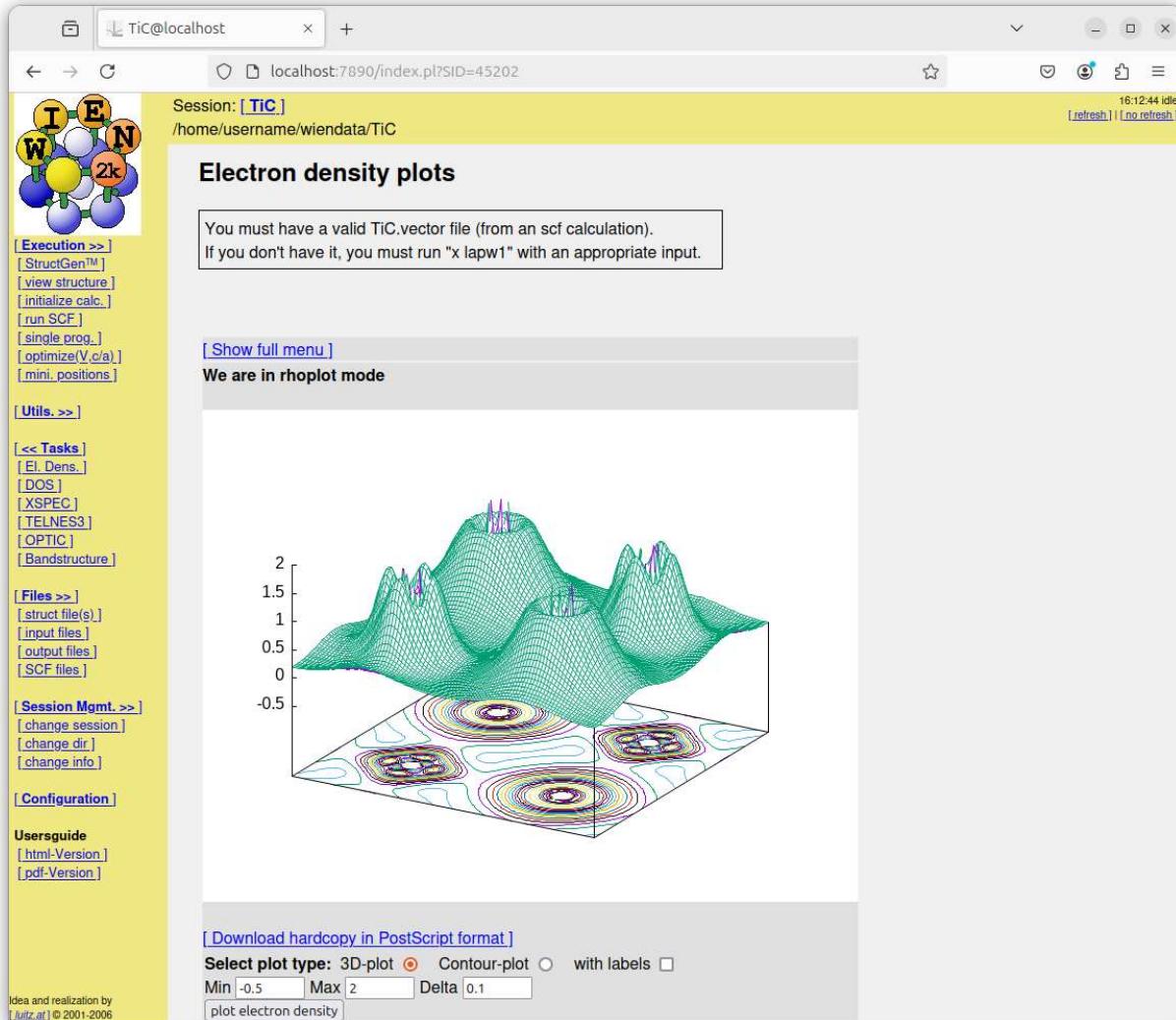
89. In the left menu, click “El. Dens.” under “Tasks”

90. Click the “rhoplot” button

91. Type -0.5 for Min and 2 for Max, then click “plot electron density”:



92. This gives us the following plot (compare to Figure 3.9 in the WIEN2k usersguide):



## Plot density of states (DOS)

93. In the left menu, click on “DOS” under “Tasks”

94. Click on “x lapw2 -qtl”:

**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 qt1](#) Calculate partial charges with QTL program  so  interactively

**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 input-file for TETRA

[x tetra](#) Calculate partial DOS  interactively

[view TiC.output](#) Check output of TETRA

**OPTIONAL: Calculate renormalized DOS**

[x rendos](#) (requires a previous partial DOS with case.int like: total 1 s,p,d 2 s,p ...)  interactively

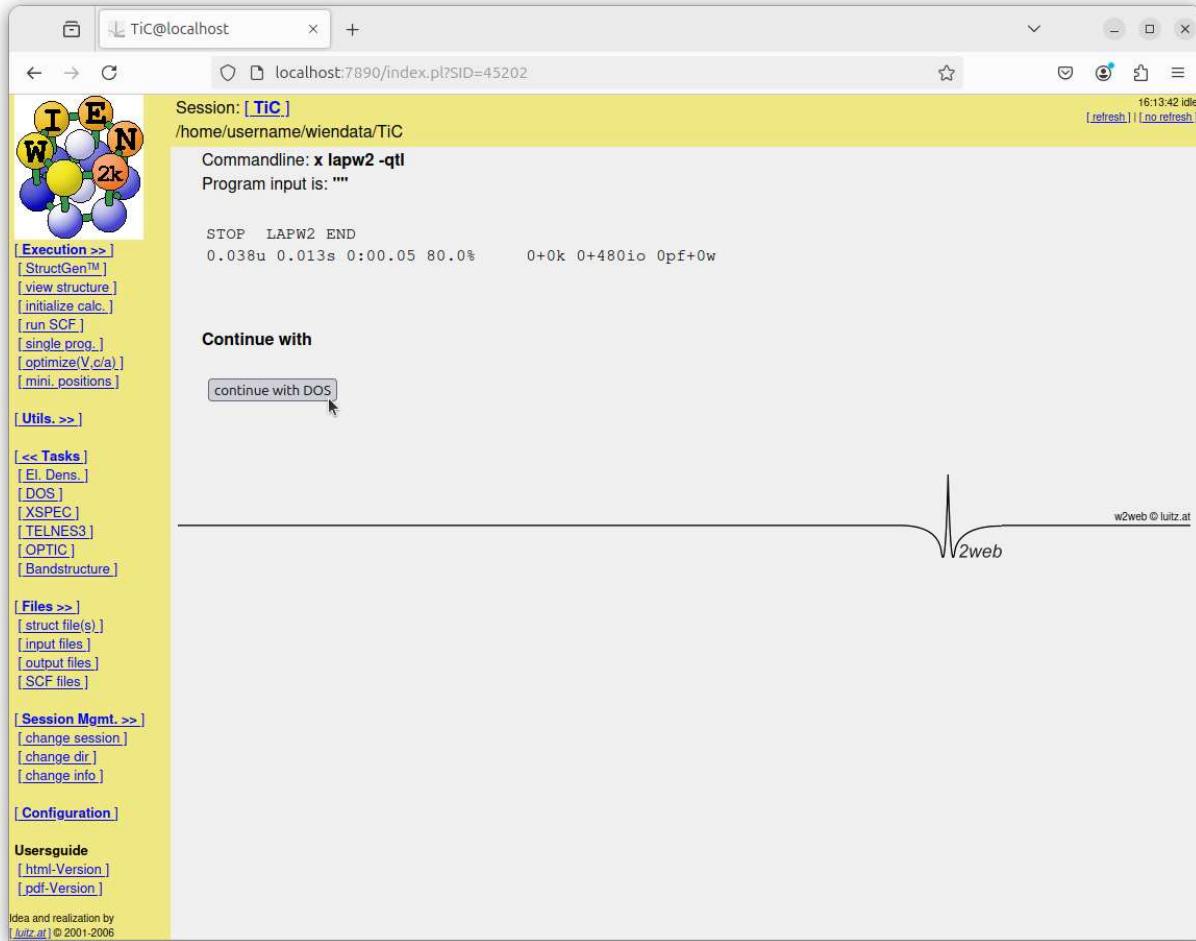
[dospot](#) Plot DOS  using renormalized DOS or download DOS-data for plotting with your plotting program:

[save\\_lapw -dos](#) with name:

Idea and realization by [luitz.at](#) © 2001-2006

w2web © luitz.at

## 95. Click on “continue with DOS”:



96. Click “edit TiC.int”

97. Type the file so that it looks like:

```
TiC
-0.50 0.002 1.500 0.003 #EMIN, DE, EMAX, Gauss-broadening
6 N 0.000 KSEL=-1 #Number of DOS-CASES
0 1 tot
1 4 Ti d
1 5 Ti eg
1 6 Ti t2g
2 2 C s
2 3 C p
SUM: 0 2
2 5
```

Session: [TiC.]  
 /home/username/wiendata/TiC/TiC.int

File:  
 /home/username/wiendata/TiC/TiC.int

Header from TiC.qtl:

