

## WIEN2k TiC Example

Ubuntu 24.04.1 LTS

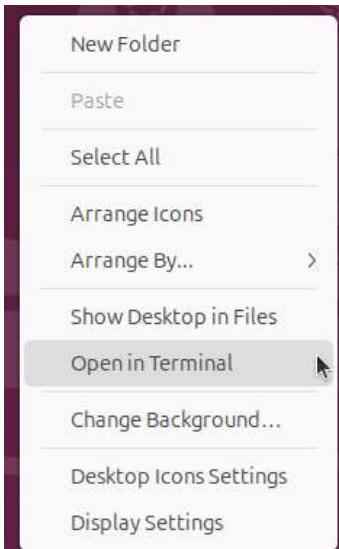
WIEN2k\_24.1 (Release 1/8/2024)

ifx version 2025.0.4

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

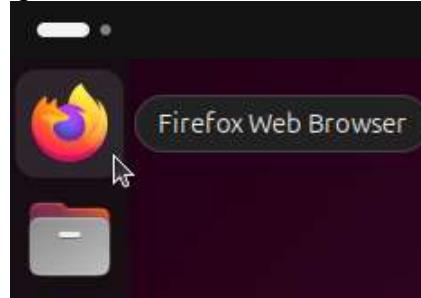
#####
# w2web installer
# Copyright (C) 2001 luitz.at
#####

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

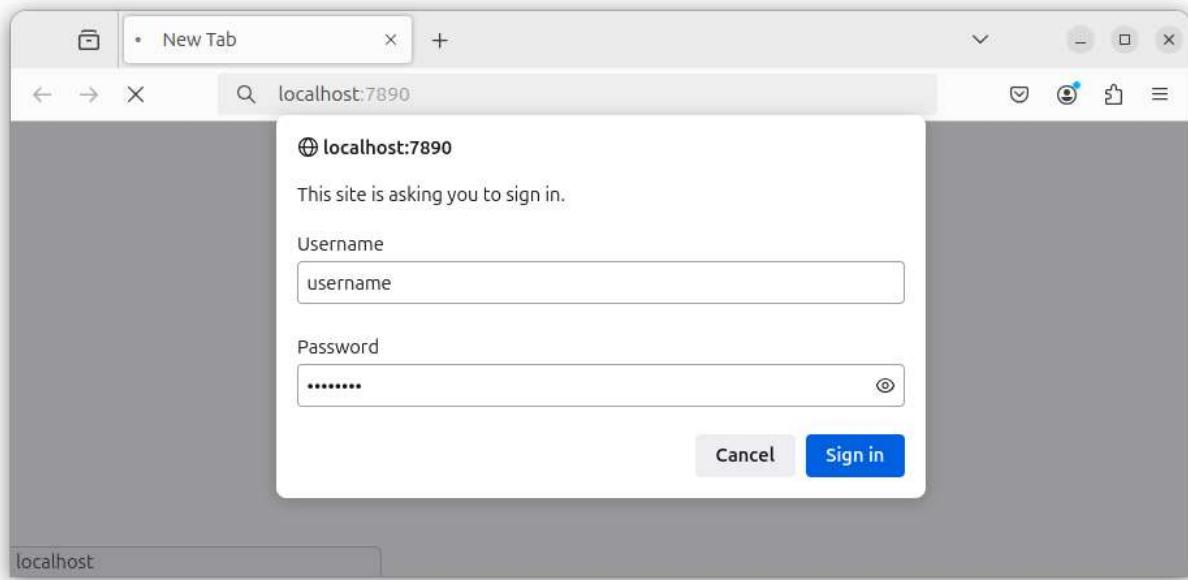
w2web failed to bind port 7890 - port already in use!
You may want to try w2web -p portnumber
username@computername:~/Desktop$ 
```

Open Firefox and login to w2web

3. Click on the Firefox icon to open Firefox:

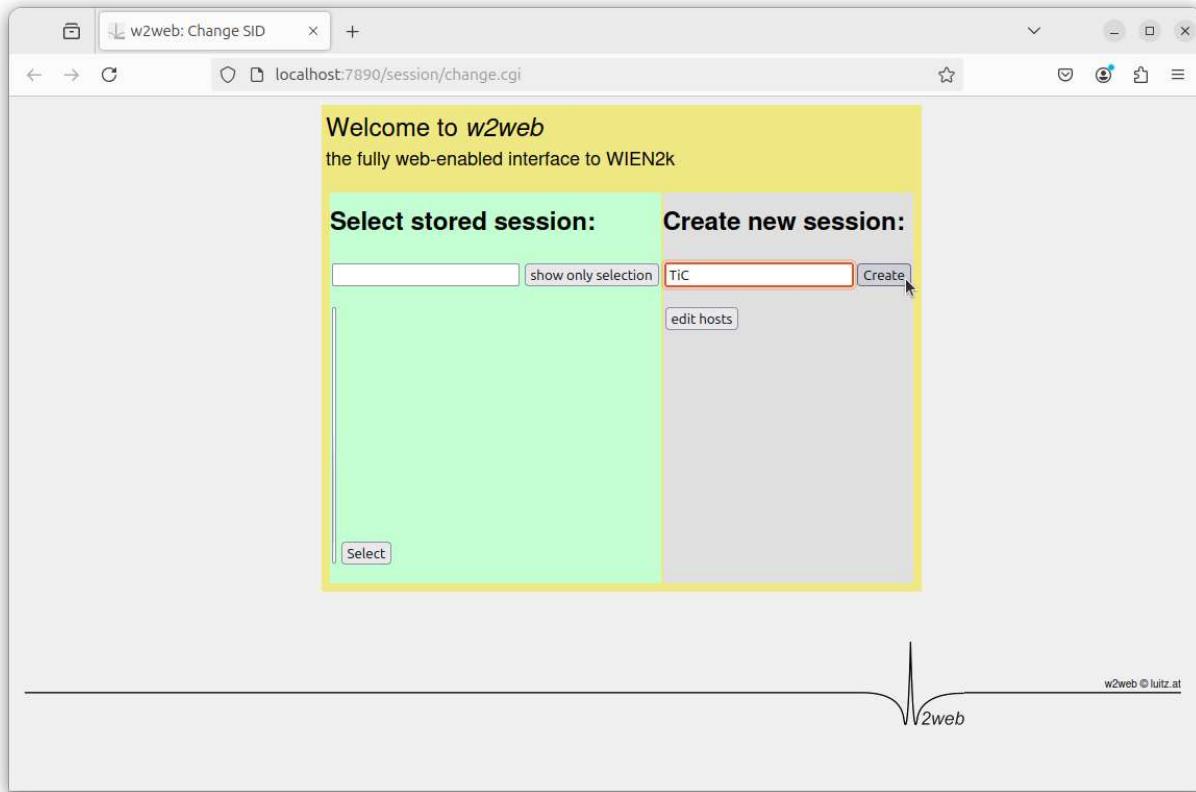


4. Enter url <http://localhost:7890>, type your w2web username and password, then click “Sign in” to login to w2web:

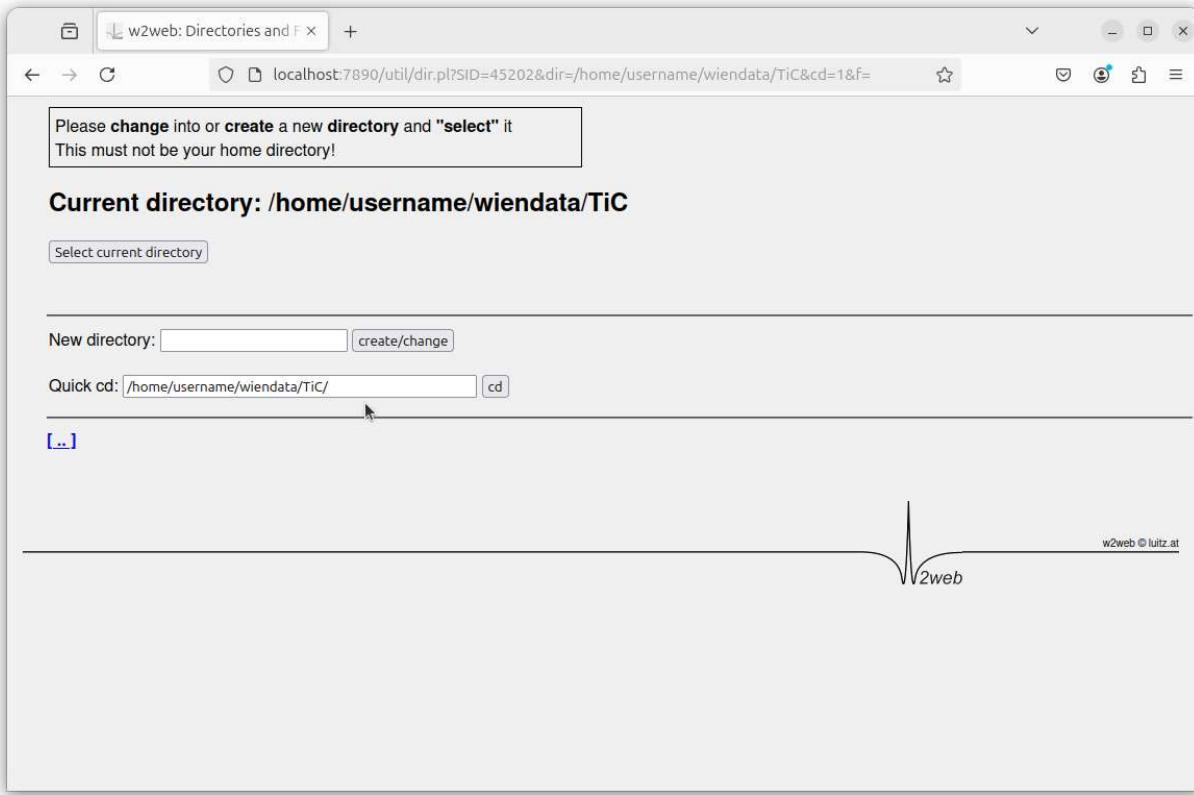


Create a new session (calculation)

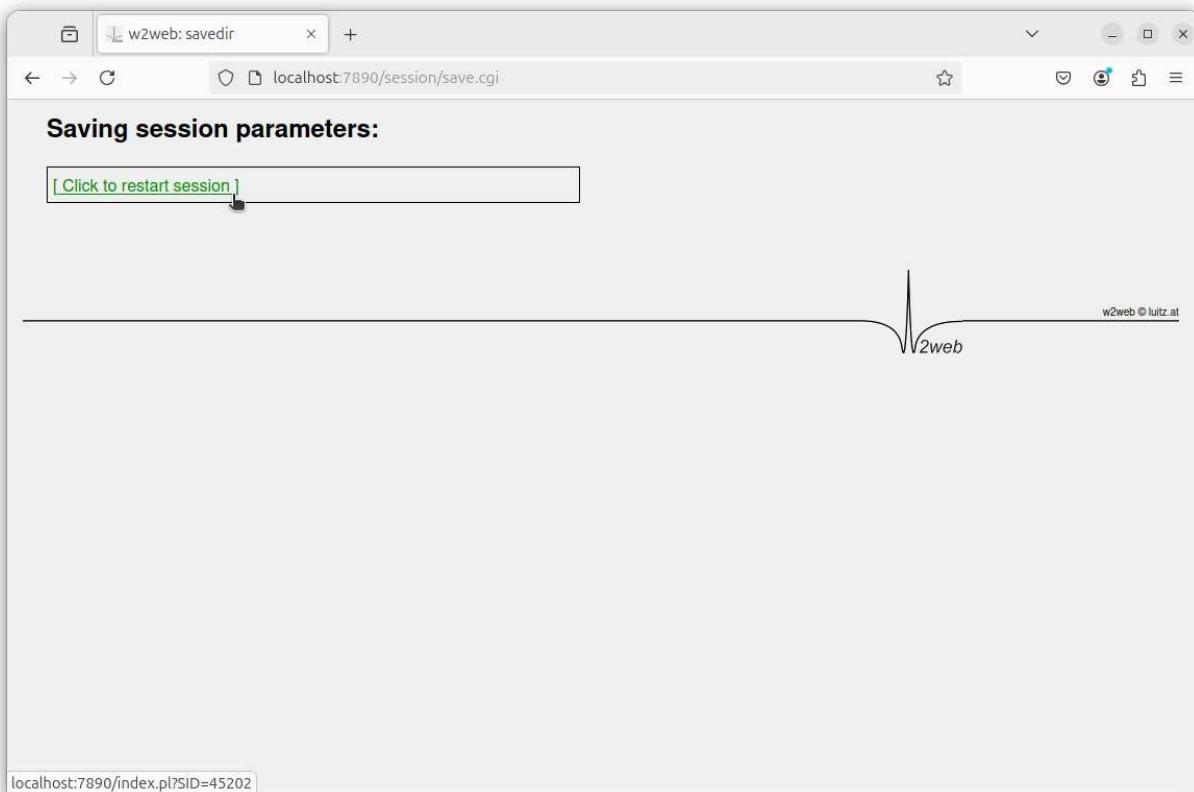
5. Enter “TiC” in the “Create new session:” box and then click the “Create” button:



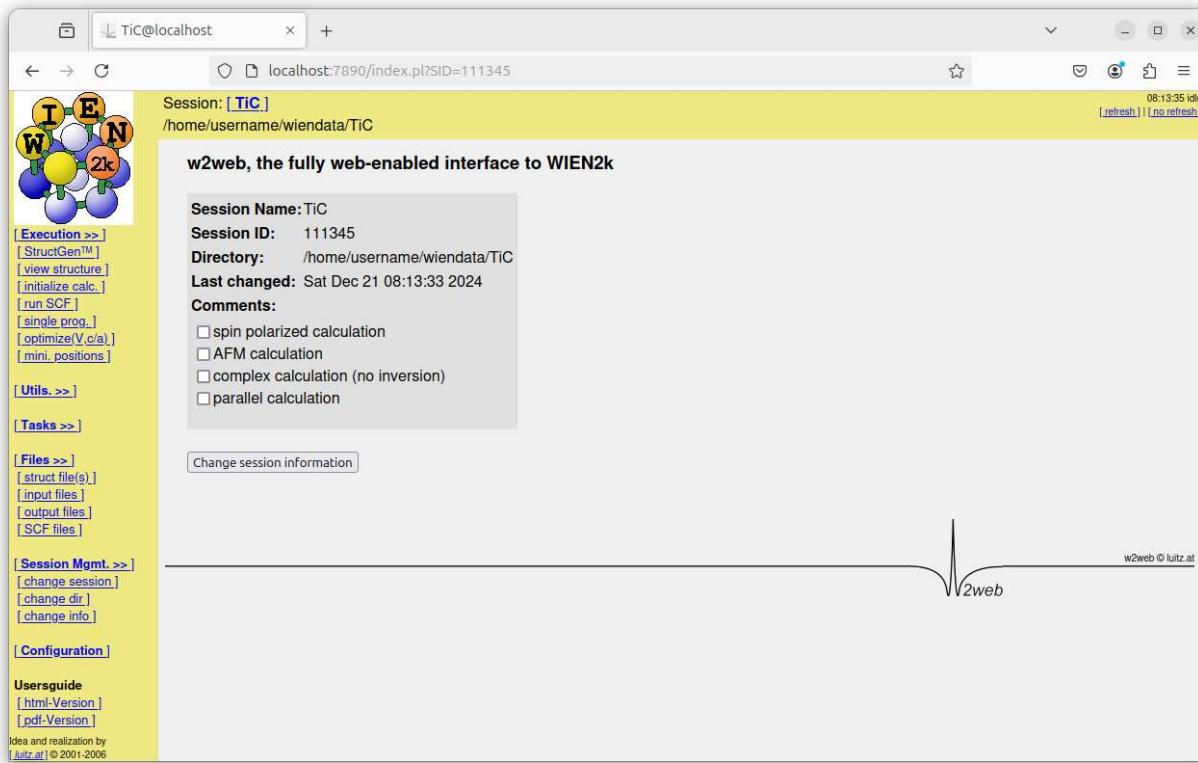
6. The “New directory” box will contain “TiC”, click the “create/change” button
7. The directory “TiC” is created and “TiC” will appear in the “Quick cd.” box:



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 main content area has a yellow header bar with the session information: "Session: [TiC.] /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 form field "Number of atoms: [2]" and a "Generate template" button. Below this is an "Alternatively:" section with instructions for cif2struct and xyz2struct conversion, and a "Use selected CIF/TXT file" button. At the bottom, there is a note about uploading files and a copyright notice for LSDY-V2006.

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, there is a sidebar with various menu options such as Execution, Tasks, Files, Session Mgmt., Configuration, and Usersguide. The main area displays a crystal structure model with atoms labeled T, E, N, W, and 2k. Below the model, several buttons like 'Execution >>', 'StructGen™.', and 'view structure' are visible.

The central part of the screen shows the following parameters:

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

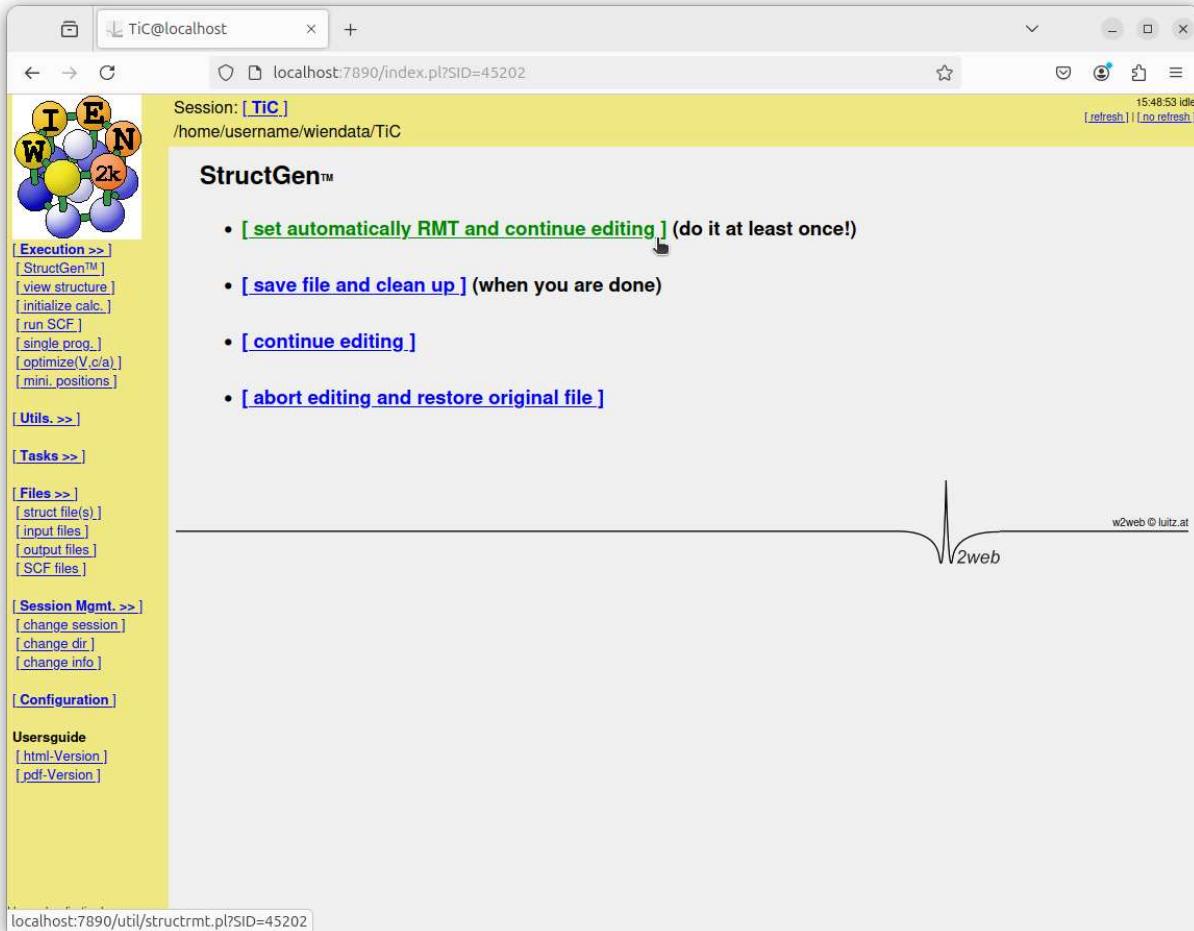
|                      |                     |                      |
|----------------------|---------------------|----------------------|
| a = 4.328            | b = 4.328           | c = 4.328            |
| $\alpha = 90.000000$ | $\beta = 90.000000$ | $\gamma = 90.000000$ |

- Inequivalent Atoms: 2**
- Atom 1:** Ti (highlighted in red) with Z = 0.000, RMT = 2.0000. Buttons: [remove atom], [remove], [split], [add position]. Position: Pos 1: x = 0.00000000, y = 0.00000000, z = 0.00000000.
- Atom 2:** c (highlighted in red) with Z = 0.000, RMT = 2.0000. Buttons: [remove atom], [remove], [split], [add position]. Position: Pos 1: x = 0.5, y = 0.5, z = 0.5.
- Number of symmetry operations: generate**
- You have to click "Save Structure" for changes to take effect!**
- Save Structure** button (highlighted in red)

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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**

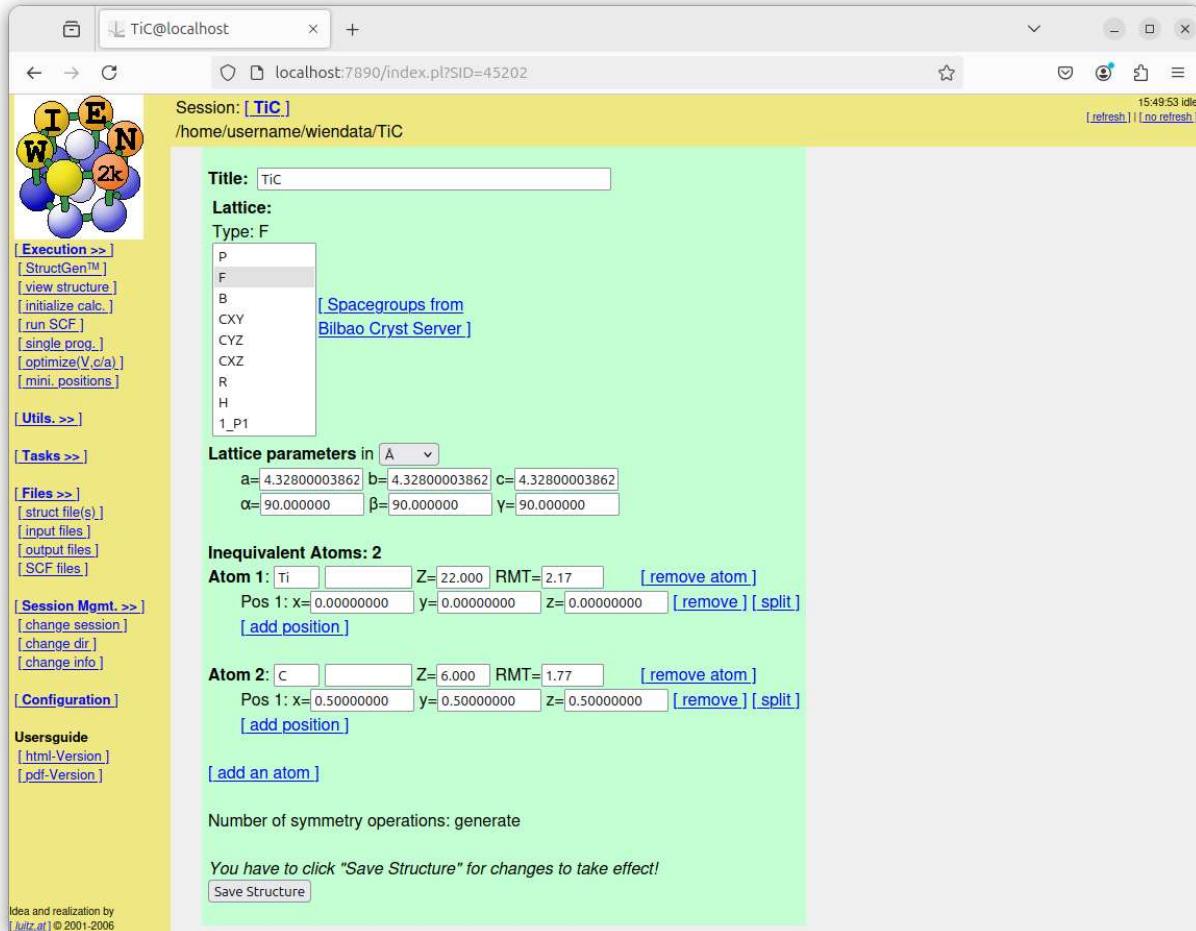
**Alternatively** you can specify the sphere radii explicitly by element using a syntax like: Fe:2.0,C:1.77,...  
Note: It is your responsibility that RMTs will not lead to overlapping spheres.  
Specify a comma separated list of **name:radius** as indicated above:

**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 the StructGen™ software interface running in a web browser (localhost:7890/index.pl?SID=45202). The left sidebar contains a molecular model of TiC and various navigation links like 'Execution >>', 'StructGen™', and 'Session Mgmt. >>'. The main panel displays the following input fields:

- Title:** TiC
- Lattice:** F (selected from a dropdown menu)
- 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 in red), Z = 22.000, RMT = 2.0000  
Pos 1: x = 0.00000000, y = 0.00000000, z = 0.00000000
  - Atom 2:** C (highlighted in red), 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]**

## 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)", there are several configuration options with checkboxes. One option, "select spin-polarized calculation", has its checkbox checked. Below this, there is a section for "Precision level (0-3; 0n-3n for non-metals, default=1)" which is also checked. Other options like RMT reduction, VXC option, energy separation, RKMAX, TEMP, and TEMPS are listed but not checked. A "CHECK BATCH VALUES" button is at the bottom of this section. Below this is a section titled "Individual mode (phase 1)". It contains a note about running steps for antiferromagnets, self-generated structures, supercells, and surfaces. At the bottom, there is a row of buttons: "x nn", "view outputnn", "x sgroup", "view outputsgroup", "x symmetry", "check TiC.in1\_st", "Click here for more info.", "check TiC.in2\_st", "Prepare input files", "view TiC.outputtd and cp TiC.in0\_std TiC.in0", "check if gmax>gmin", and "Perform spin-polarized calc.?". The "x nn" button is highlighted with a red box.

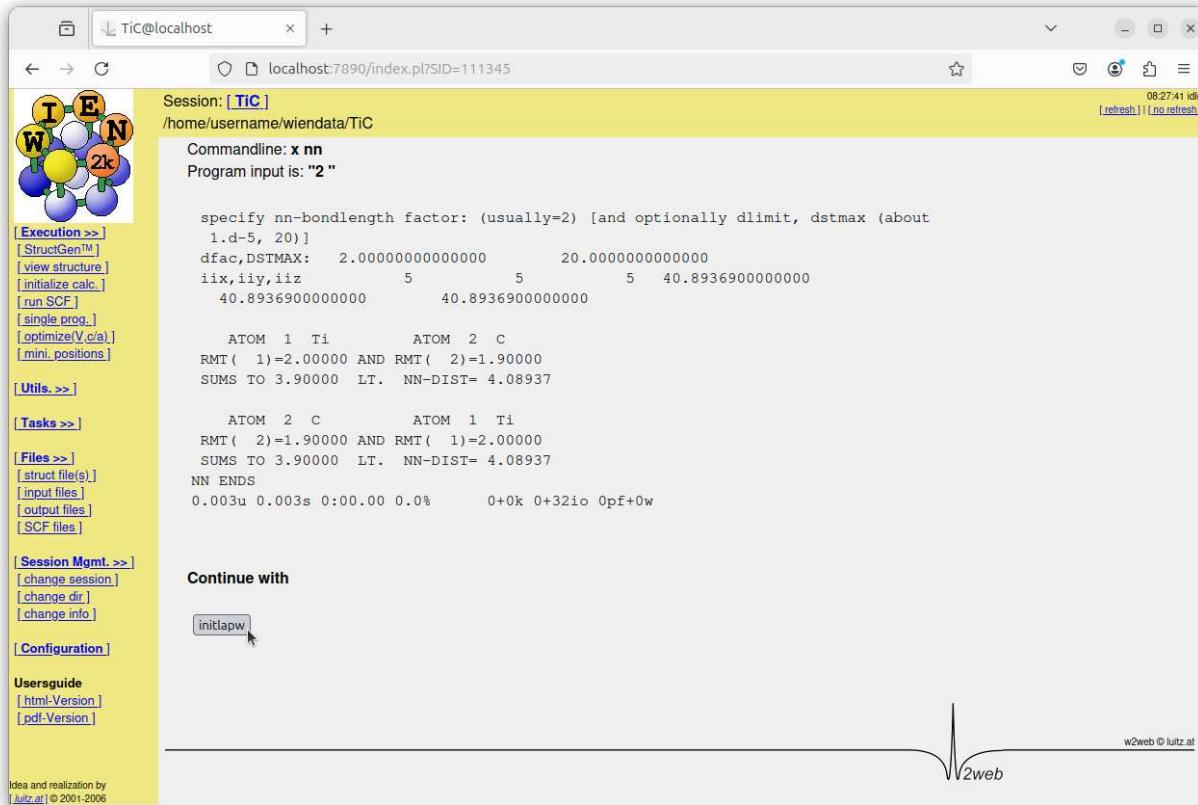
30. By default 2 should be given in the box, click the “Execute!” button:

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:

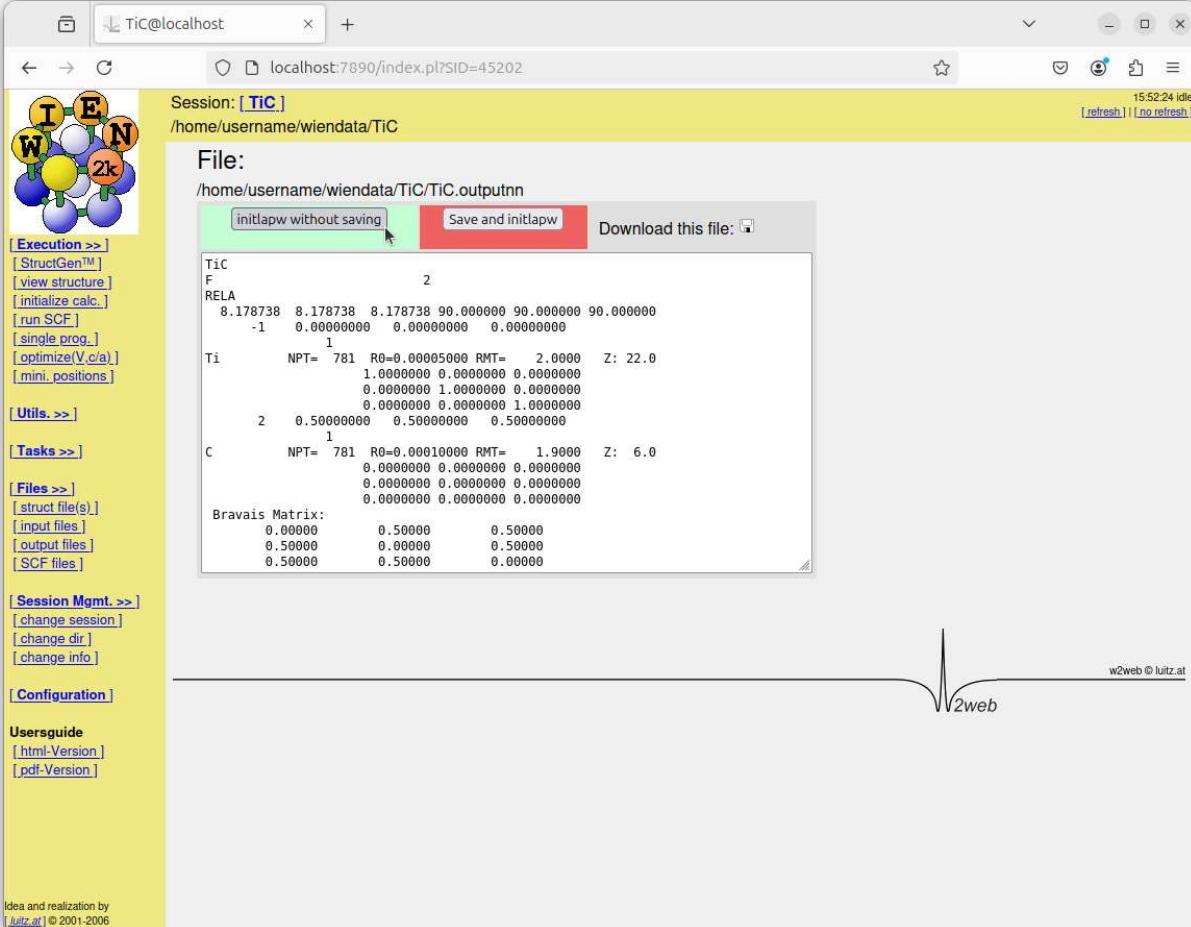
- [Execution >>]
  - [StructGen™]
  - [view structure]
  - [initialize calc.]
  - [run SCF]
  - [single prog.]
  - [optimize(V,c/a)]
  - [mini. positions]
- [Utils. >>]
- [Tasks >>]
- [Files >>]
  - [struct file(s)]
  - [input files]
  - [output files]
  - [SCF files]
- [Session Mgmt. >>]
  - [change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

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31. Click the “initlapw” button:



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



The screenshot shows a web browser window titled "TiC@localhost" at "localhost:7890/index.pl?SID=45202". The page displays a session named "TiC" located at "/home/username/wiendata/TiC". A molecular structure diagram is visible on the left, showing atoms labeled I, E, W, N, and 2x. The main content area shows the file path "/home/username/wiendata/TiC.outputnn". Below this, there are three buttons: "initlapw without saving" (highlighted with a green box), "Save and initlapw" (red box), and "Download this file: ". The text area contains the following data:

```

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

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

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

RELAX

|                 |            |  |
|-----------------|------------|--|
| Ti              | F          | 2                                      |
| 8.178738        | 8.178738   | 8.178738 90.000000 90.000000 90.000000 |
| -1              | 0.00000000 | 0.00000000 0.00000000                  |
| Ti              | NPT= 781   | R0=0.00005000 RMT= 2.0000 Z: 22.0      |
|                 | 1          | 1.00000000 0.00000000 0.00000000       |
|                 |            | 0.00000000 1.00000000 0.00000000       |
|                 |            | 0.00000000 0.00000000 1.00000000       |
| C               | NPT= 781   | R0=0.00010000 RMT= 1.9000 Z: 6.0       |
|                 | 1          | 0.00000000 0.00000000 0.00000000       |
|                 |            | 0.00000000 0.00000000 0.00000000       |
|                 |            | 0.00000000 0.00000000 0.00000000       |
| Bravais Matrix: |            |  |
| 0.00000         | 0.50000    | 0.50000                                |
| 0.50000         | 0.00000    | 0.50000                                |
| 0.50000         | 0.50000    | 0.00000                                |

w2web © luitz.at

34. Click the “x sgroup” button
35. Click the “initlapw” 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 I, E, N, W, and 2k. The session information is shown as "Session: [TiC]" and "/home/username/wiendata/TiC". The commandline is "x sgroup" and the program input is "". Below this, there is a status line showing "0.000u 0.000s 0:00.00 0.0%" and "0+0k 0+8io 0pf+0w". A "Continue with" section contains a button labeled "initlapw" which is being clicked. On the left side, there is a sidebar with various menu options under "Execution >>", "Tasks >>", "Files >>", "Session Mgmt. >>", "Configuration", and "Usersguide". At the bottom left, it says "Idea and realization by [lutz.at] © 2001-2006". The right side of the page has a footer with "w2web" and "w2web © lutz.at".

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 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.

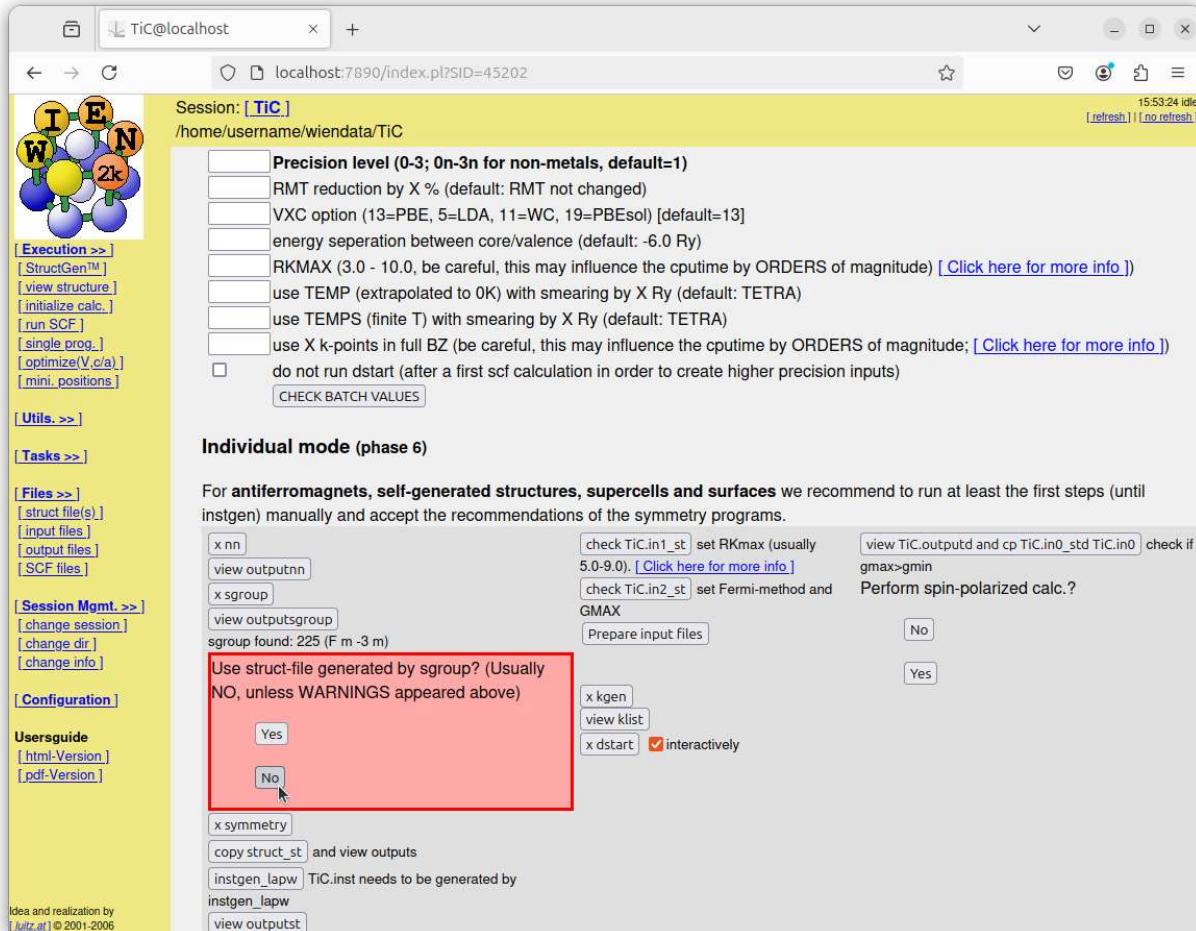
```
a          b          c
8.17873800  8.17873800  8.17873800
alpha       beta        gamma
90.00000000  90.00000000  90.00000000

===== 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):

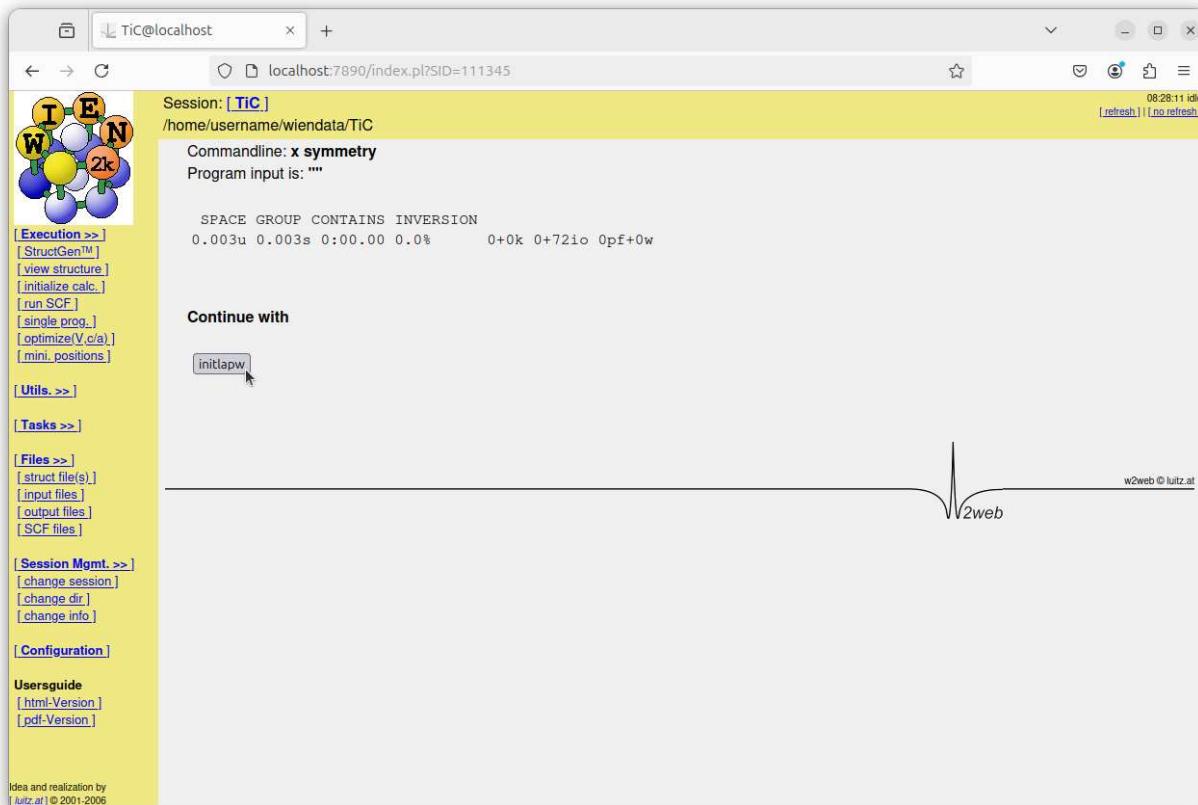
0.00000000  0.00000000  0.00000000
Ti
0.50000000  0.00000000  0.00000000
```