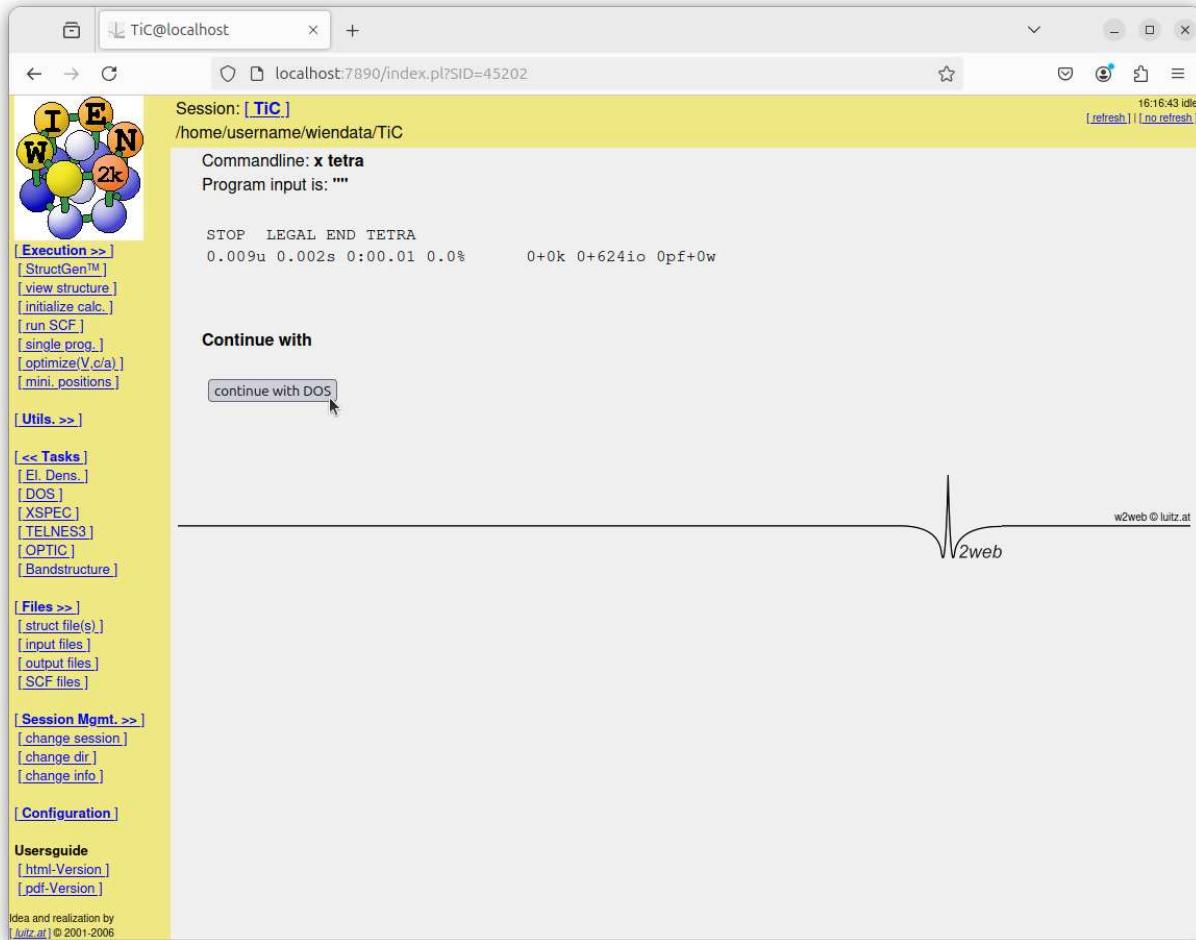
```
ATOM          COLUMN
ATOM 1: Ti: tot,s,p,d,D-eg,D-t2g,f
ATOM 2: C: tot,s,p,d,D-eg,D-t2g,f
```

**TiC**

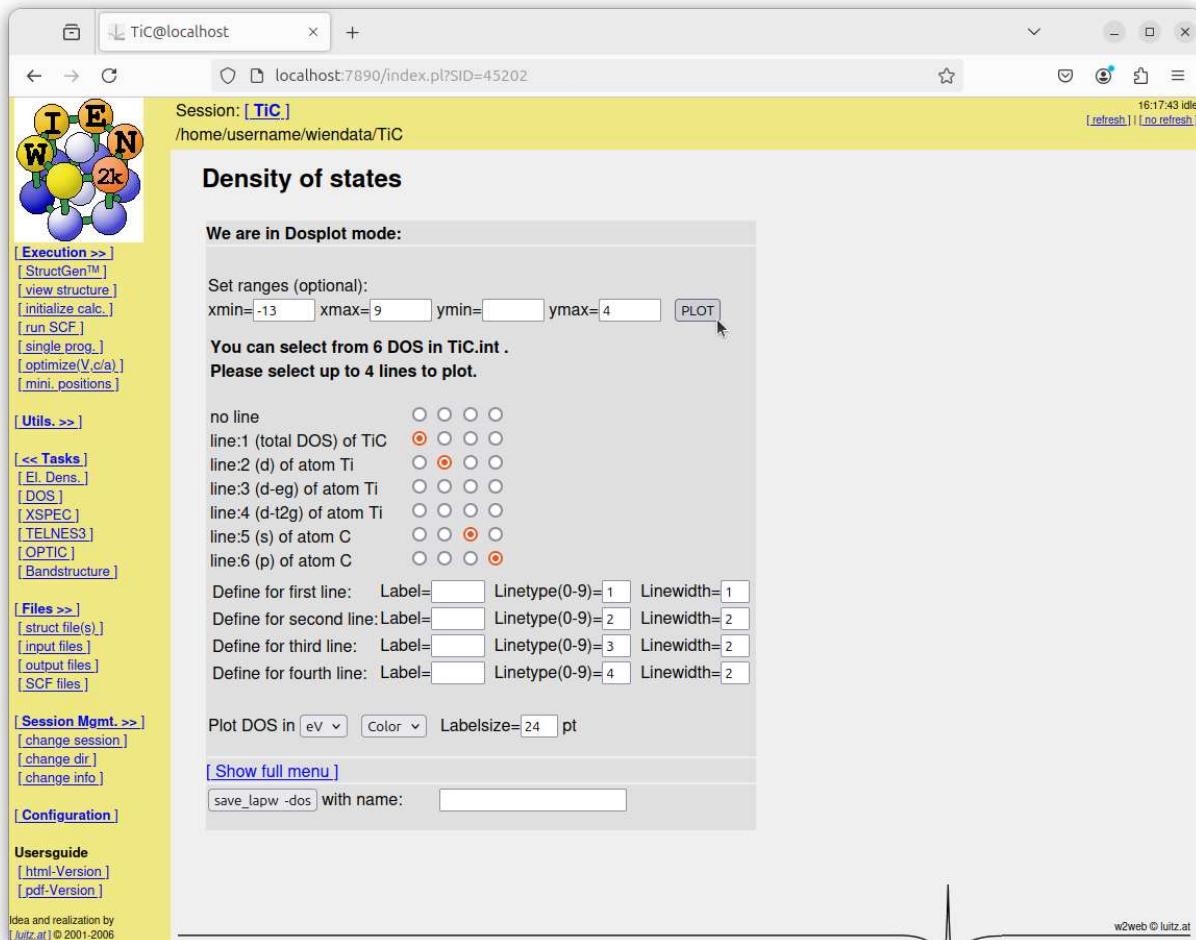
```
-0.50 0.002 1.500 0.003 # EMIN, DE, EMAX, Gauss-broadening(>de)
6 N 0.000 KSEL=-1 # NUMBER OF DOS-CASES below, G/L/B broadening (Ry),KSE
0 1 tot           # atom, case=column in gtl-header, label
1 4 Ti d
1 5 Ti eg
1 6 Ti t2g
2 2 C s
2 3 C p
SUM: 0 2          # NUMBER OF SUMMATIONS, MAXIMUM OF SUMMANDS
2 5              # this sums dos-cases 2+5 from the input above
```

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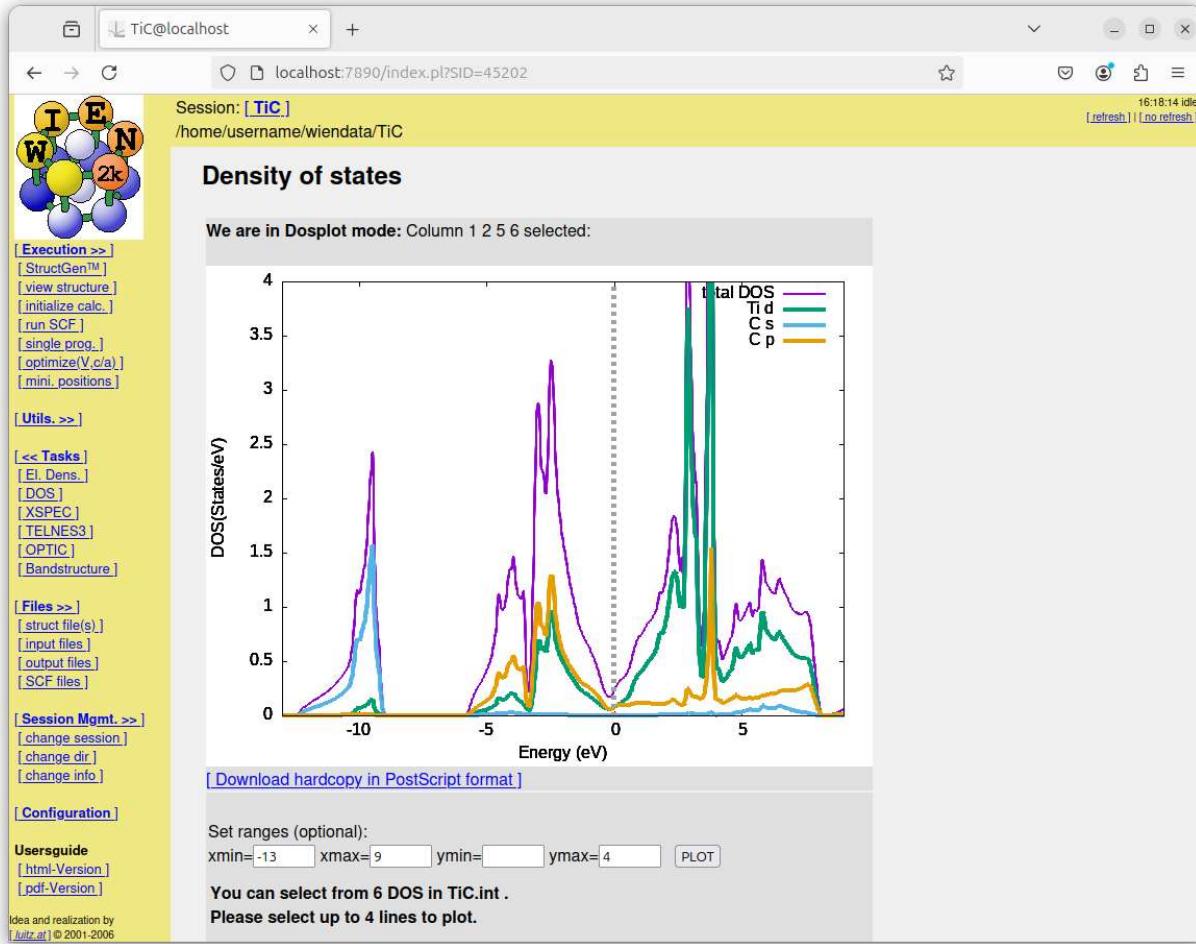
98. Click “Save and continue with DOS”
99. Click “x tetra”
100. Click “continue with DOS”:



101. Click “dosplot”
102. Type -13 for xmin, 9 for xmax, 4 for ymax and select lines 1, 2, 5 and 6. Then, click “PLOT”:

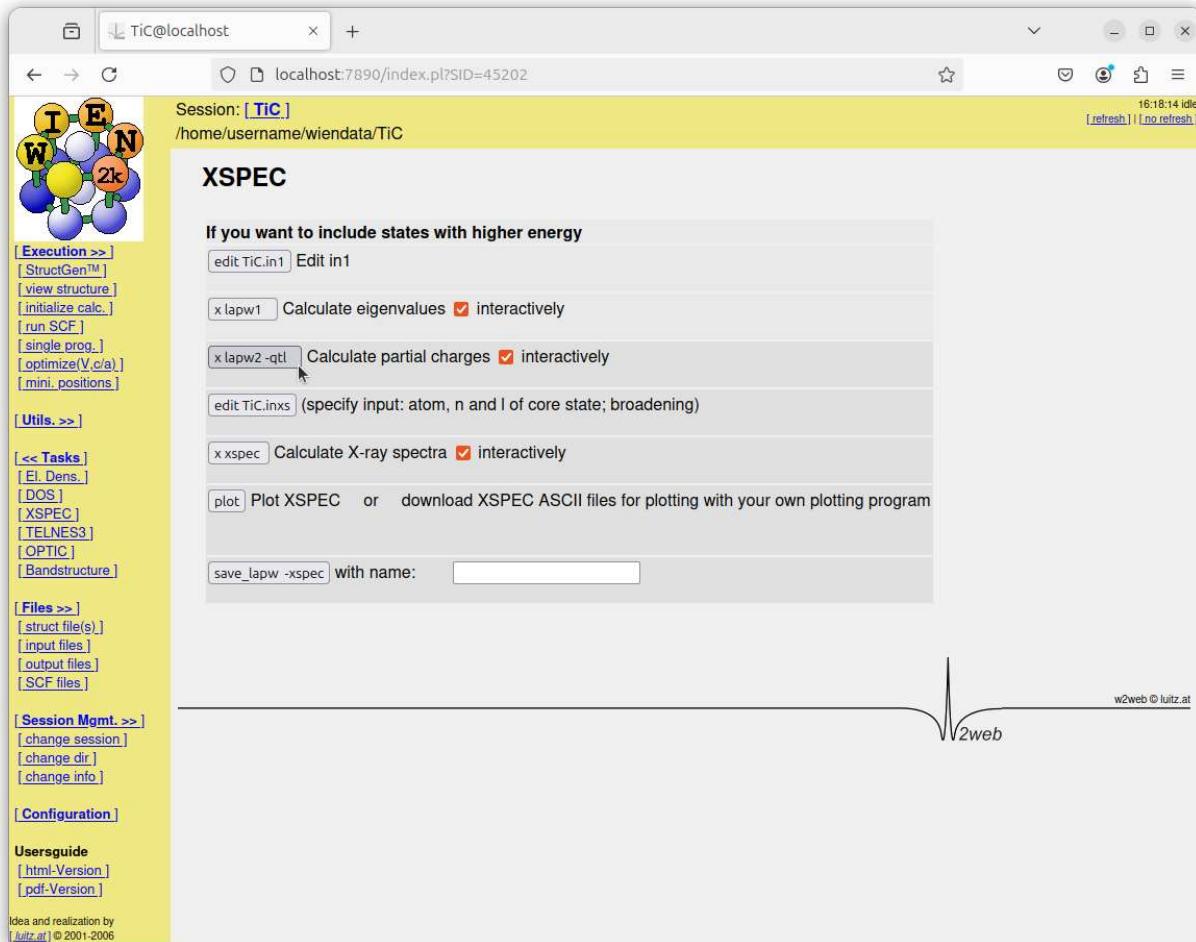


103. The resulting plot is (this is similar to Figure 3.10 in the usersguide):

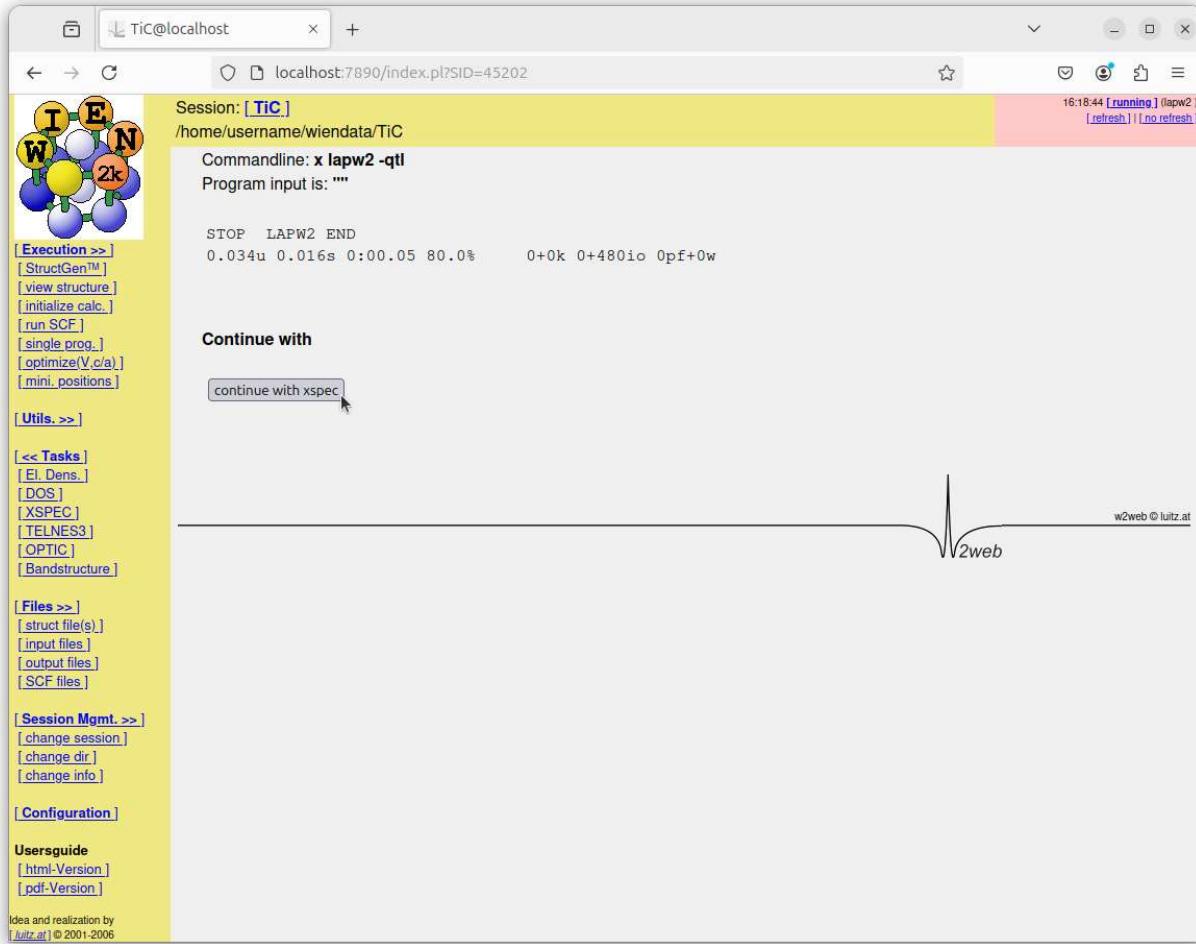


## Plot x-ray spectra

104. In the left menu, click on “XSPEC” under “Tasks”
105. Click “x lapw2 -qtl”:



106. Click “continue with xspec”:



107. Click “x xspec”

108. Click “continue with xspec”:

Session: **TiC**  
/home/username/wiendata/TiC

16:18:44 [running] (lapw2)  
[refresh] || no refresh

Commandline: **x xspec**  
Program input is: ""

```

Start INITXSPEC
STOP INIT_XSPEC - done
0.000u 0.001s 0:00.00 0.0%    0+0k 0+16io 0pf+0w
Start TETRA
STOP  LEGAL END TETRA
0.005u 0.003s 0:00.00 0.0%    0+0k 0+304io 0pf+0w
Start TXSPEC
STOP TXSPEC DONE
0.027u 0.007s 0:00.03 66.6%   0+0k 0+360io 0pf+0w
Start LORENTZ
STOP Lorentz done
0.015u 0.000s 0:00.01 100.0%   0+0k 0+56io 0pf+0w
> stop
> xspec done
0.062u 0.028s 0:00.09 88.8%   0+0k 0+768io 0pf+0w

```

Continue with

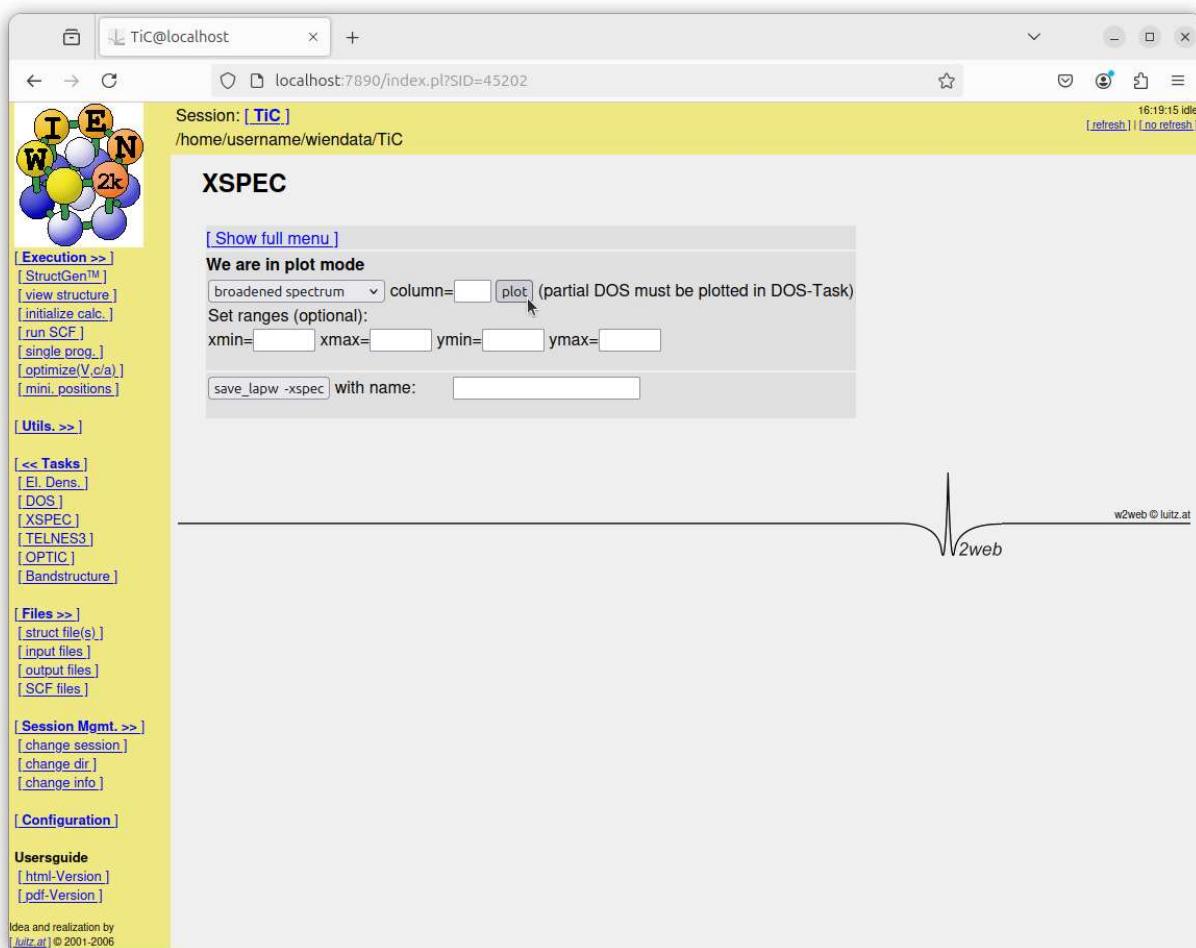
continue with xspec

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2web

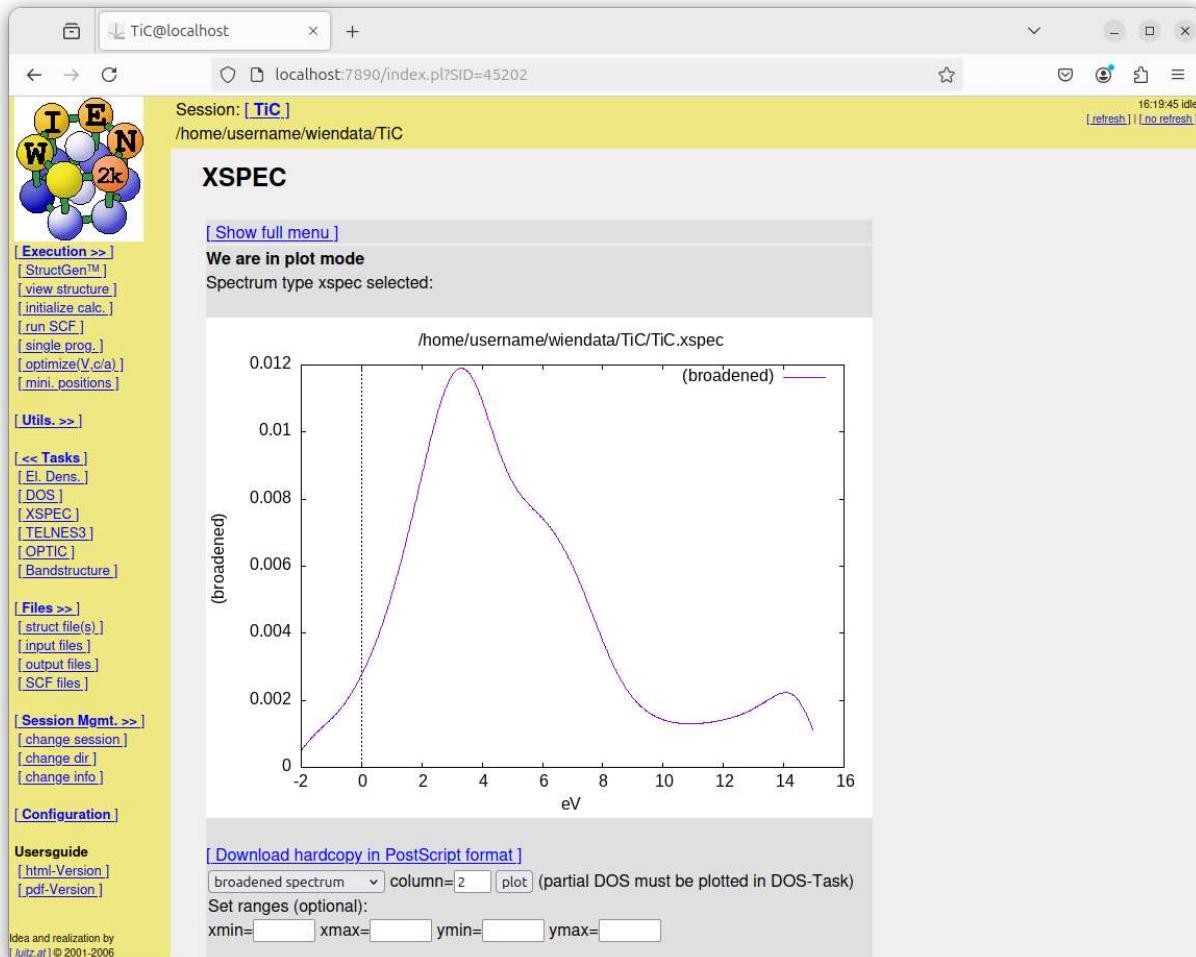
Idea and realization by  
[luitz.at](http://luitz.at) © 2001-2006

109. Click "plot"

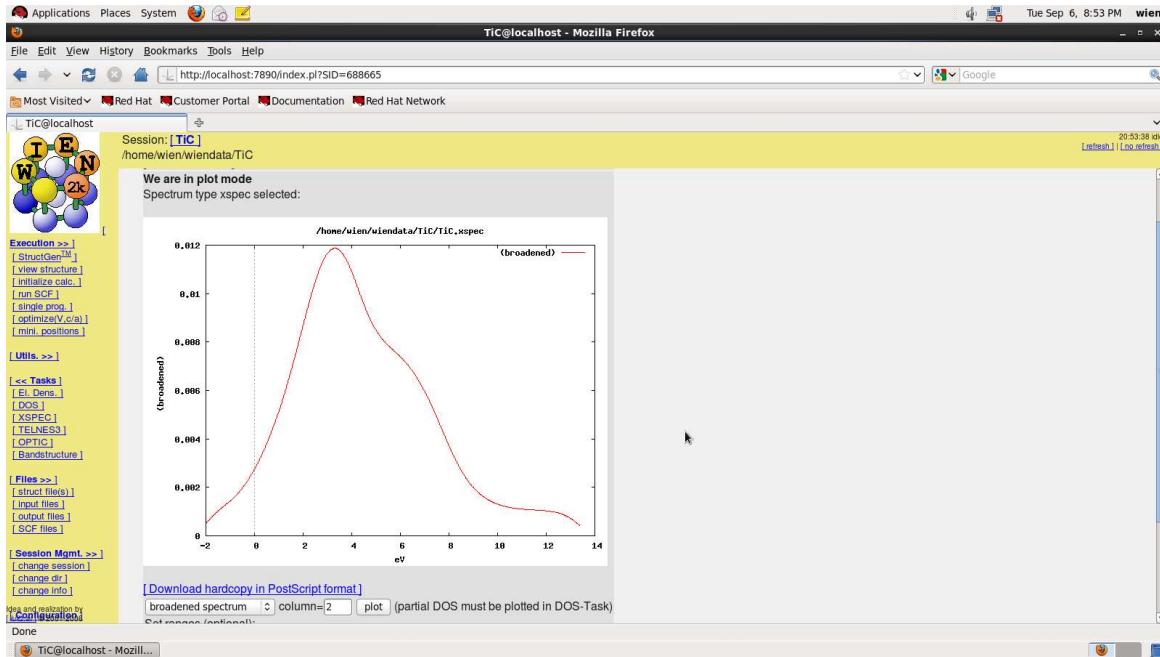
110. Click "plot":



111. The resulting plot (versions 24.1-23.2) is shown below (this is similar to Figure 3.12 in the usersguide):



However, there seems to be some difference in the eV axis compared to WIEN2k versions 11.1-13.1:



## Plot bandstructure

112. In the left menu, click on “Bandstructure” under “Tasks”
113. Click on “create TiC.klist\_band” with fcc selected:

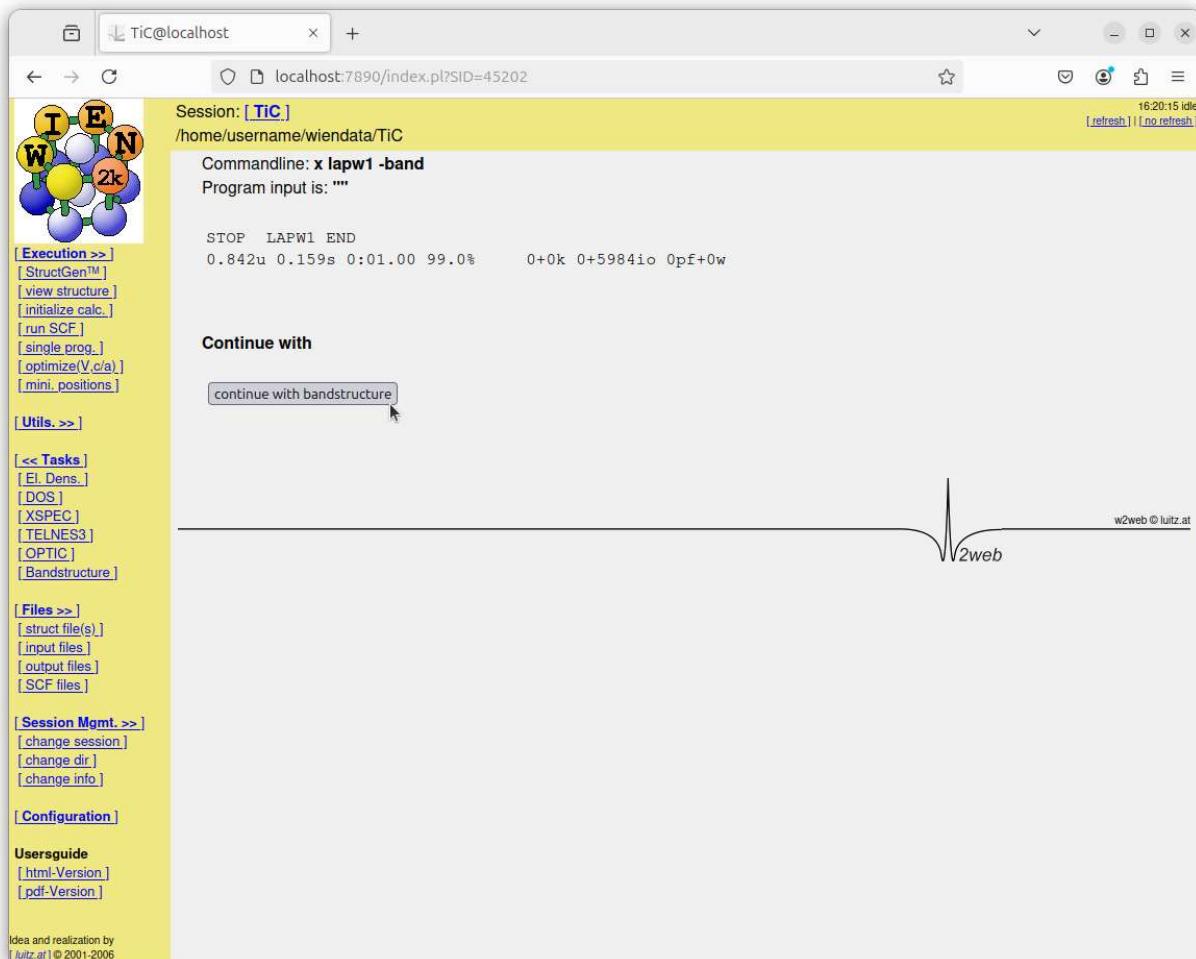
The screenshot shows a web-based interface for a TiC session. The top bar displays the session name "TiC@localhost" and the URL "localhost:7890/index.pl?SID=45202". The status bar indicates "16:20:15 idle" and provides refresh and no-refresh buttons.

The main content area is titled "Band structure". It contains several input fields and buttons:

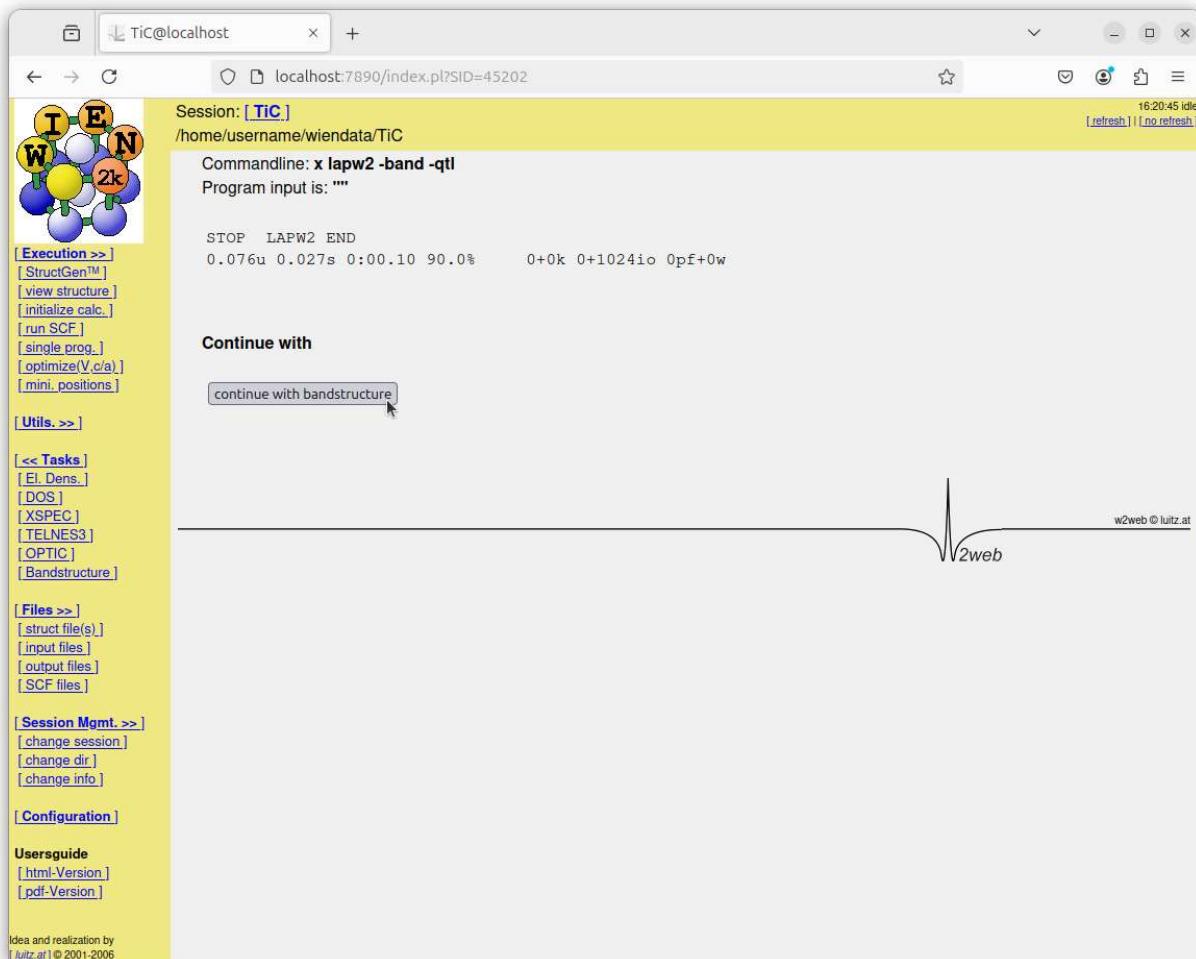
- "The required k-mesh for bandstructure plotting can be generated by:" dropdown set to "fcc", button "create TiC.klist\_band", link "[Brillouinzones from Bilbao Cryst Server.]"
- "or Generate k-mesh using XCrysden" button, followed by "(save klist as TiC.klist\_band)"
- "x lapw1-band" button, "Calculate Eigenvalues" checkbox checked, "interactively" checkbox checked
- "needed only for continuous lines in the plot (not for non-symmorphic spacegroups)!"
- "x irrepl" button, "Calculate irreducible representations" checkbox unchecked, "so" checkbox unchecked, "interactively" checkbox checked
- "for band character plots only!"
- "x lapw2-band-qt1" button, "Calculate partial charges ("qt1"-file)" checkbox unchecked, "so" checkbox unchecked, "interactively" checkbox checked
- "edit TiC.insp" button, "Insert correct EF"
- "x spaghetti" button, "Calculate bandstructure" checkbox unchecked, "so" checkbox unchecked, "interactively" checkbox checked
- "plot bandstructure" button, "Plot bandstructure" or "download Xmgrace files for plotting with xmgrace"
- "save\_lapw -band" button, "With name:" input field

A small diagram of a crystal lattice with atoms labeled I, E, N, W, and 2k is visible on the left. The left sidebar contains a navigation tree with sections like "Execution >>", "StructGen™", "View structure", etc., and "Configuration" with "Usersguide" links. A footer note at the bottom left credits "Idea and realization by [luitz.at] © 2001-2006". The bottom right corner features a stylized "2web" logo.

114. Click on “x lapw1 -band”
115. Click “continue with bandstructure”:



116. Click on “x lapw2 -band -qtl”
117. Click “continue with bandstructure”:



118. Edit TiC.insp by clicking “edit TiC.insp”, change jatom to 1, jtype to 6, Fermi energy to 0.7425 (or could enter 0.7429613770 shown on the screen):

Session: **TiC**  
/home/username/wiendata/TiC

**File:**  
/home/username/wiendata/TiC/TiC.insp

continue with bandstructure without saving **Save and continue with bandstructure** Download this file:

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/username/wiendata/TiC/TiC.scf: EF (TETRAH.M.)= 0.7429613770
```

```
### Figure configuration
5.0 3.0 # paper offset of plot
10.0 15.0 3.0 # xszie,ysize [cm], linebreak-parameter
1.0 4 # major ticks, minor ticks
1.0 1 1 # character height, font switch, header (0/1)
1.1 2 4 # line width, line switch, color switch