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

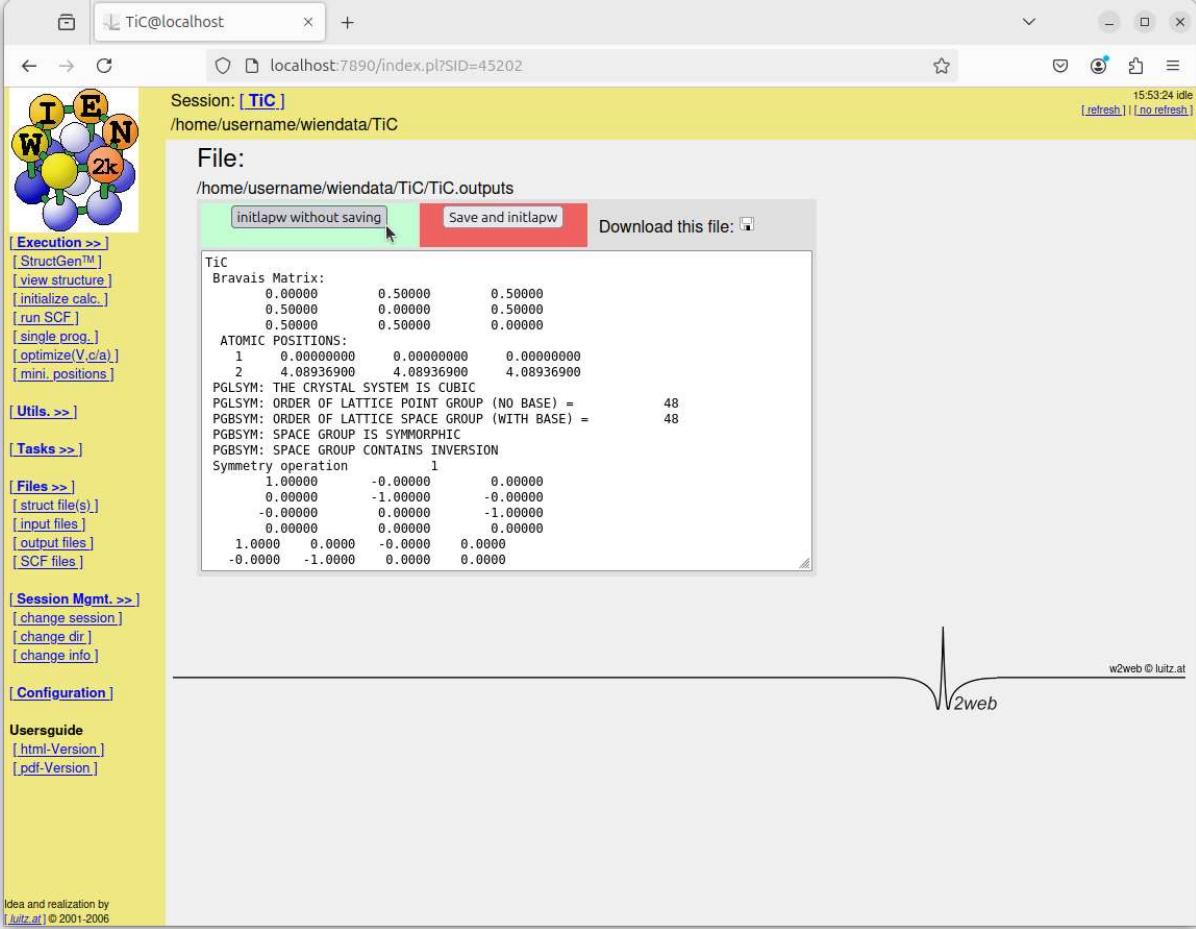


39. Click the “x symmetry” button

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 a session named "TiC" located at "/home/username/wiendata/TiC". On the left, there's a sidebar with various navigation links under categories like "Execution >>", "Tasks >>", "Files >>", "Session Mgmt. >>", and "Configuration". The main content area shows a molecular model of TiC with atoms labeled I, E, N, W, and 2x. Below the model, several buttons are visible: "initlapw without saving" (highlighted with a red box), "Save and initlapw", and "Download this file: ". The text output section contains crystallographic information:

```

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

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

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

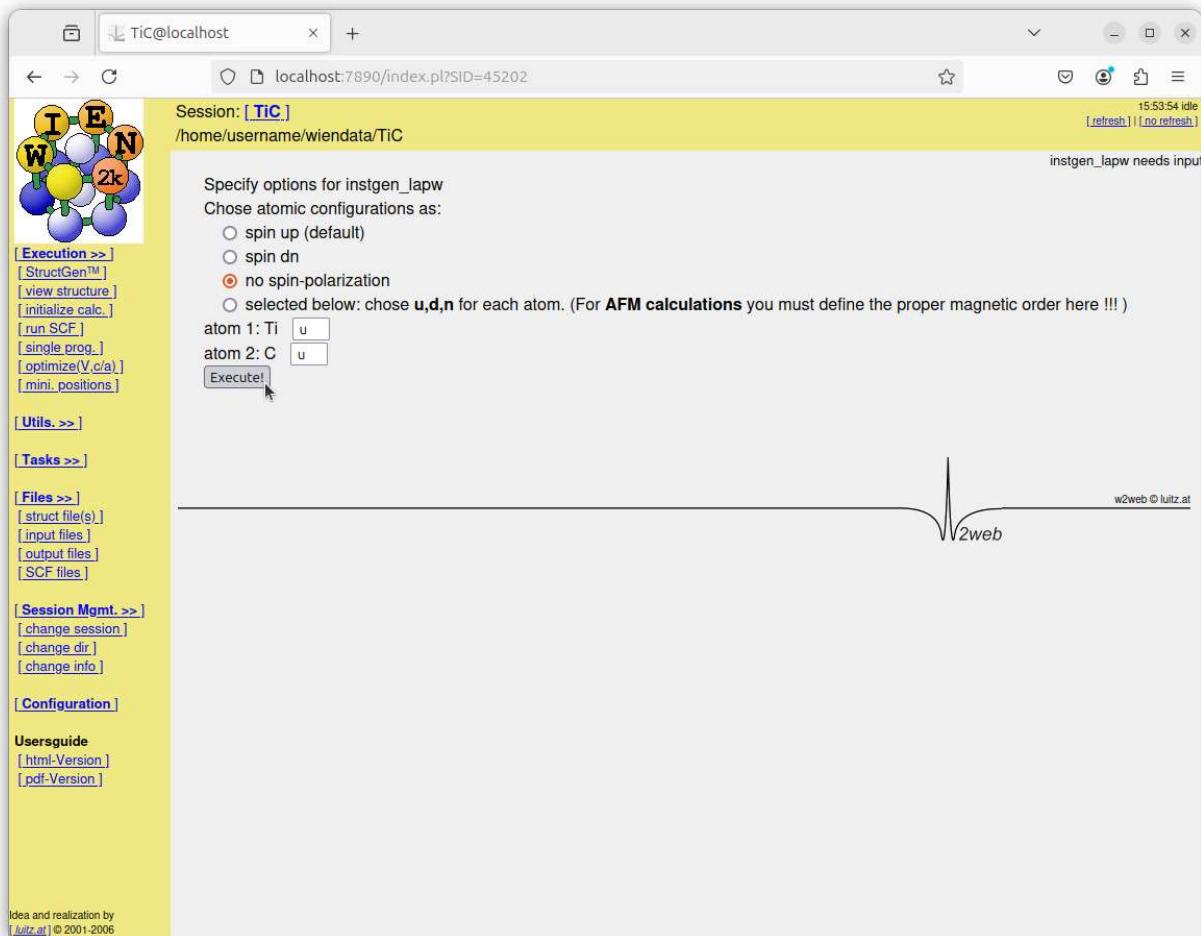
TiC
Bravais Matrix:
  0.00000   0.50000   0.50000
  0.50000   0.00000   0.50000
  0.50000   0.50000   0.00000

ATOMIC POSITIONS:
  1  0.0000000   0.0000000   0.0000000
  2  4.08936900  4.08936900  4.08936900

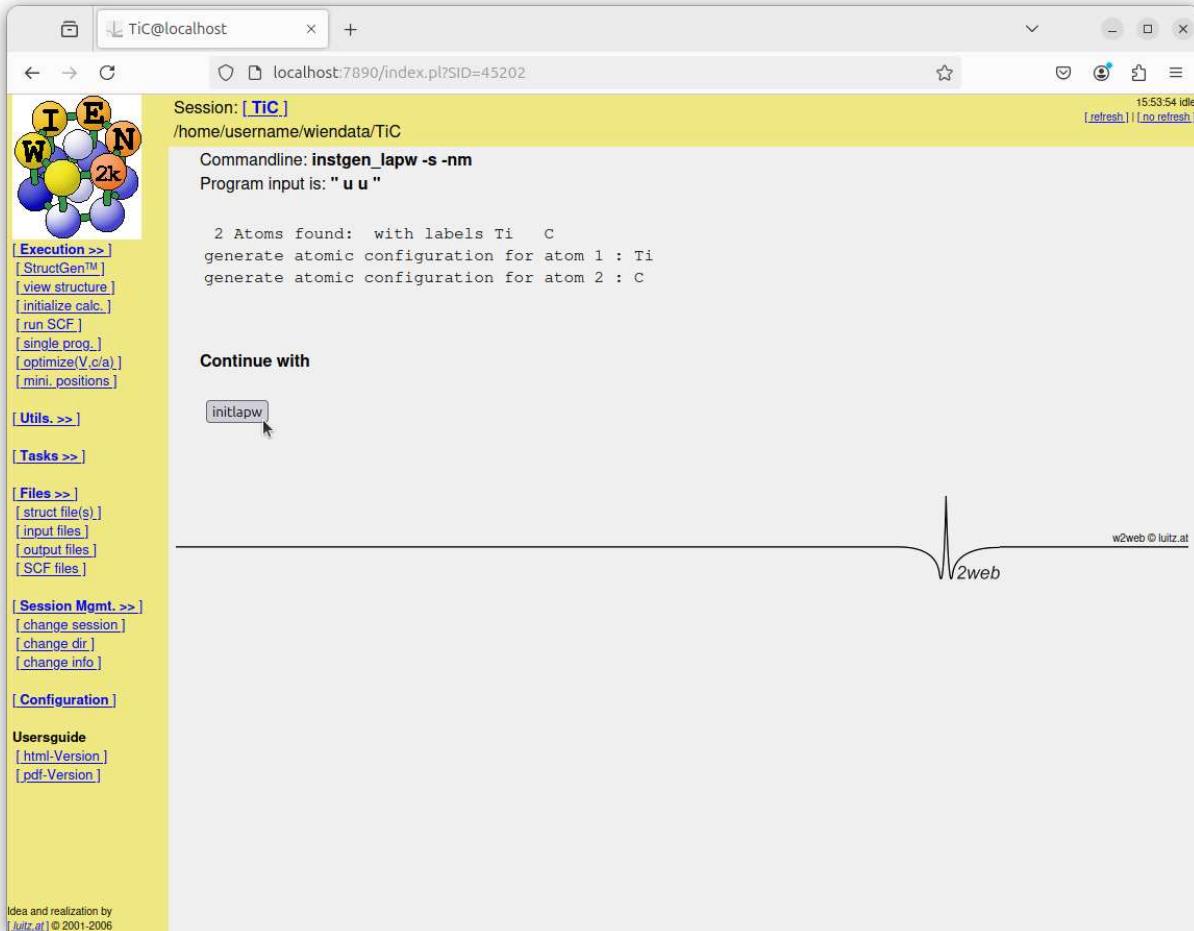
PGLSM: THE CRYSTAL SYSTEM IS CUBIC
PGLSM: ORDER OF LATTICE POINT GROUP (NO BASE) = 48
PGBSM: ORDER OF LATTICE SPACE GROUP (WITH BASE) = 48
PGBSM: SPACE GROUP IS SYMMORPHIC
PGBSM: SPACE GROUP CONTAINS INVERSION
Symmetry operation 1
  1.00000   -0.00000   0.00000
  0.00000   -1.00000   -0.00000
  -0.00000   0.00000   -1.00000
  0.00000   0.00000   0.00000
  1.00000   0.00000   -0.00000
  -0.00000   -1.00000   0.00000
  0.00000   1.00000   0.00000
  
```

In the bottom right corner of the main content area, there is a logo for "w2web" with the text "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 execution and management options like "Execution >>", "StrucGen™", "view structure", etc. The main content area has a yellow header "Select Exchange Correlation Potential:" with a dropdown set to "PBE-GGA (Perdew-Burke-Ernzerhof 96)". Below it, there's a section for "ENERGY to separate core and valence states:" with a text input field containing "-6.0" and a note about charge localization. A button labeled "Execute!" is highlighted with a cursor. The bottom right corner features a small logo "w2web © iuiz.at".

## 48. Click the “initlapw” button:

TiC@localhost

localhost:7890/index.pl?SID=111345

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

08:28:41 idle  
 [refresh] || [no refresh]

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   |

LSTART ENDS  
 0.114u 0.003s 0:00.11 100.0% 0+0k 0+968io 0pf+0w

Continue with

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**initlapw**

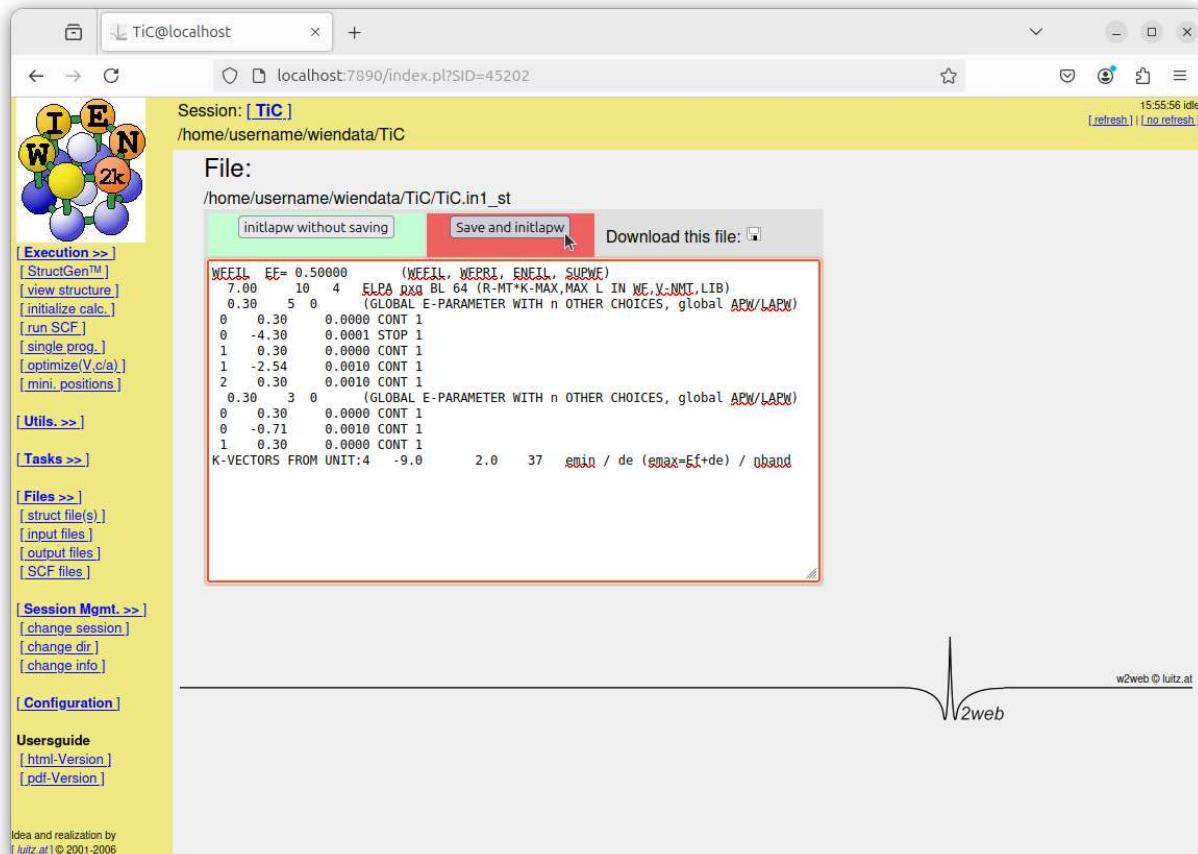
49. Click the “view outputst” button  
50. Click the “initlapw without saving” button:

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, W, N, 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:



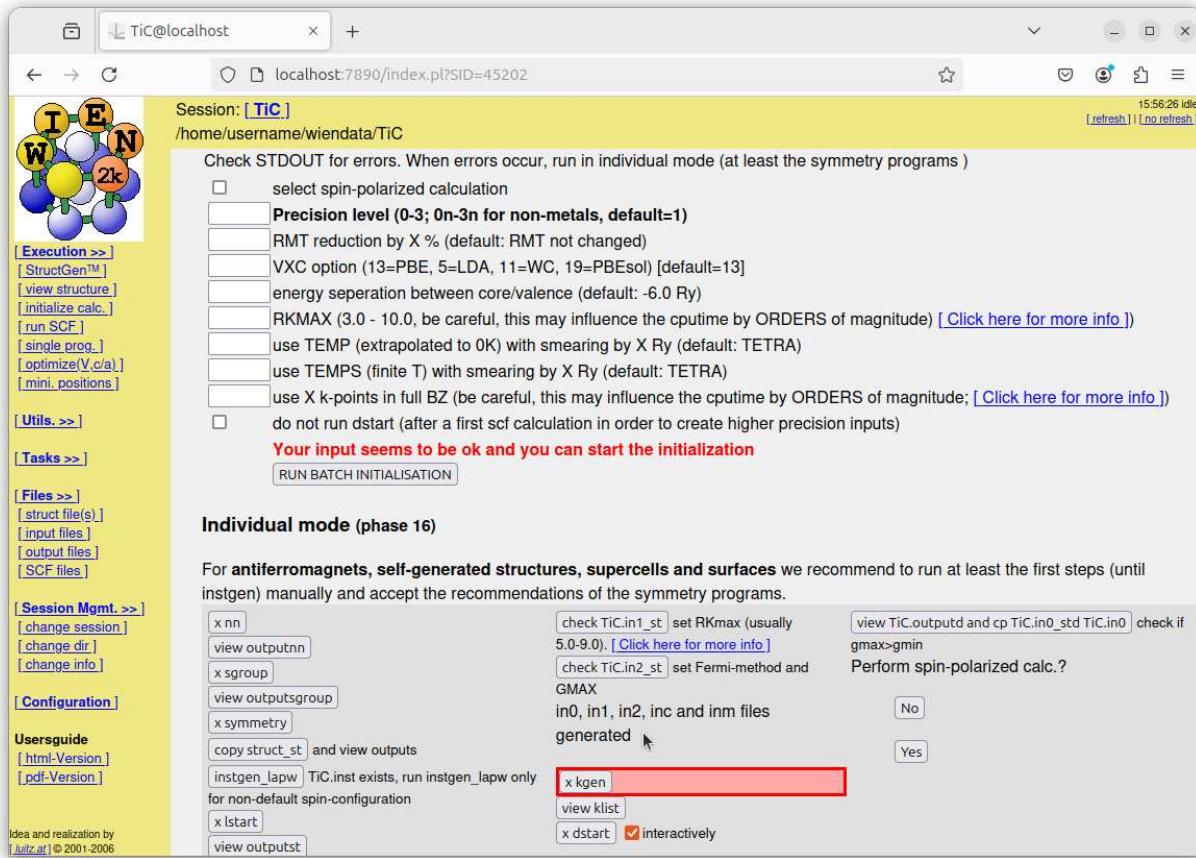
54. Click the “check TiC.in2\_st” button
55. Click the “initlapw without saving” button:

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
```

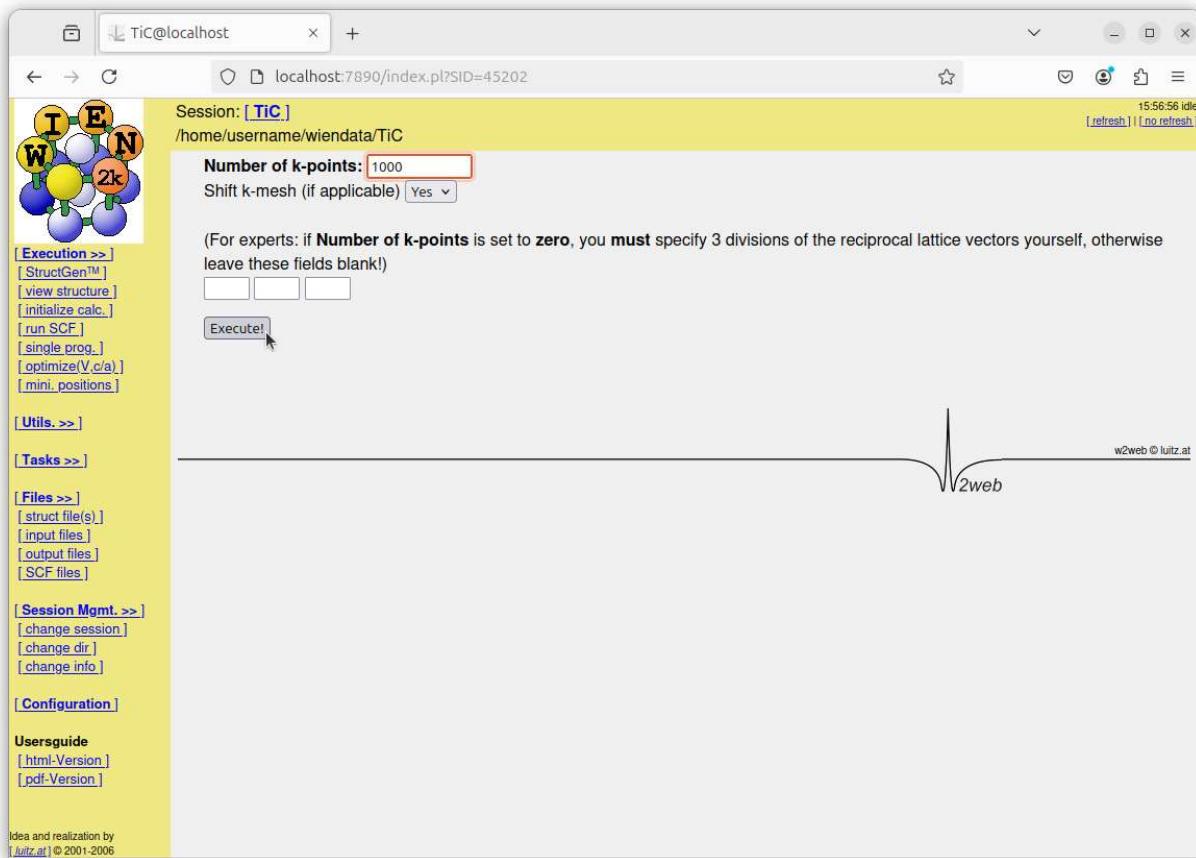
At the top of the file view, there are three buttons: "initlapw without saving" (highlighted in green), "Save and initlapw" (red), and "Download this file: ". The bottom right corner of the page has a "w2web" logo.

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

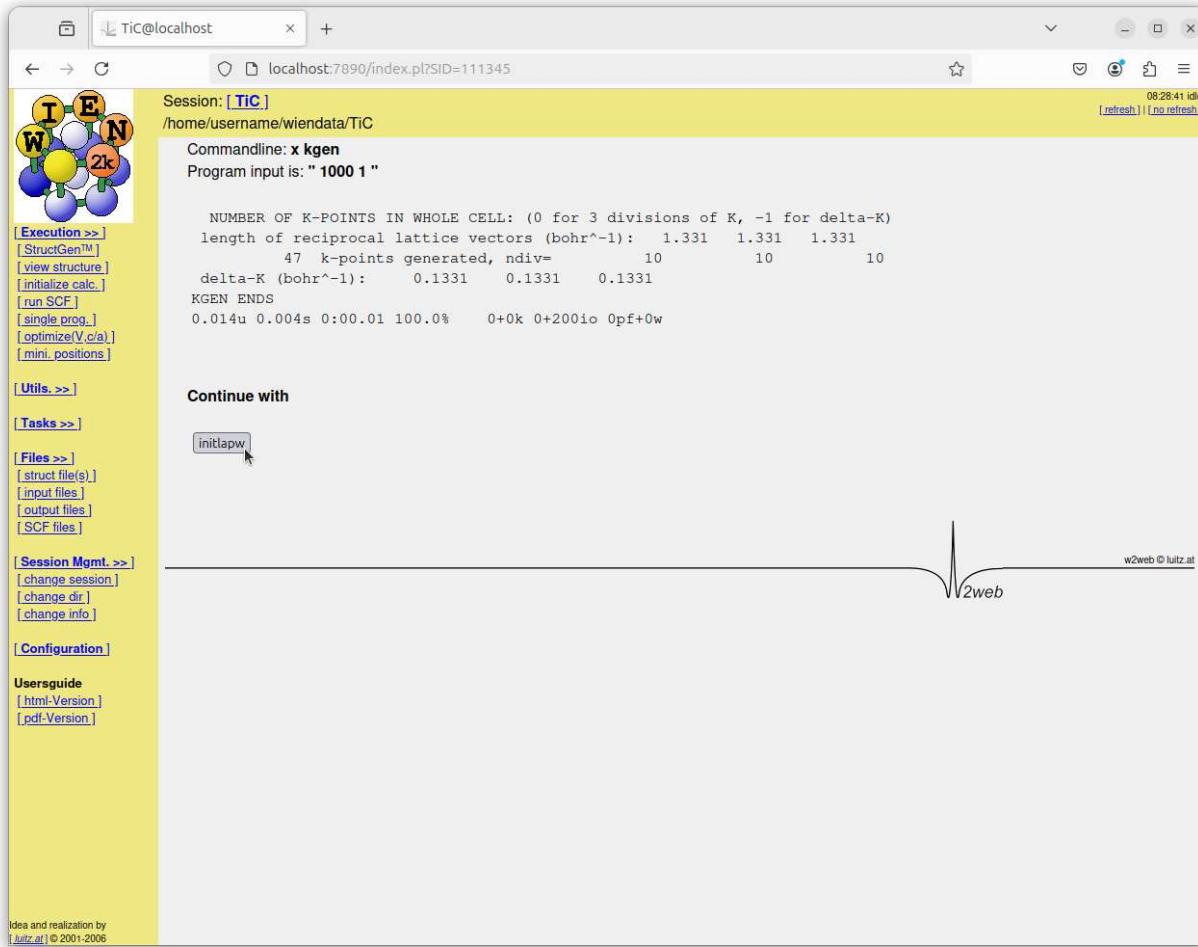


57. Click the “x kgen” button

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



## 59. Click the “initlapw” button:



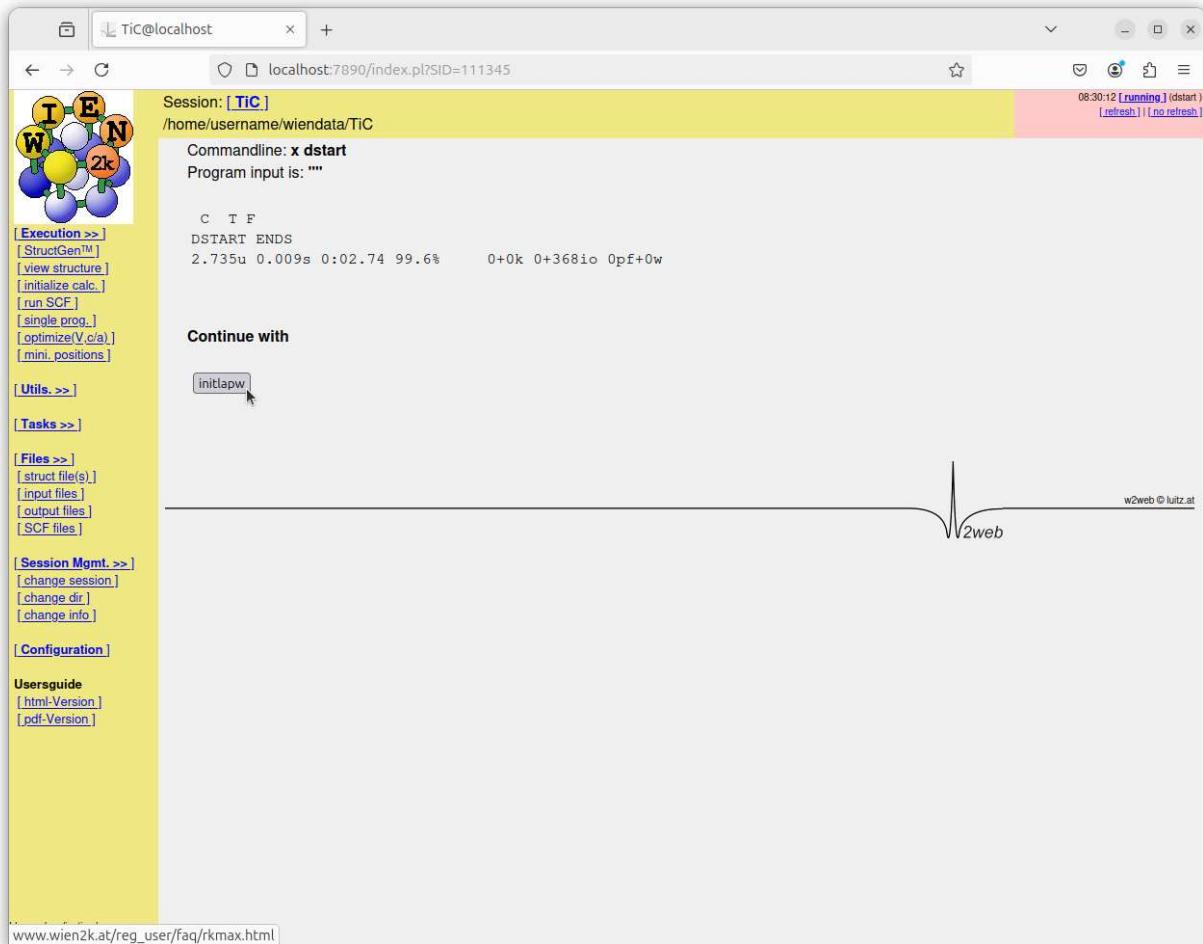
60. Click the “view klist” button

61. Click the “initlapw without saving” button:

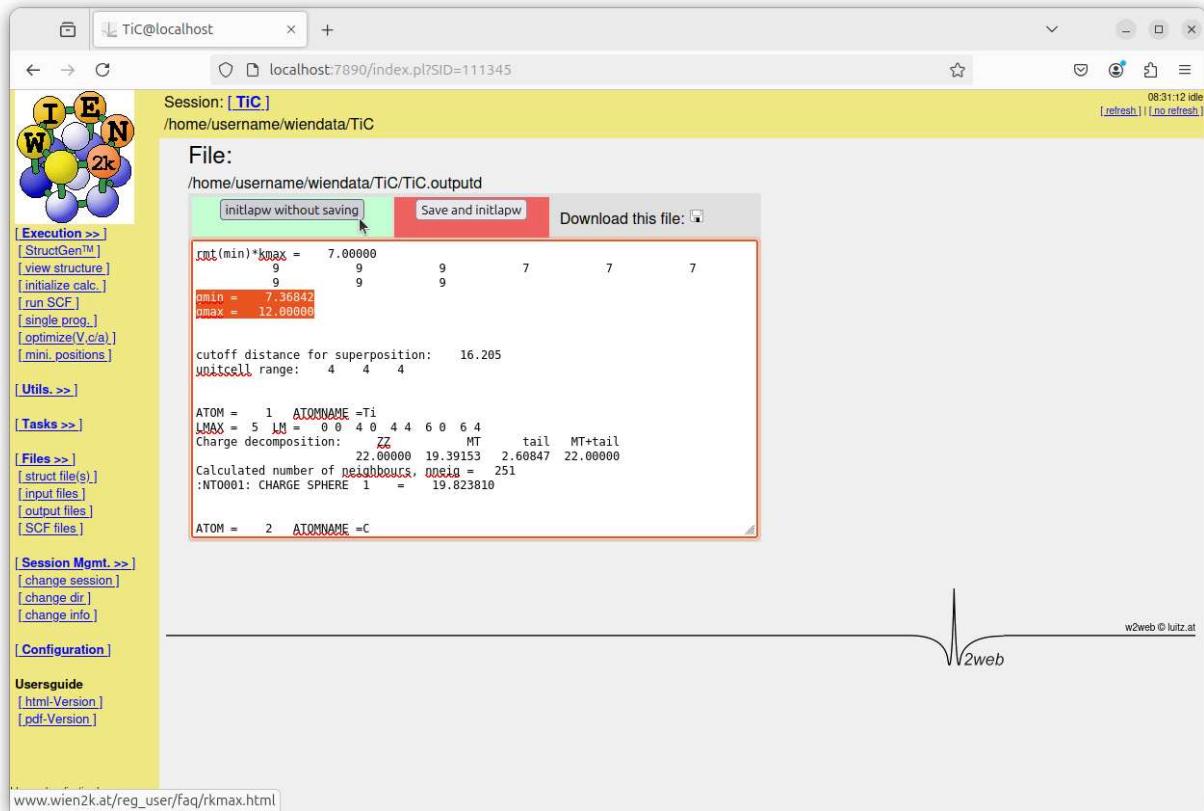
The screenshot shows a web browser window titled "TiC@localhost" with the URL "localhost:7890/index.pl?SID=45202". The page displays a session named "TiC" with the path "/home/username/wiendata/TiC". On the left, there is a sidebar with various menu options like "Execution >>", "Tasks >>", "Files >>", "Session Mgmt. >>", and "Configuration". The main area shows a table of data labeled "TiC.klist" with columns for indices (1-20) and coordinates (x, y, z). At the top right of the table, there are three buttons: "initlapw without saving" (highlighted in green), "Save and initlapw" (red), and "Download this file: ". The bottom right corner features a logo for "w2web" with the text "w2web © luitz.at".

|   | 1 | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20   |      |
|---|---|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|------|------|
| x | 0 | 1  | 2  | 3  | 4  | 5  | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  | 10 | 4  | 5  | 6  | 7  | 8    | 1.0  |
| y | 0 | -1 | -2 | -3 | -4 | -5 | 0  | -1 | -2 | -3 | -4 | -5 | -6 | -7 | -8 | 0  | 1  | 2  | 3  | -4   | -7.0 |
| z | 0 | 10 | 10 | 10 | 10 | 10 | 10 | 10 | 10 | 10 | 10 | 10 | 10 | 10 | 10 | 10 | 10 | 10 | 10 | 1000 | k, d |

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 the Wien2k web interface with the following details:

- Molecular Structure:** A ball-and-stick model of a TiC unit cell is displayed, showing atoms labeled Ti, C, N, E, W, and 2k.
- Session Information:** Session name: TiC, Path: /home/username/wiendata/TiC.
- File:** /home/username/wiendata/TiC/TiC.outputd
- Buttons:** initlapw without saving (highlighted), Save and initlapw, Download this file.
- Text Output:**

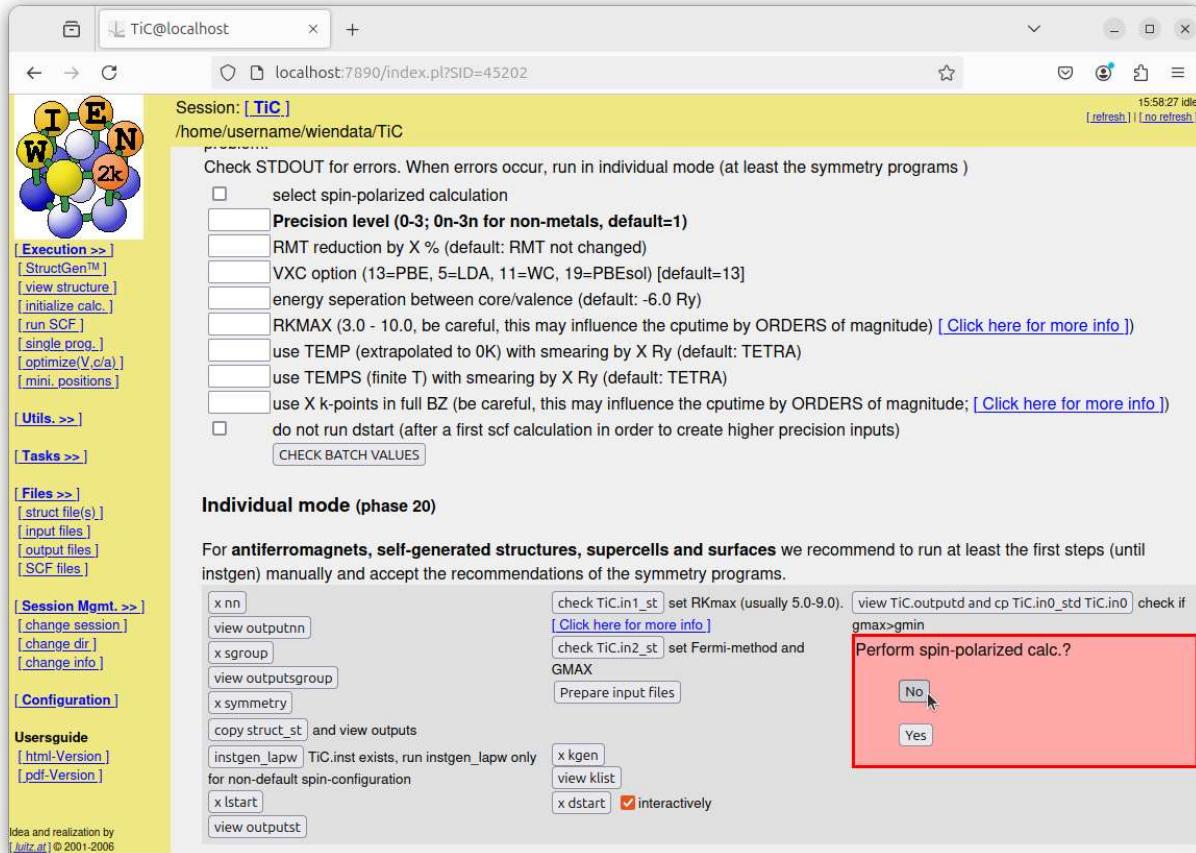
```
rmt(min)*kmax = 7.00000
 9      9      9      7      7      7
 9      9      9
dmin = 7.36842
dmax = 12.00000