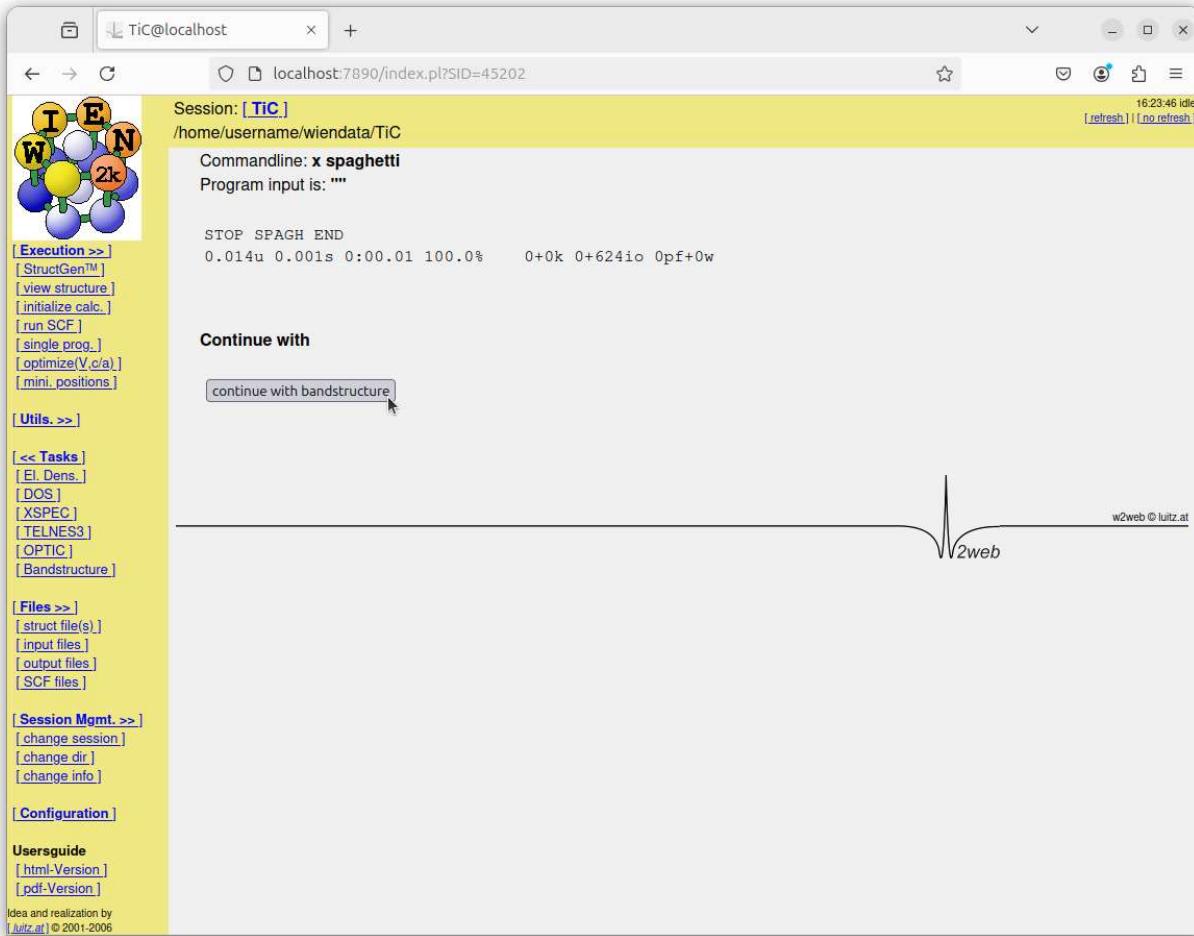
### Data configuration
-14.0 8.0 2 # energy range, energy switch (1:Ry, 2:eV)
1 0.7425 # Fermi switch, Fermi-level (in Ry units)
1 999 # number of bands for heavier plotting 1,1
1 6| 0.2 # jatom, icol, size of heavier plotting
```

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

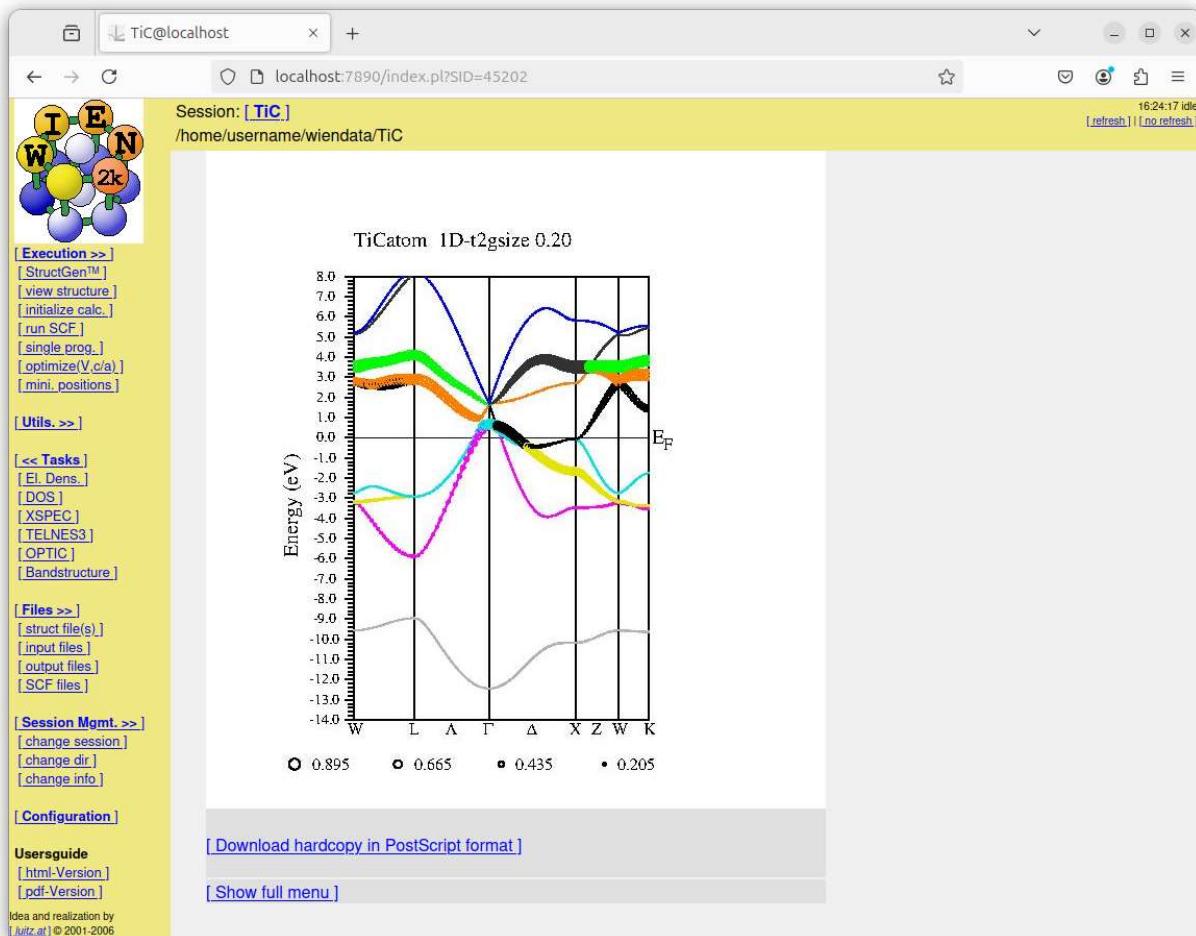
```
Line switch:
```

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2web

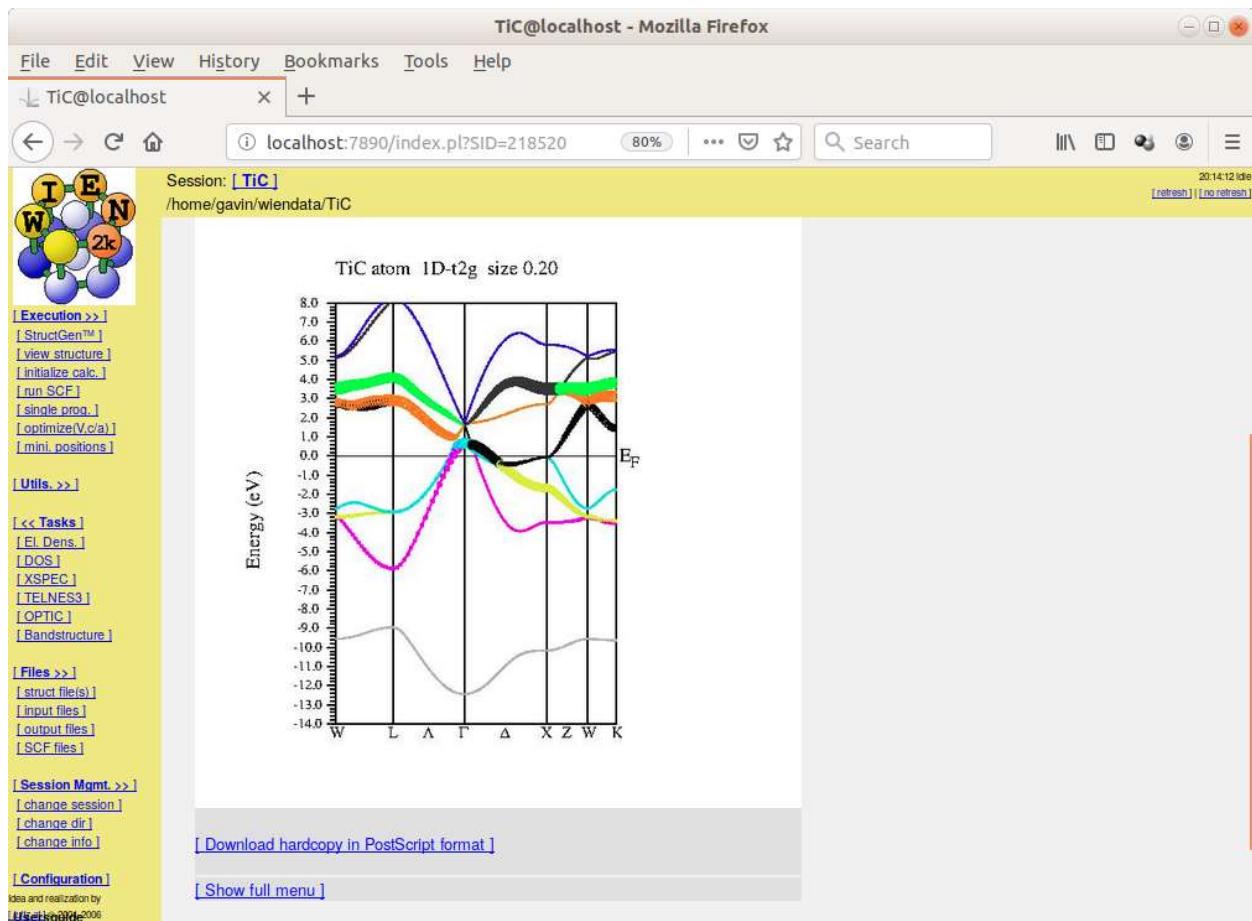
119. Click “Save and continue with bandstructure”
120. Click “x spaghetti”
121. Click “continue with bandstructure”:



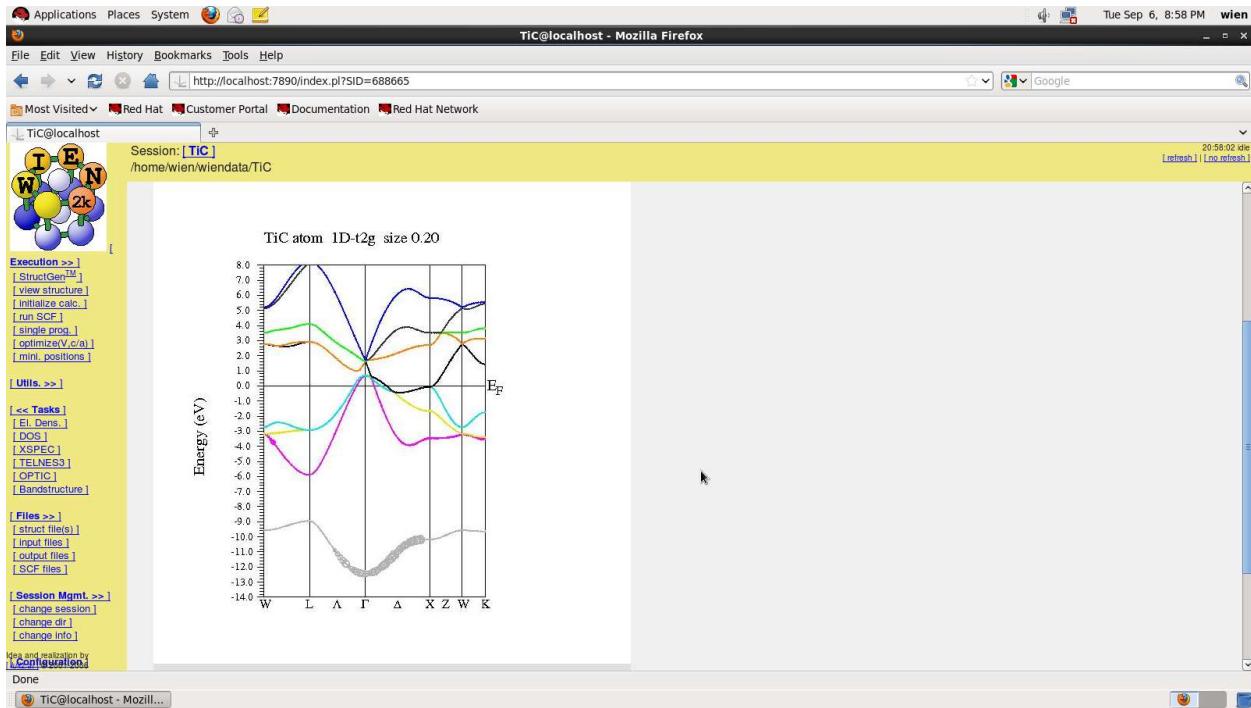
122. Click “plot bandstructure”, the creates the following plot (version 24.1-23.2):



WIEN2k versions 14.1-19.1 did not have the labels for the circle sizes:



There are some noticeable differences compared to WIEN2k versions 11.1-13.1:

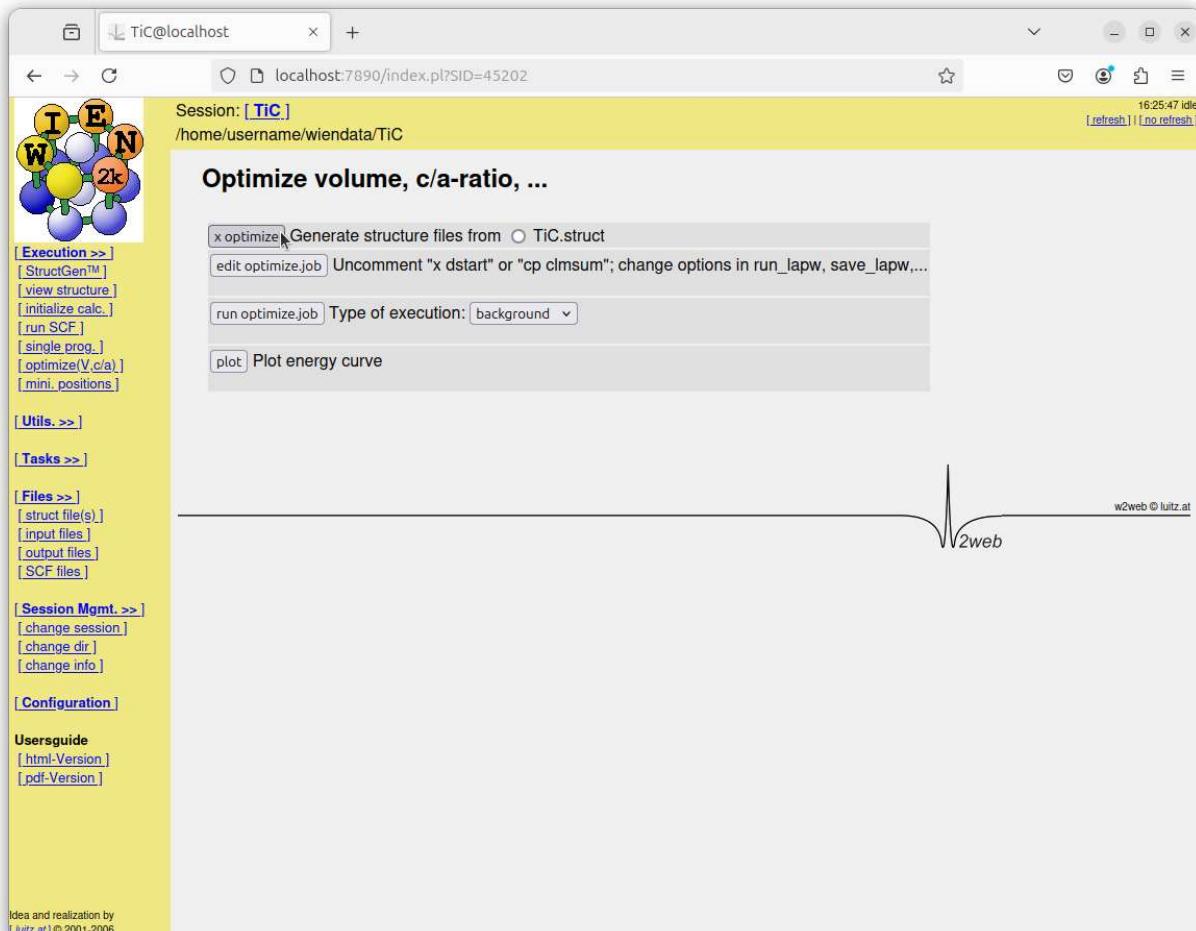


## Plot volume optimization

123. In the left menu, click on “optimize(V,c/a)” under “Execution”

Note: Click link “Save Calculation with save\_lapw”, if prompted. Check “Save calculation in a directory as specified” and type “TiC\_scf” in the “Save name or directory” box and click the “save” button. Can also save by clicking “save\_lapw” under “Utils.” in the left menu. Finally, click on “optimize(V,c/a)” under “Execution” again.

124. Click “x optimize”:



125. With “vary VOLUME with constant a:b:c ratio” selected, enter -10, -5, 0, 5, and 10 into the box each on its own line  
 126. Click “Execute!”:

**optimizer**

1) vary VOLUME with constant a:b:c ratio

For option 1-4: specify structure changes in % (each value in separate line)

-10  
-5  
0  
5  
10

For option 5: specify number of structures: 6, 9 (3x3), 16 (4x4), 25 (5x5), 36

For option 6: specify number of structures: 10, 27 (3x3x3), 64 (4x4x4), 125 (5x5x5) 16 specify the % change: 1.0

For option 7: specify number of structures: 15, 81 (3x3x3x3), 256 (4x4x4x4)

**Execute!**

Session: [ TIC ]  
 /home/username/wiendata/TiC

16:26:18 idle  
[\[refresh\]](#) | [\[no refresh\]](#)

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127. Click “continue with optimizer”:

Session: [TiC]  
 /home/username/wiendata/TiC