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

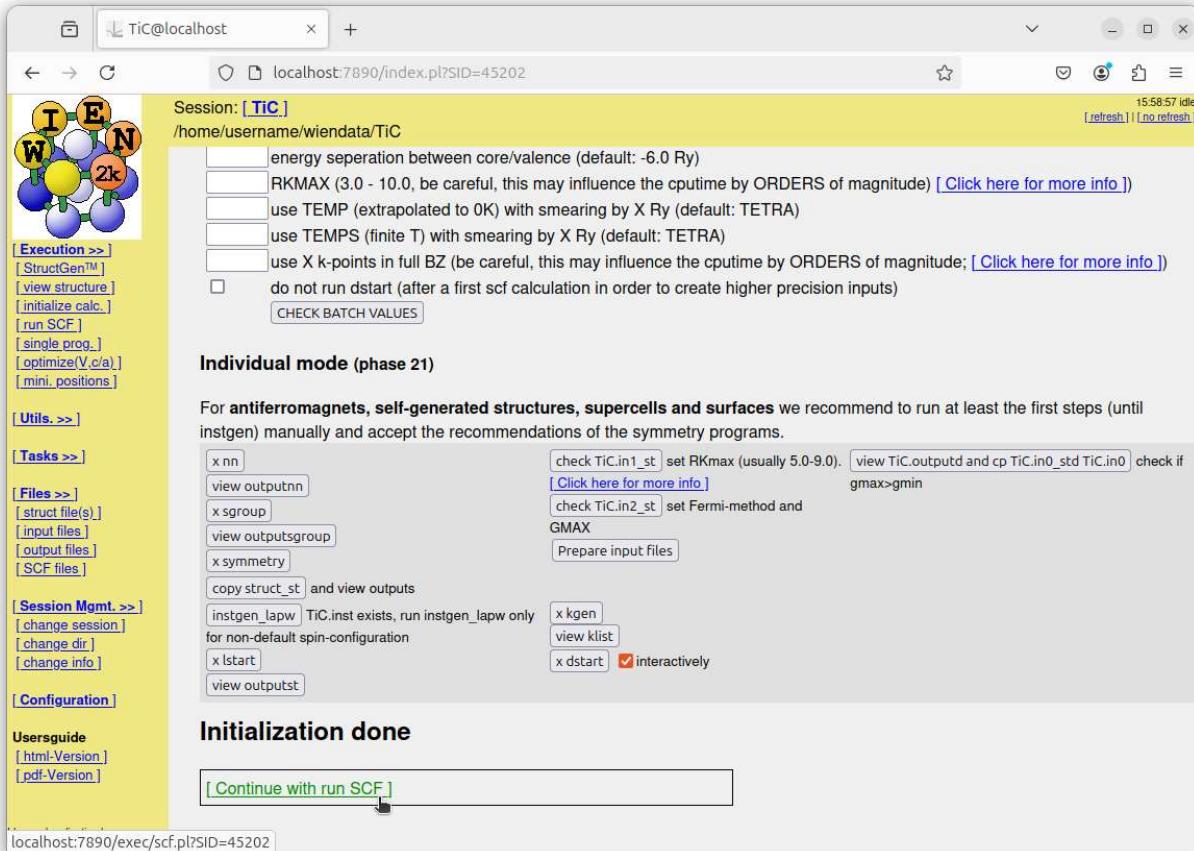
ATOM = 1 ATOMNAME =Ti
LMAX = 5 LN = 0 0 4 0 4 4 6 0 6 4
Charge decomposition: ZZ MT tail MT+tail
                      22.00000 19.39153 2.60847 22.00000
Calculated number of neighbours, openig = 251
:NT0001: CHARGE SPHERE 1 = 19.823810

ATOM = 2 ATOMNAME =C
```
- Left Sidebar:**
  - [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]
- Bottom:** www.wien2k.at/reg\_user/faq/rkmax.html

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

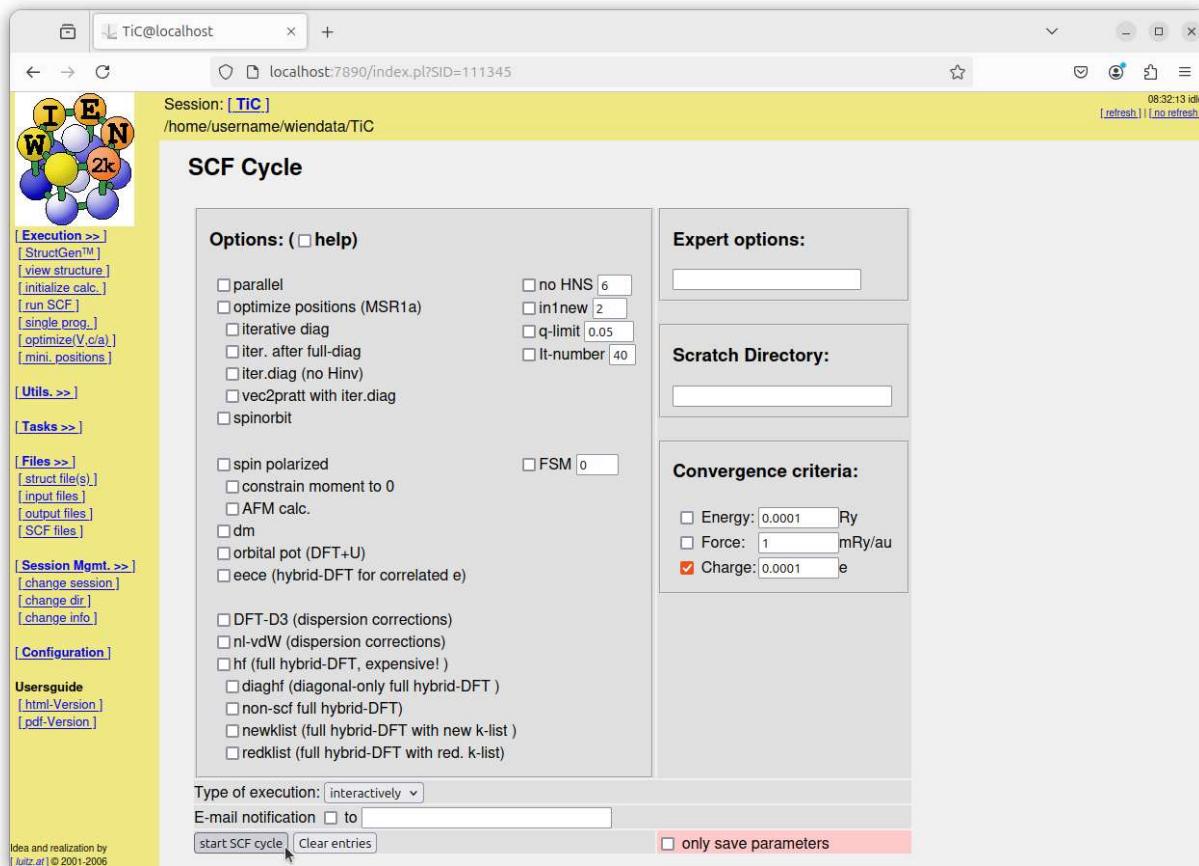


67. Click the “Continue with run SCF” link:

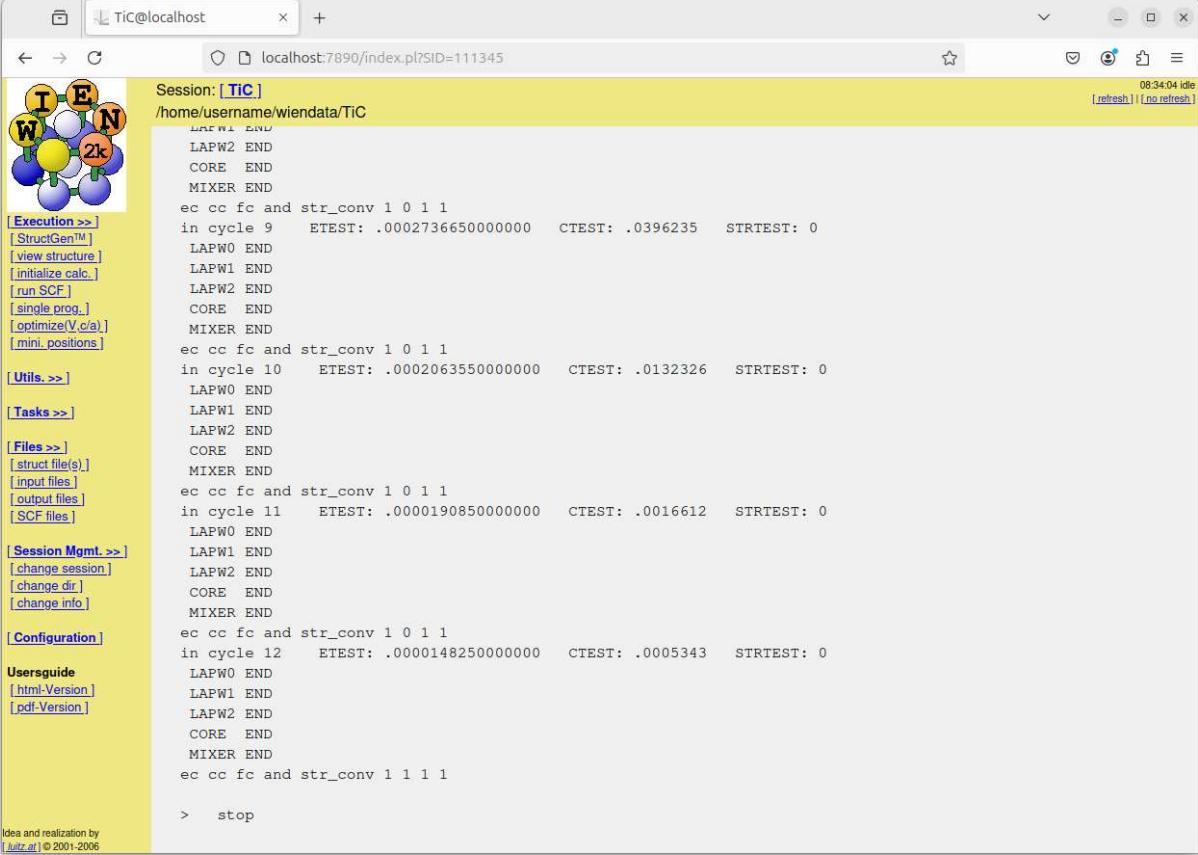


## Run the calculation

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 12 cycles:



```

Session: [TiC]
/home/username/wiendata/TiC
08:34:04 idle
[refresh] | [no refresh]

LAPW1 END
LAPW2 END
CORE END
MIXER END

ec cc fc and str_conv 1 0 1 1
in cycle 9    ETEST: .0002736650000000    CTEST: .0396235    STRTEST: 0
LAPW0 END
LAPW1 END
LAPW2 END
CORE END
MIXER END

ec cc fc and str_conv 1 0 1 1
in cycle 10   ETEST: .0002063550000000    CTEST: .0132326    STRTEST: 0
LAPW0 END
LAPW1 END
LAPW2 END
CORE END
MIXER END

ec cc fc and str_conv 1 0 1 1
in cycle 11   ETEST: .0000190850000000    CTEST: .0016612    STRTEST: 0
LAPW0 END
LAPW1 END
LAPW2 END
CORE END
MIXER END

ec cc fc and str_conv 1 0 1 1
in cycle 12   ETEST: .0000148250000000    CTEST: .0005343    STRTEST: 0
LAPW0 END
LAPW1 END
LAPW2 END
CORE END
MIXER END

ec cc fc and str_conv 1 1 1 1

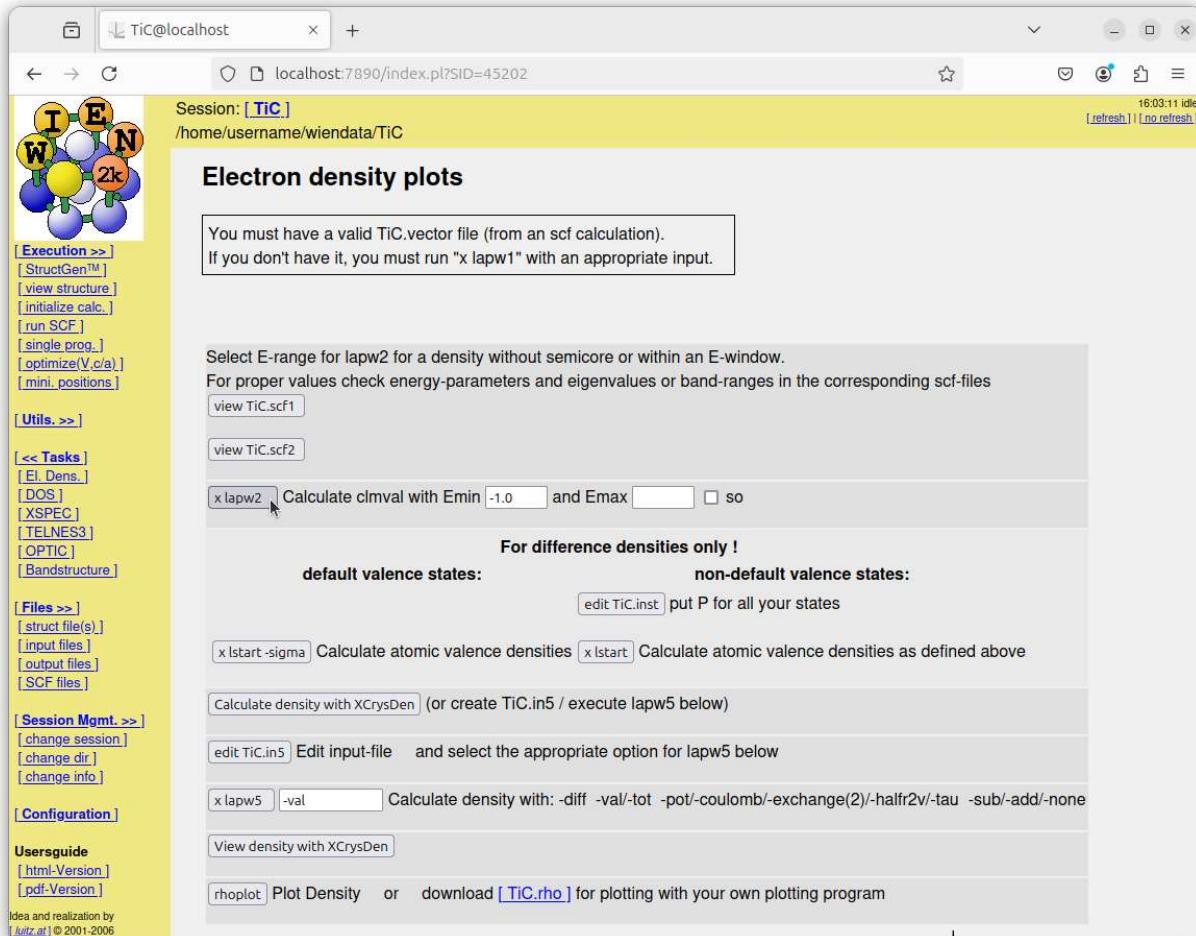
> stop

```

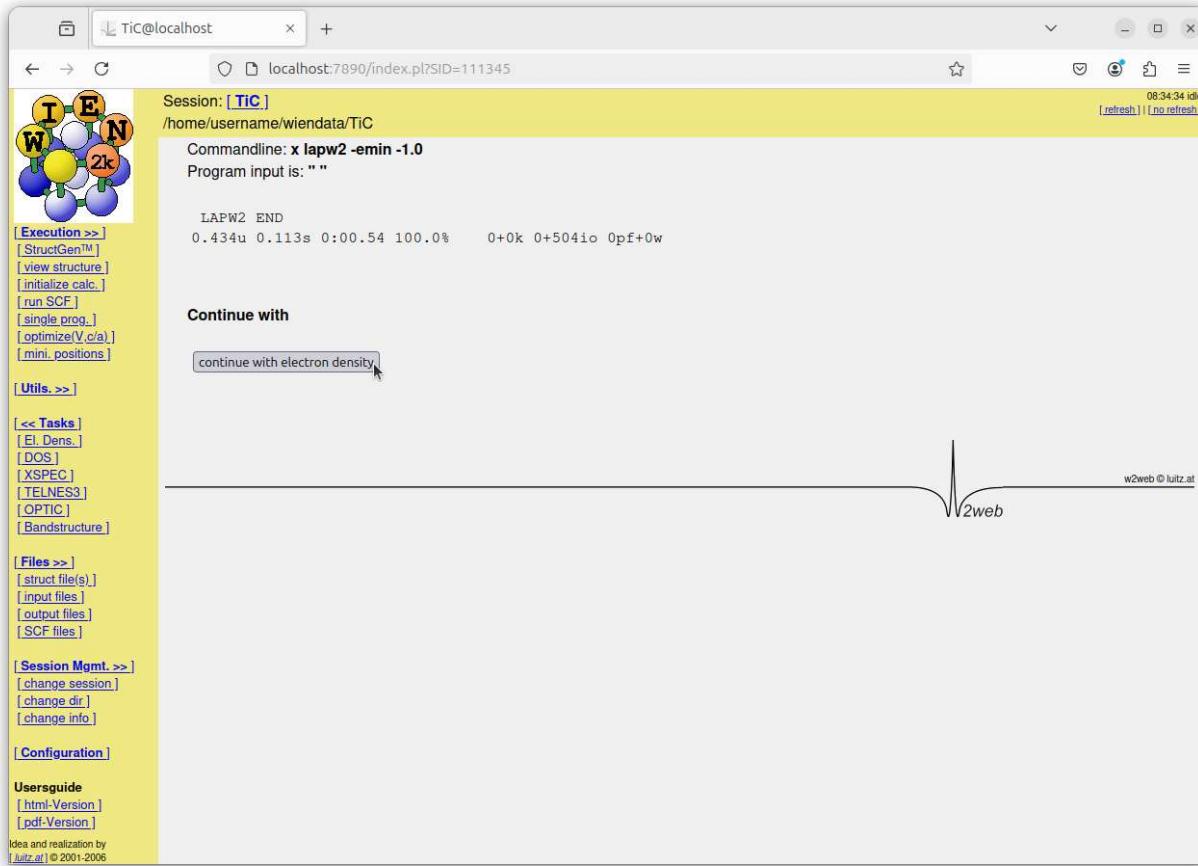
Idea and realization by  
[altz.at] © 2001-2006

## 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:

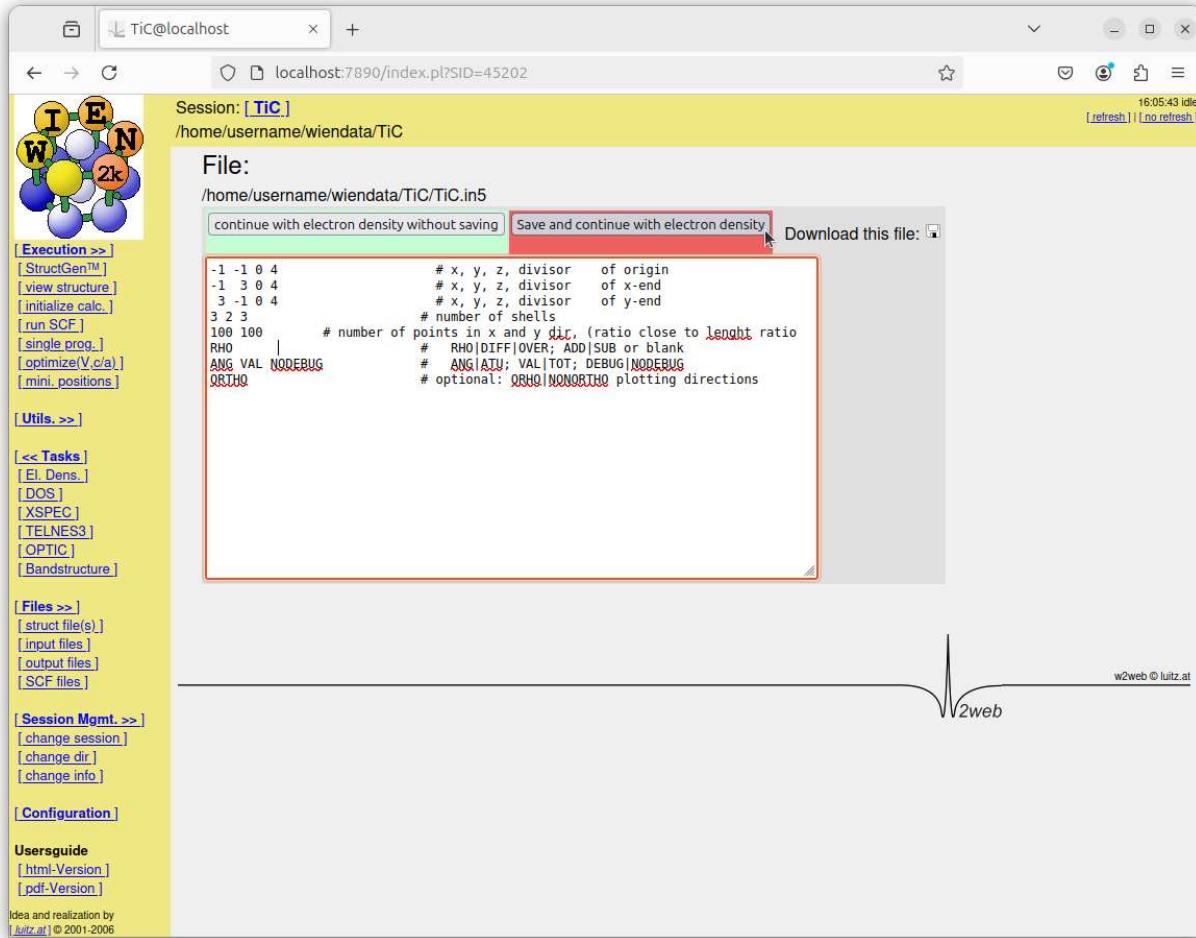
-1 -1 0 4 #origin of plot

-1 3 0 4 #x-end of plot

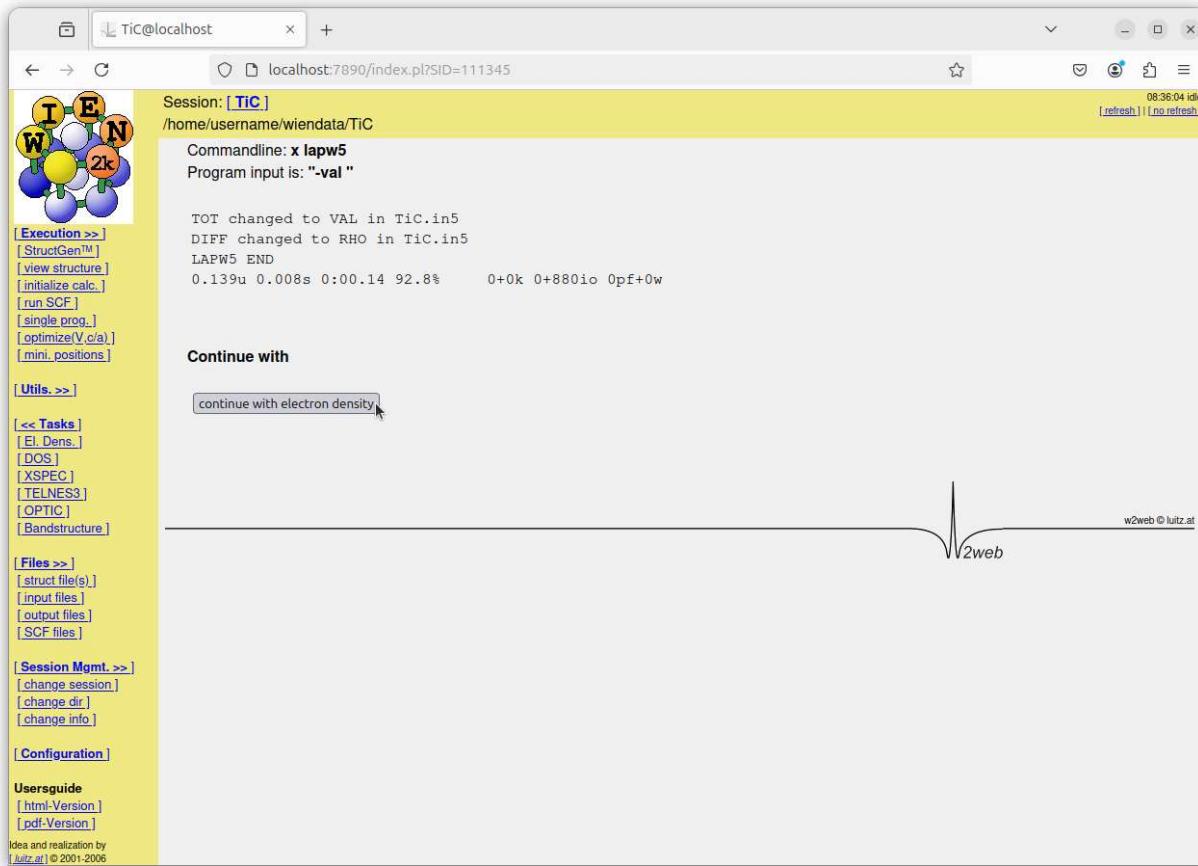
3 -1 0 4 #y-end of plot

ADD was removed

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

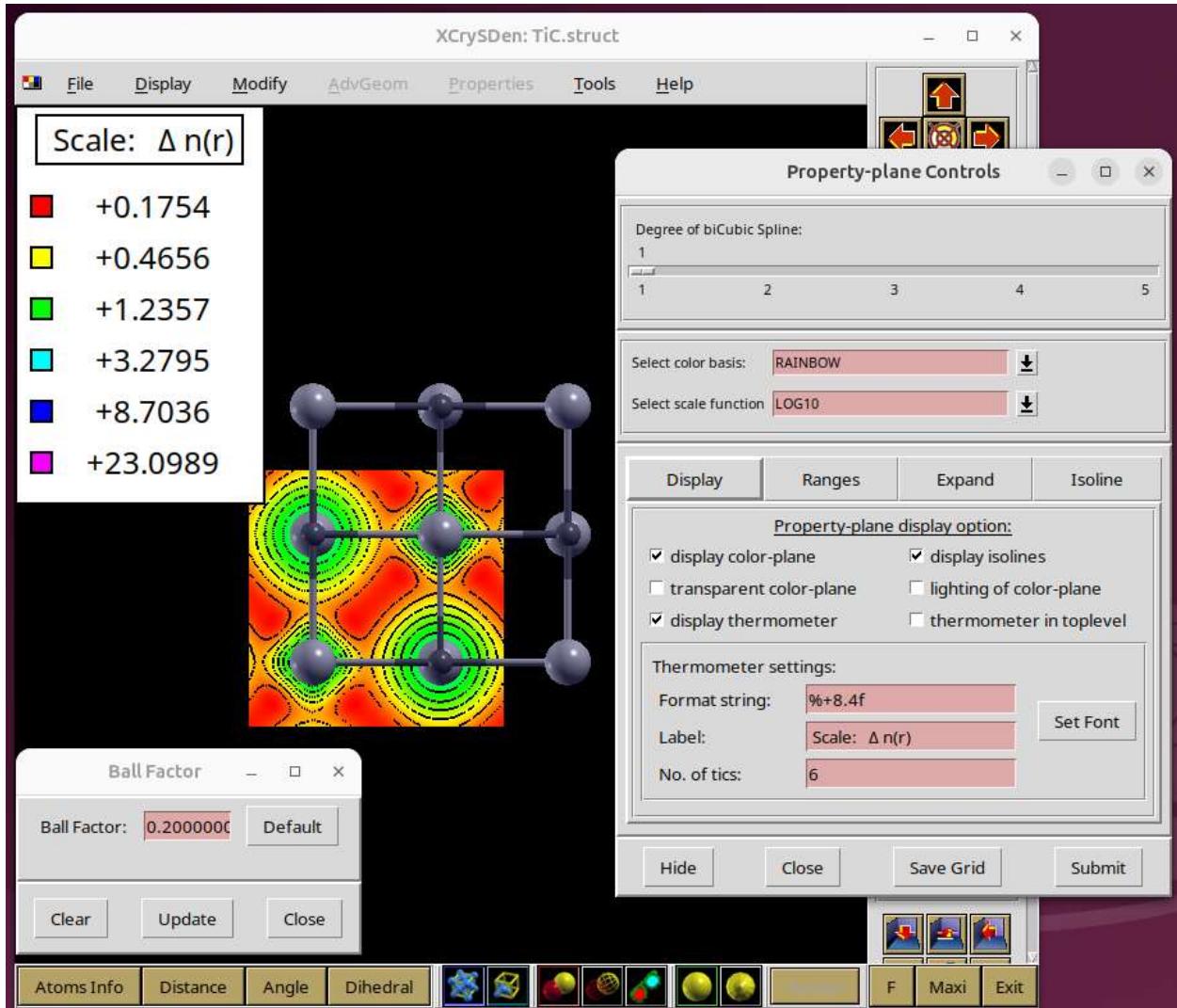


77. Click the “x lapw5” button  
 78. Click the “continue with electron density” button:



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

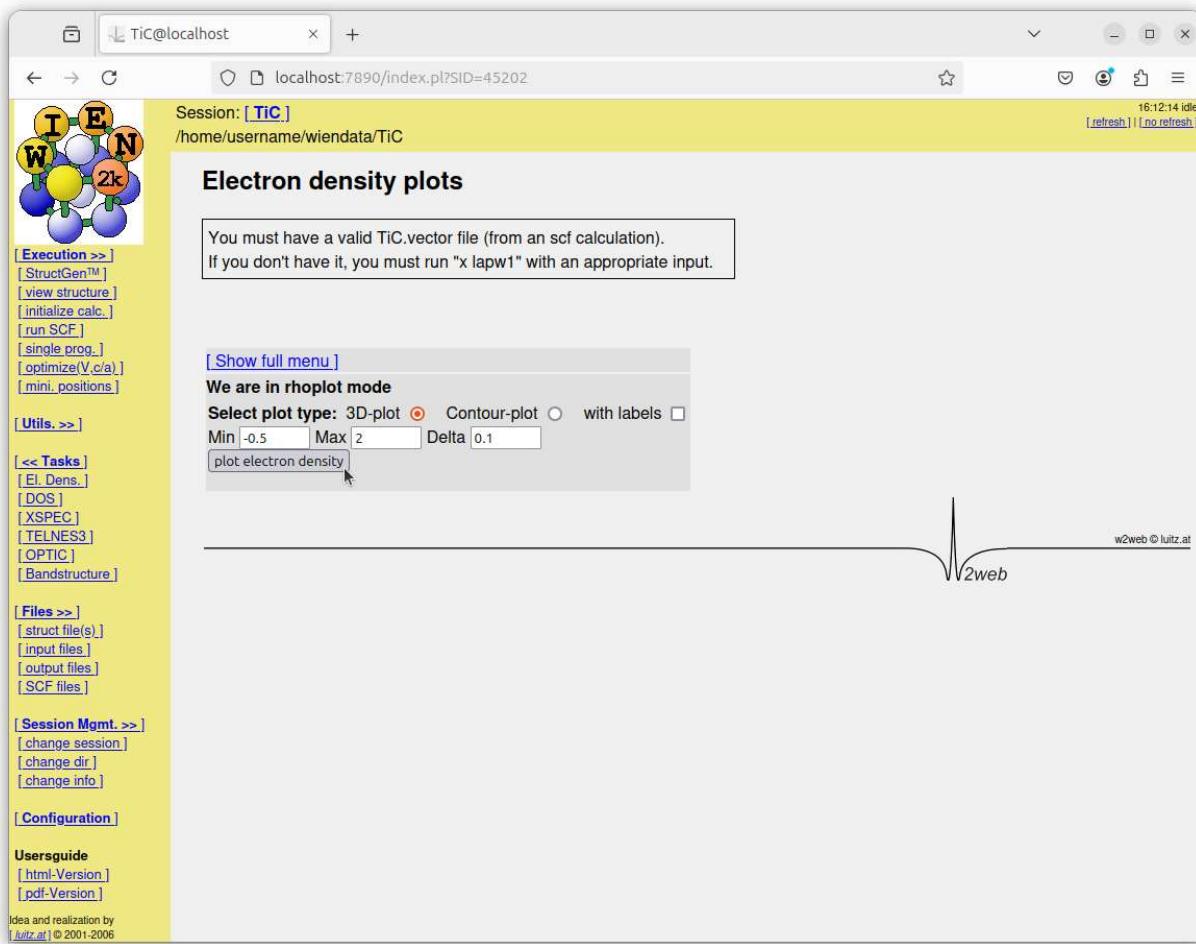
87. The following results (compare to Figure 3.8 in the WIEN2k usersguide [2]):



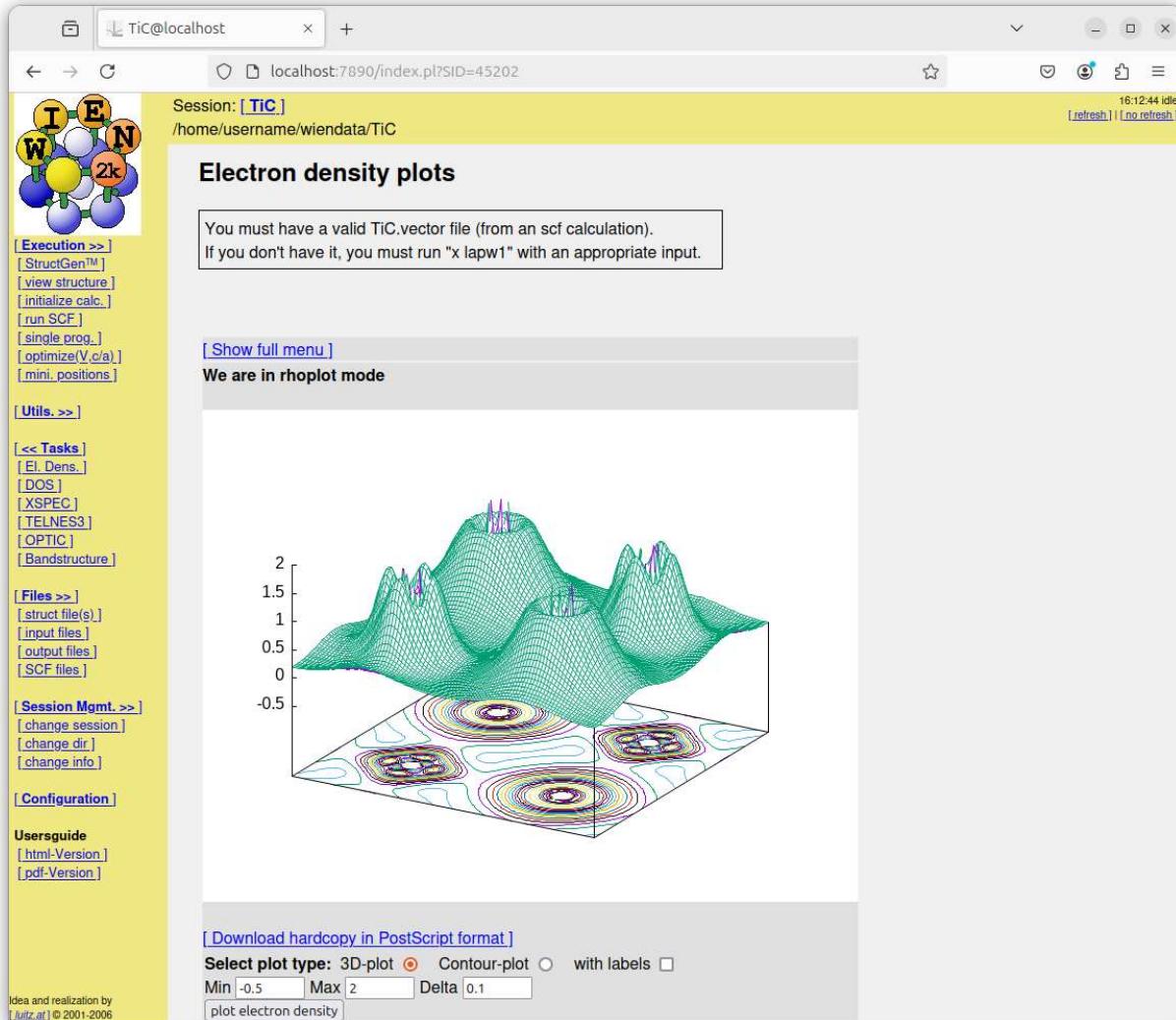
[2] [http://www.wien2k.at/reg\\_user/textbooks/usersguide.pdf](http://www.wien2k.at/reg_user/textbooks/usersguide.pdf)

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”:



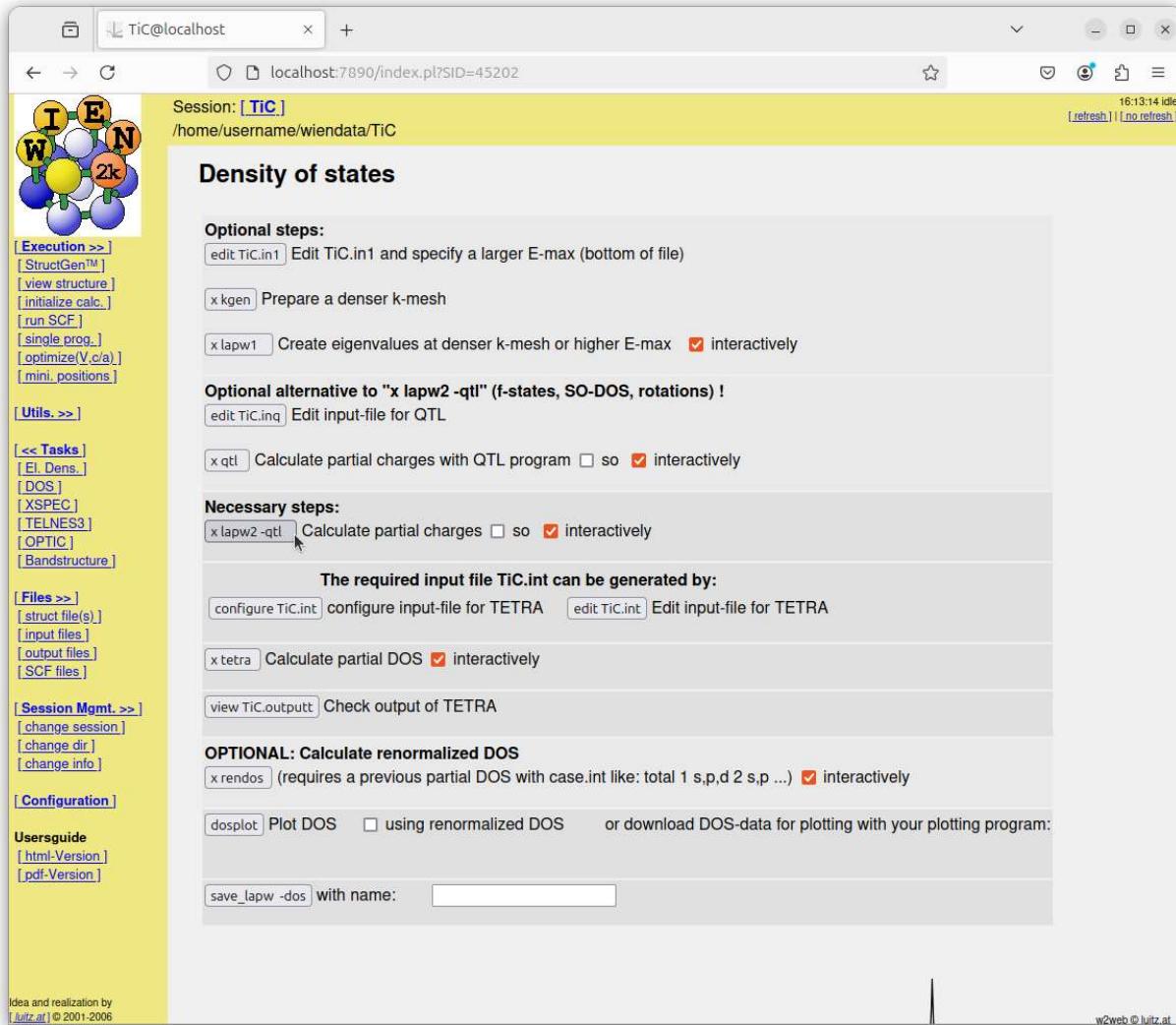
92. This gives us the following plot (compare to Figure 3.9 in the WIEN2k usersguide):



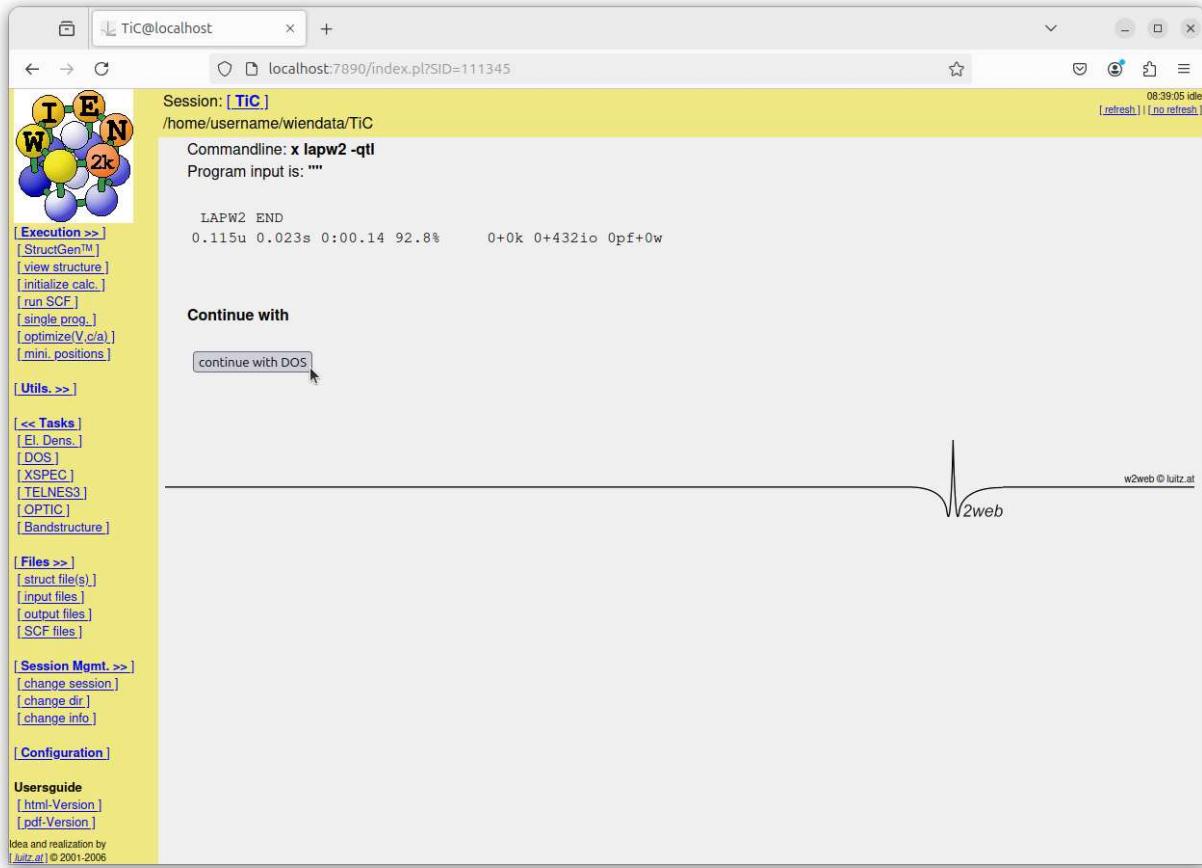
## Plot density of states (DOS)

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

94. Click on “x lapw2 -qtl”:



## 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

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

Header from TiC.qtl:

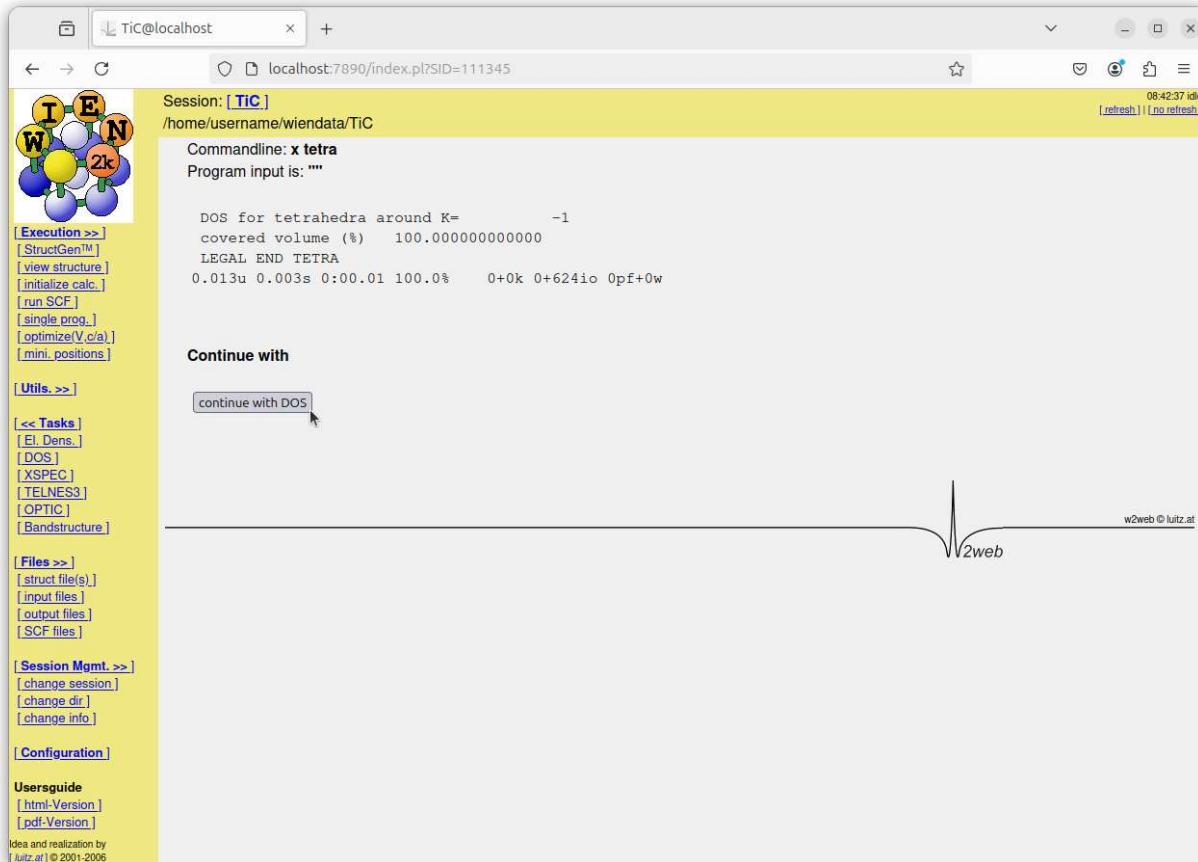
```
ATOM          COLUMN
ATOM 1: Ti: tot,s,p,d,D-eg,D-t2g,f
ATOM 2: C: tot,s,p,d,D-eg,D-t2g,f
```

**TiC**

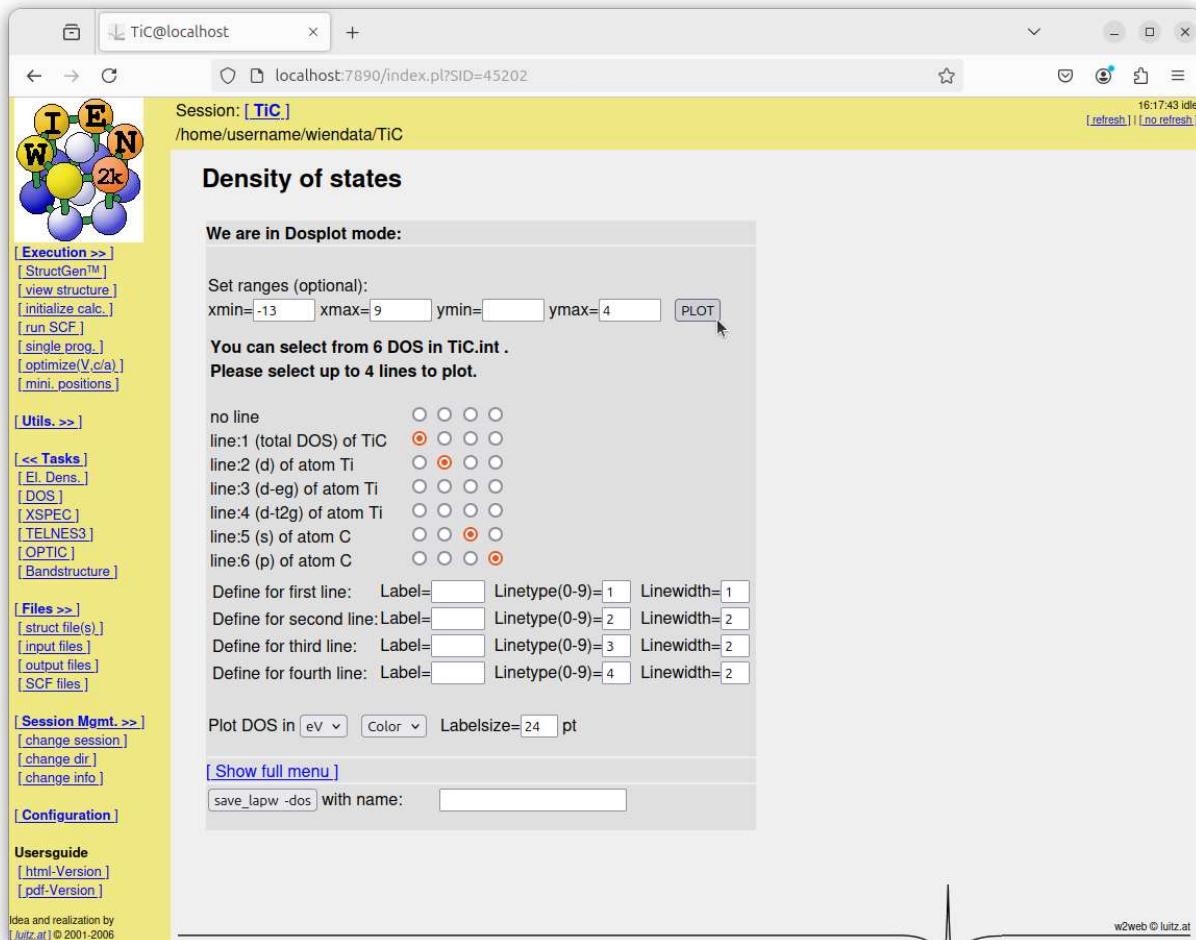
```
-0.50 0.002 1.500 0.003 # EMIN, DE, EMAX, Gauss-broadening(>de)
6 N 0.000 KSEL=-1 # NUMBER OF DOS-CASES below, G/L/B broadening (Ry),KSE
0 1 tot           # atom, case=column in gtl-header, label
1 4 Ti d
1 5 Ti eg
1 6 Ti t2g
2 2 C s
2 3 C p
SUM: 0 2          # NUMBER OF SUMMATIONS, MAXIMUM OF SUMMANDS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