```
[1] VARY VOLUME with CONSTANT RATIO A:B:C
[2] VARY C/A RATIO with CONSTANT VOLUME (tetr and hex lattices)
[3] VARY C/A RATIO with CONSTANT VOLUME and B/A (orthorh lattice)
[4] VARY B/A RATIO with CONSTANT VOLUME and C/A (orthorh lattice)
[5] VARY A and C (2D-case) (tetragonal or hexagonal lattice)
[6] VARY A, B and C (3D-case) (orthorhombic lattice)
[7] VARY A, B, C and Gamma (4D-case) (monoclinic lattice)
[8] VARY C/A RATIO and VOLUME (2D-case) (tetr and hex lattices)

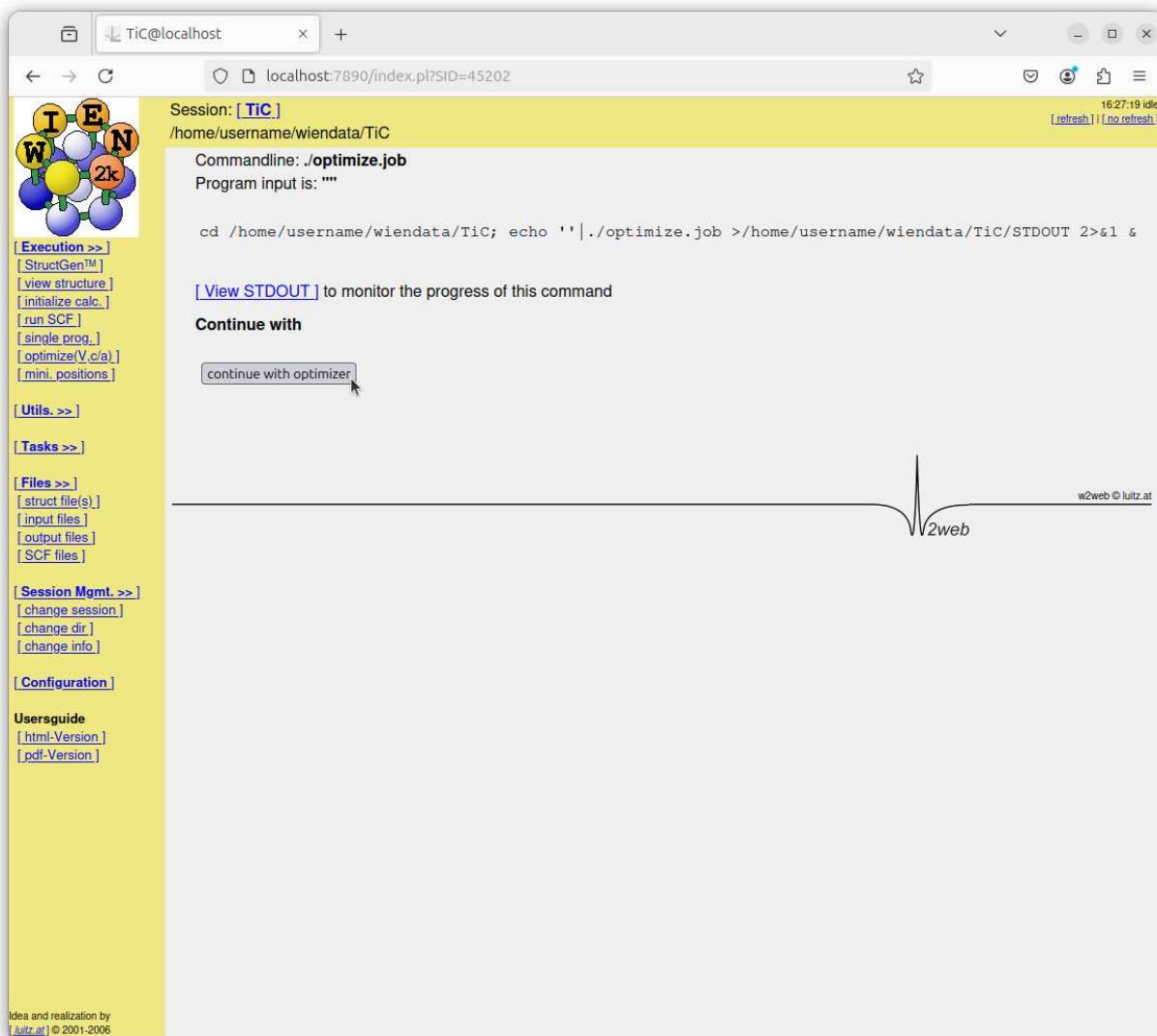
*****
Generating TiC_initial.struct
next time this file will be used as template unless you remove it explicitly.
*****
NUMBER OF STRUCTURE CHANGES ?
PLEASE ENTER VALUE      1 (IN %)
PLEASE ENTER VALUE      2 (IN %)
PLEASE ENTER VALUE      3 (IN %)
PLEASE ENTER VALUE      4 (IN %)
PLEASE ENTER VALUE      5 (IN %)
Tic_vol____-10.00.struct
  7.896485  7.896485  7.896485  90.000000
Tic_vol____-5.00.struct
  8.040089  8.040089  8.040089  90.000000
Tic_vol____0.00.struct
  8.178738  8.178738  8.178738  90.000000
Tic_vol____5.00.struct
  8.312840  8.312840  8.312840  90.000000
Tic_vol____10.00.struct
  8.442749  8.442749  8.442749  90.000000
Now run optimize.job
0.001u 0.000s 0:00.00 0.0%      0+0k 0+248io 0pf+0w
```

**Continue with**

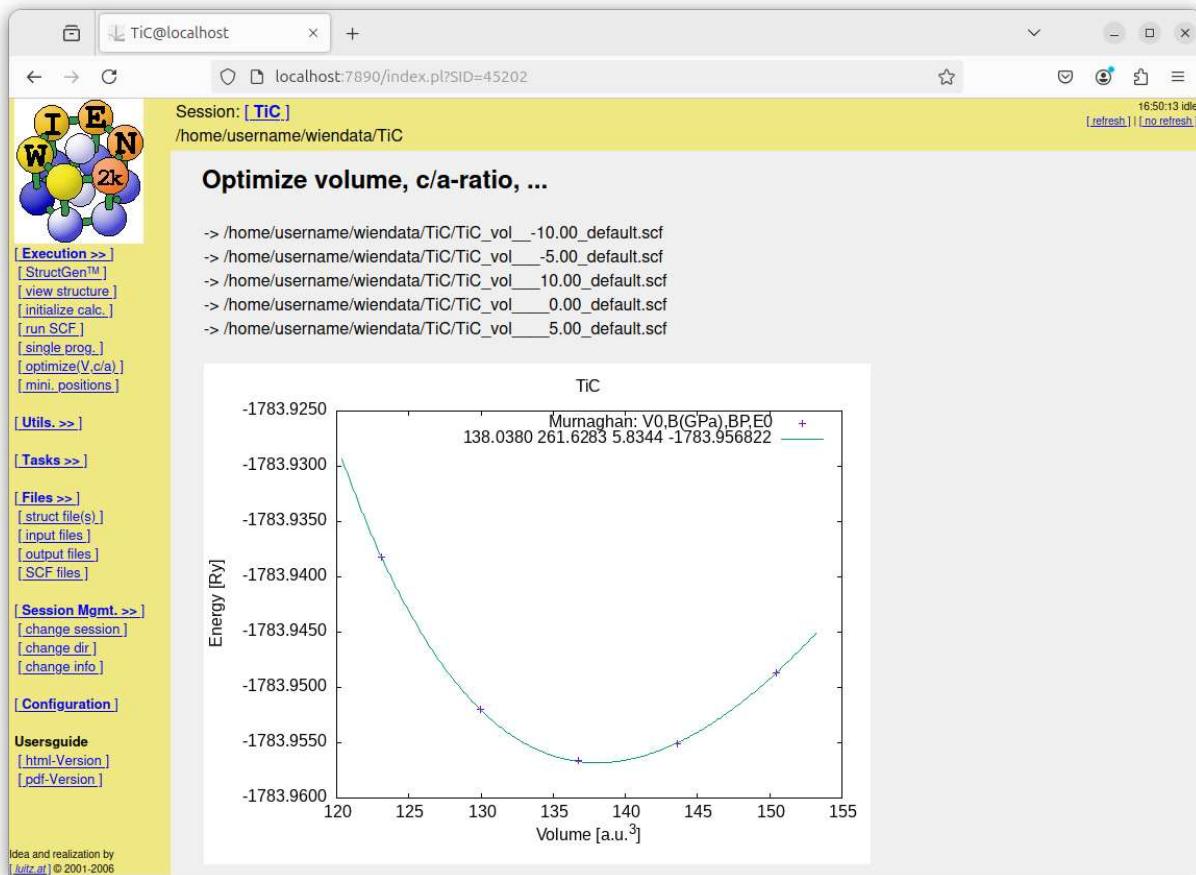
[continue with optimizer](#)

Idea and realization by  
[\[wienc.at\]](#) © 2001-2006

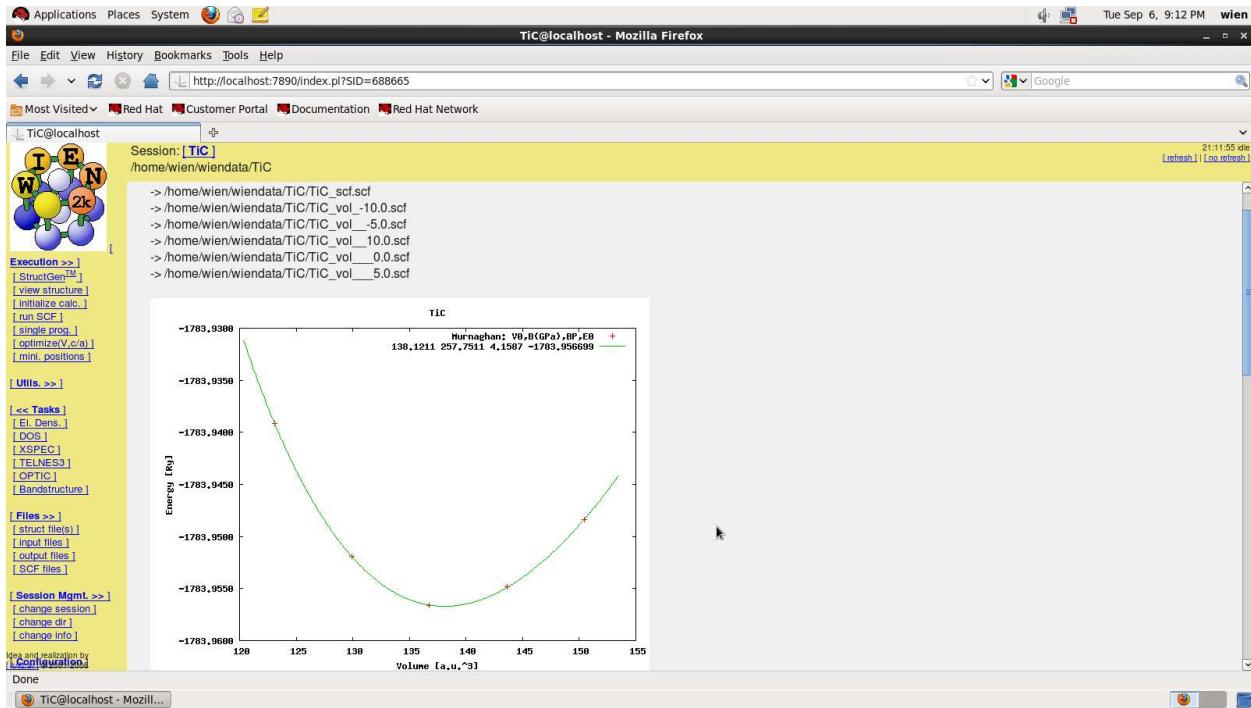
128. Click “run optimize.job”
129. Click “continue with optimizer”:



130. Wait for job to finish, then click “plot”  
 131. Click “plot” with E vs. volume selected (version 24.1-21.1):



Could compared to the differences in versions 11.1-13.1:



132. TiC example has been completed.