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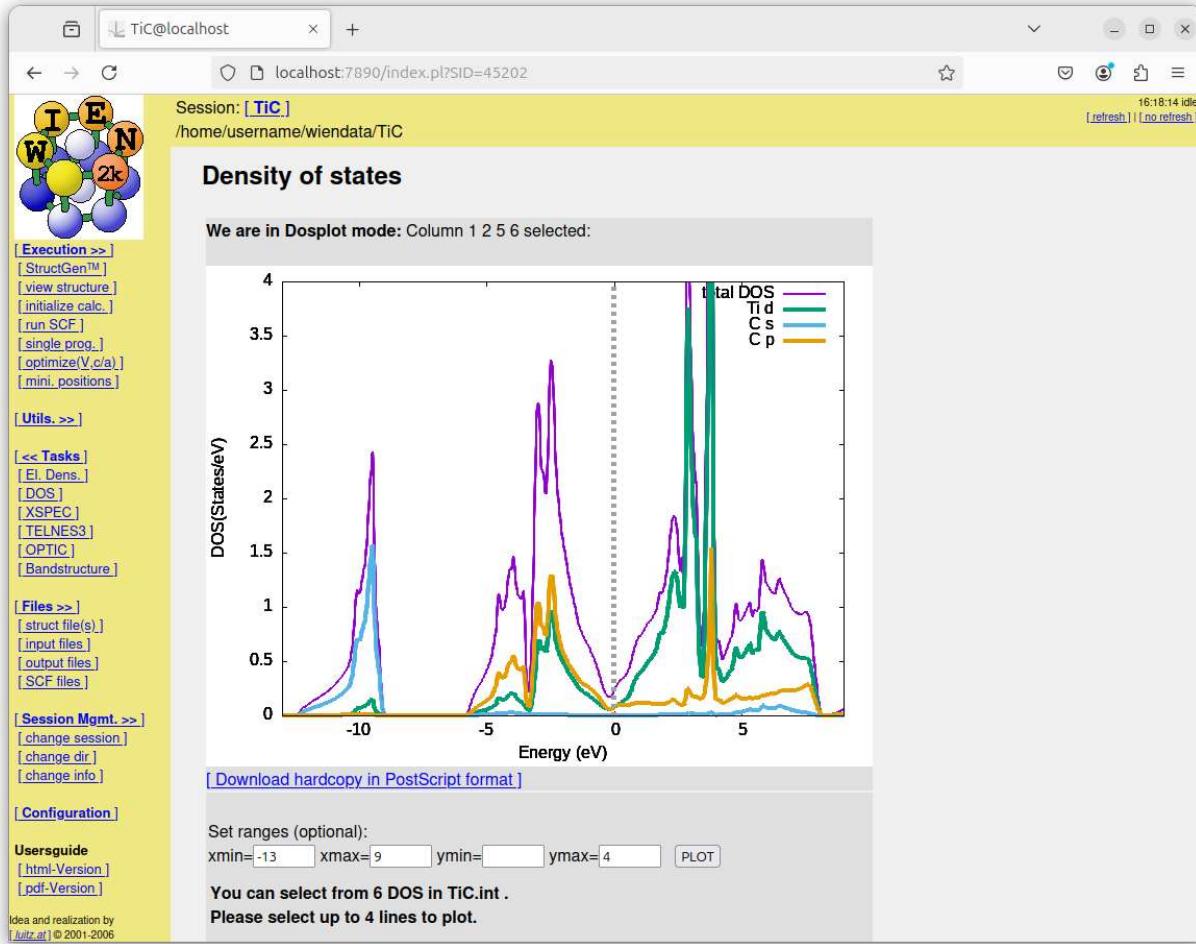
98. Click “Save and continue with DOS”  
 99. Click “x tetra”  
 100. Click “continue with DOS”:



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”:

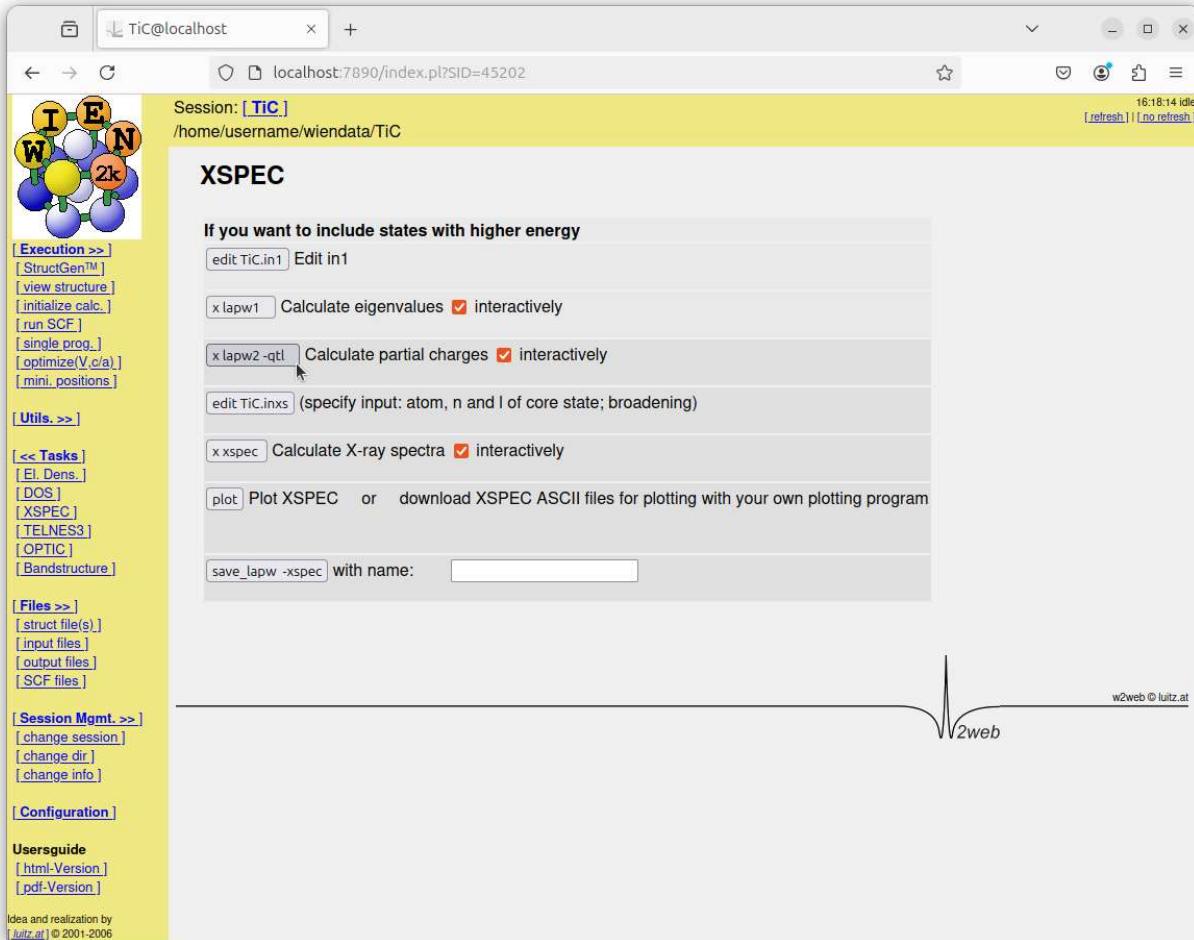


103. The resulting plot is (this is similar to Figure 3.10 in the usersguide):

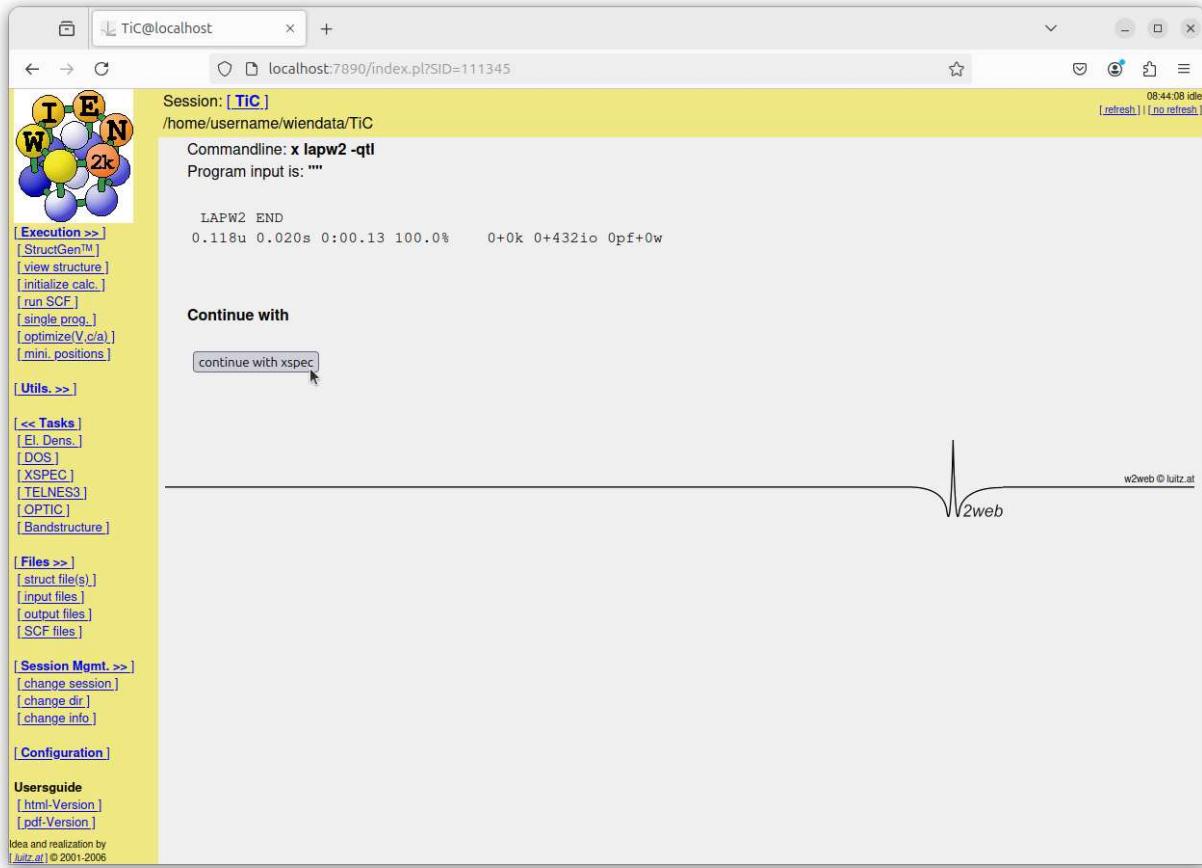


## Plot x-ray spectra

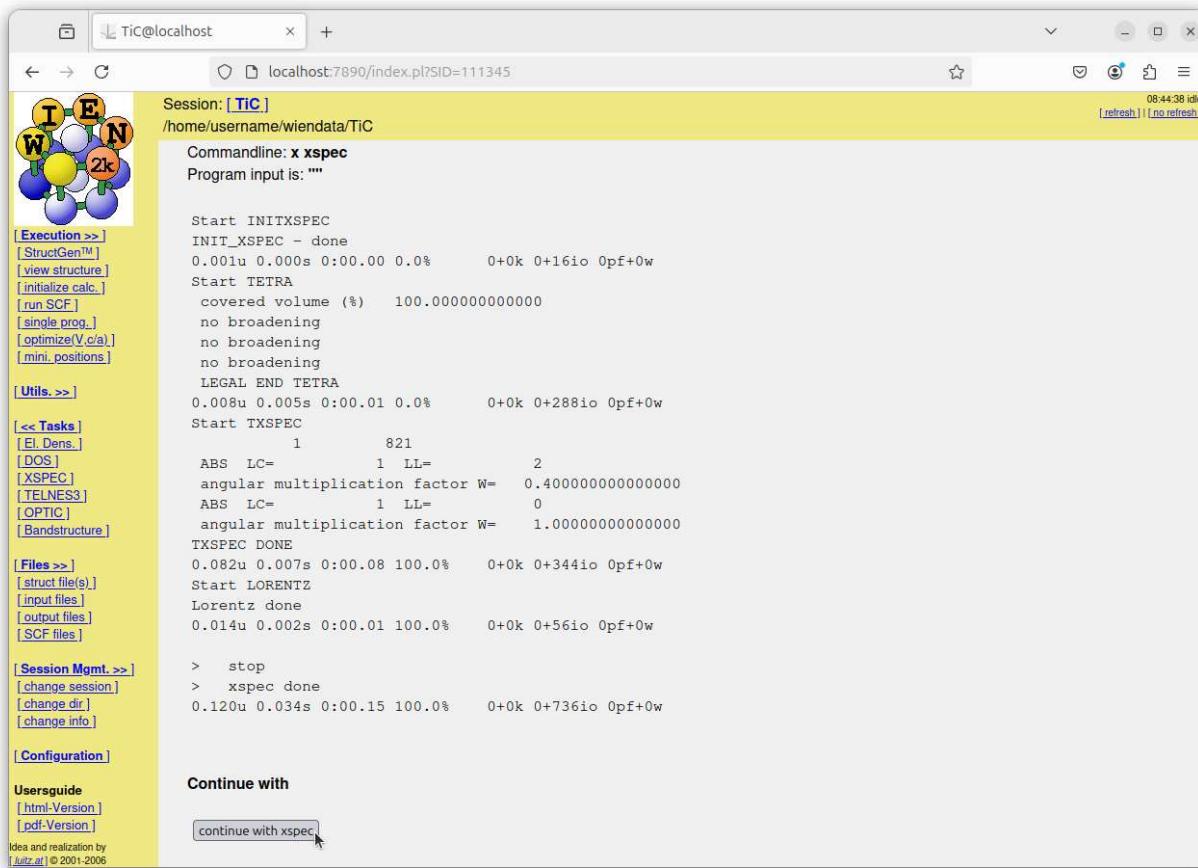
104. In the left menu, click on “XSPEC” under “Tasks”
105. Click “x lapw2 -qtl”:



106. Click “continue with xspec”:

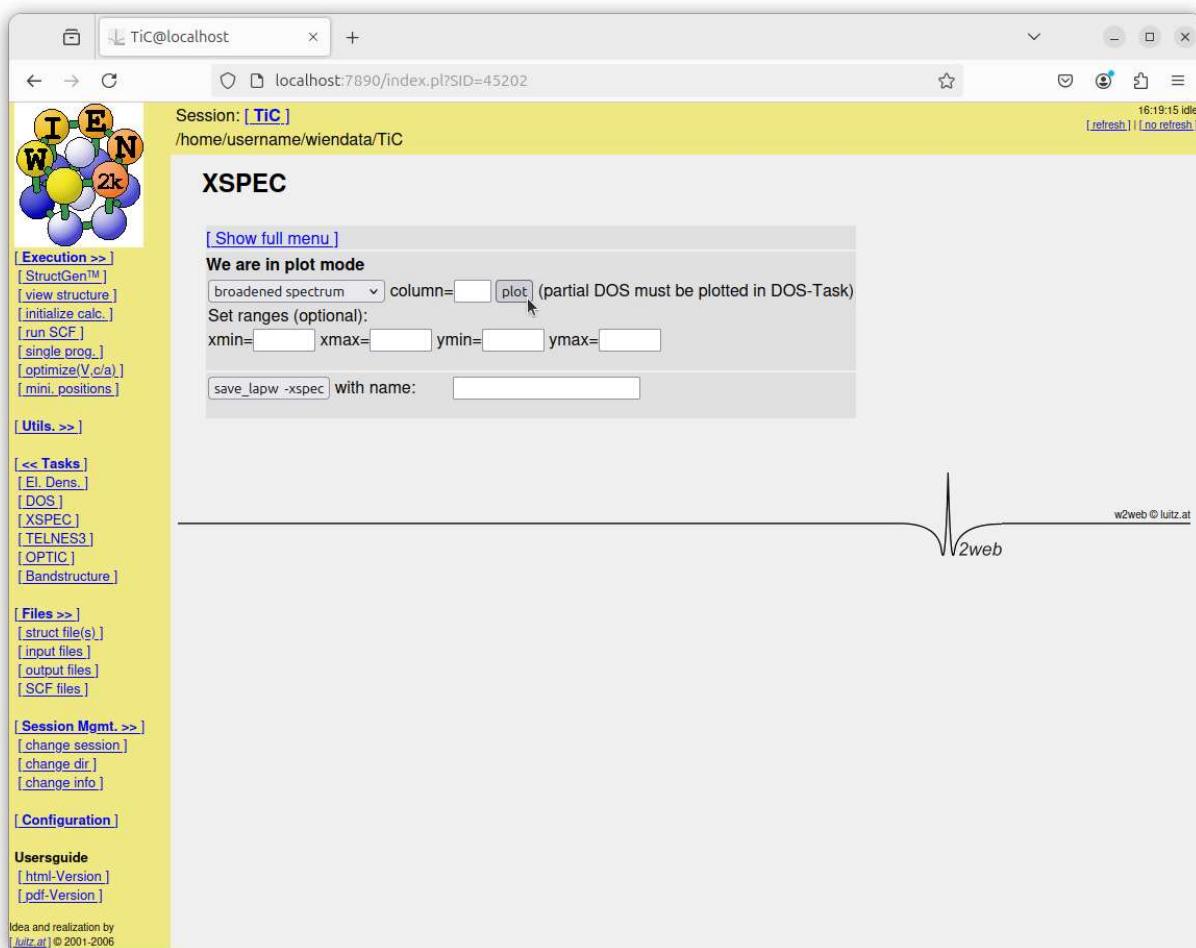


107. Click “x xspec”  
 108. Click “continue with xspec”:

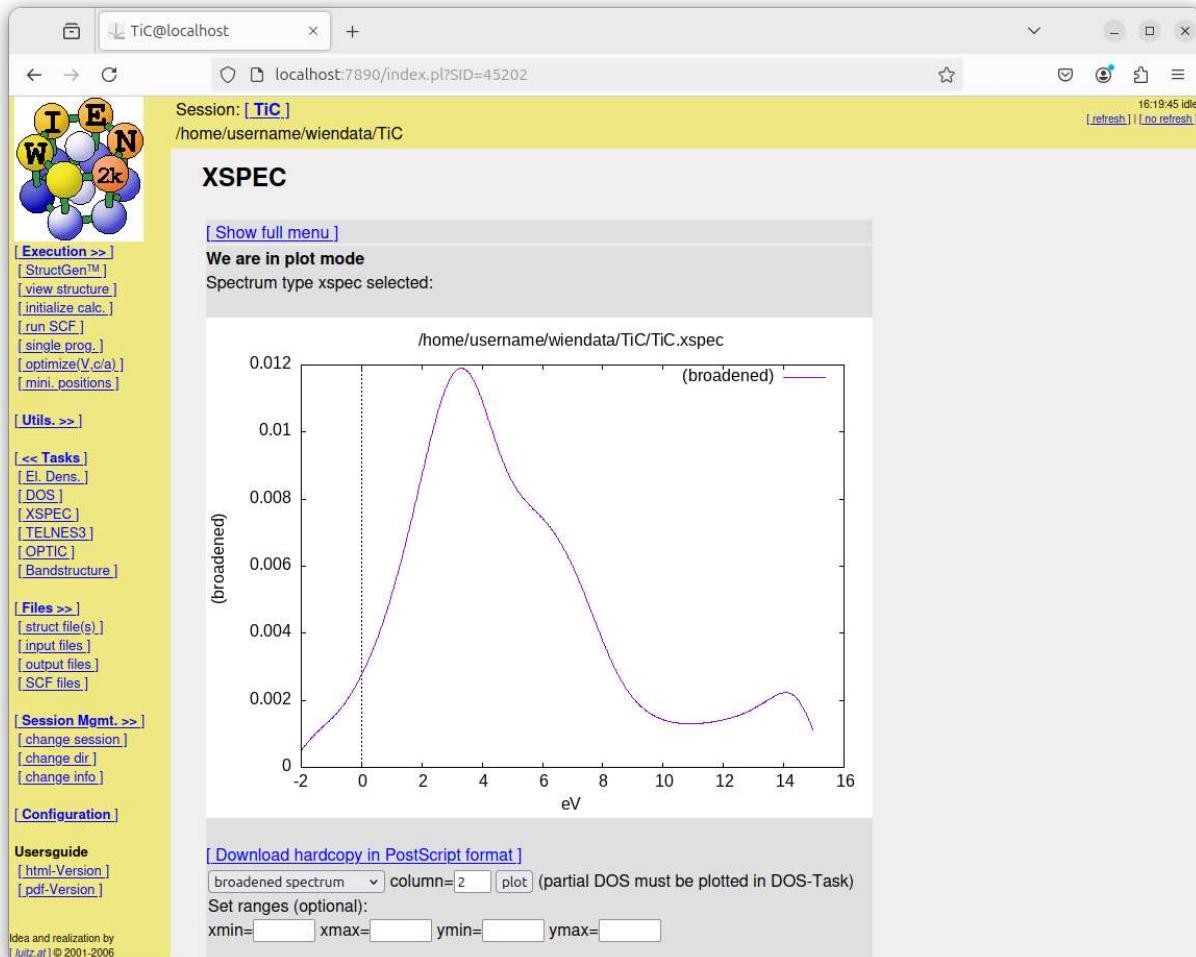


109. Click "plot"

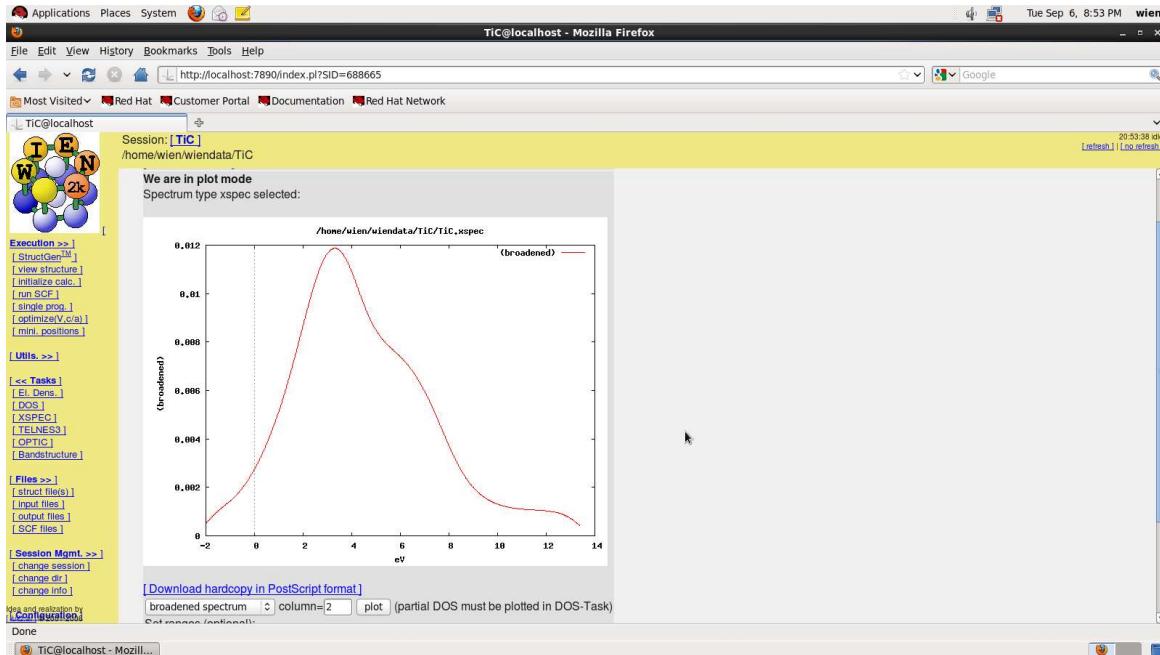
110. Click "plot":



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 the w2web interface for a session named "TiC@localhost". The main area is titled "Band structure". It displays a 3D Brillouin zone diagram with points labeled I, E, N, W, and 2k. Below the diagram, there is a sidebar with various task buttons.

**Task Buttons (Sidebar):**

- [Execution >>]
  - [StructGen™]
  - [view structure]
  - [initialize calc.]
  - [run SCF]
  - [single prog.]
  - [optimize(VCA)]
  - [mini. positions]
- [Utils. >>]
  - [<< Tasks]
  - [El. Dens.]
  - [DOS]
  - [XSPEC]
  - [TELNES3]
  - [OPTIC]
  - [Bandstructure]
- [Files >>]
  - [struct file(s)]
  - [input files]
  - [output files]
  - [SCF files]
- [Session Mgmt. >>]
  - [change session]
  - [change dir.]
  - [change info]
- [Configuration]
- Usersguide**
  - [html-Version]
  - [pdf-Version]

**Session Information:**

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

**Band structure Options:**

The required k-mesh for bandstructure plotting can be generated by:

fcc  [Brillouinzones from Bilbao Cryst Server.]

or Generate k-mesh using XCrysden (save klist as TiC.klist\_band)

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-qt1 Calculate partial charges ("qt1"-file)  so  interactively

edit TiC.insp Insert correct EF

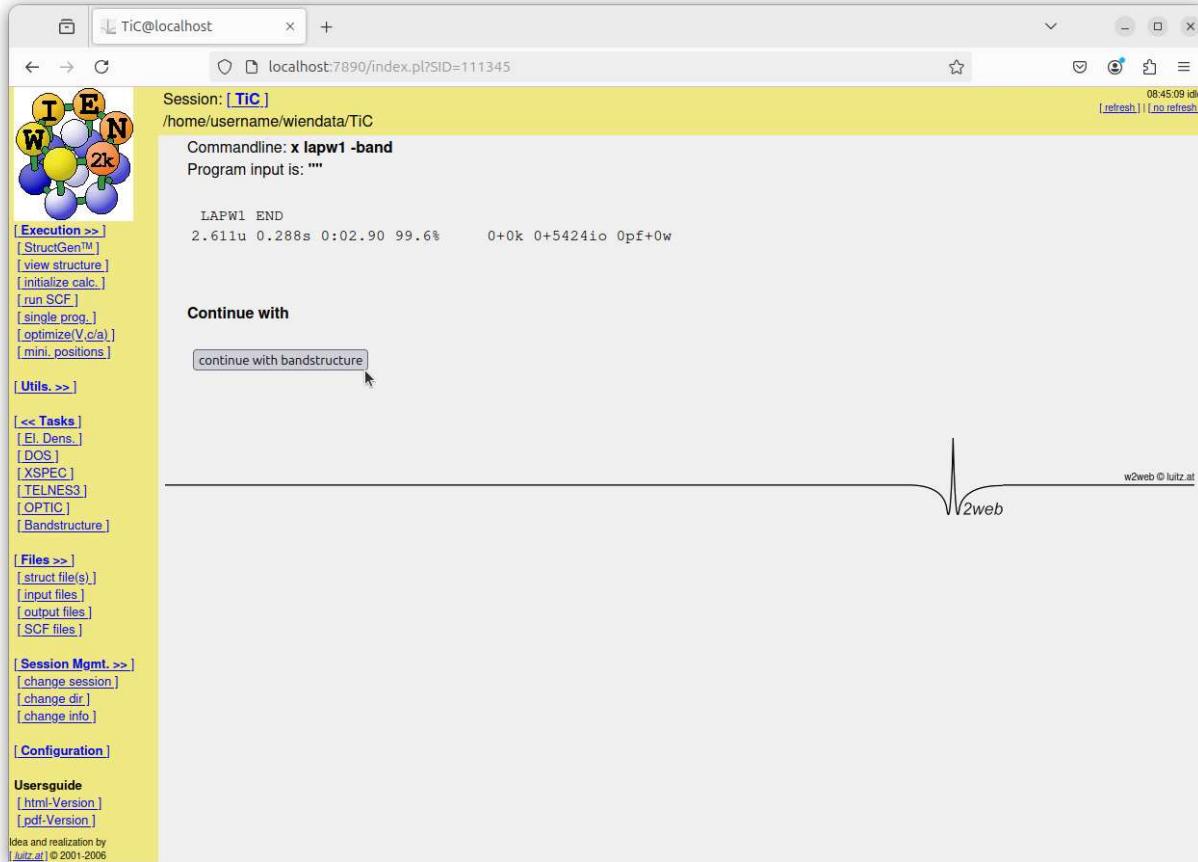
x spaghetti Calculate bandstructure  so  interactively

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

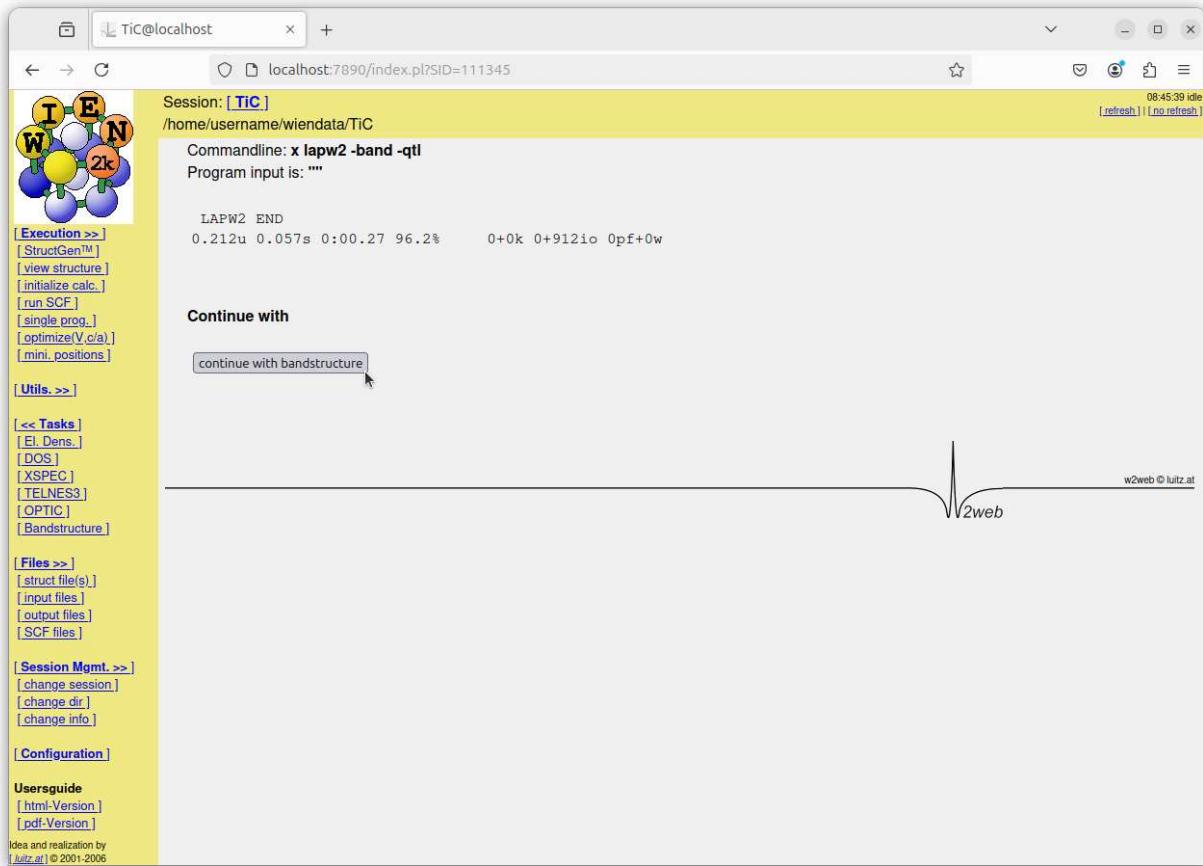
save\_lapw -band With name:

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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 0.7429563355 shown on the screen):

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

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

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.)= 0.7429563355

```

Figure configuration

```

5.0 3.0          # paper offset of plot
10.0 15.0 3.0   # xscale,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, jcol, size of heavier plotting

```

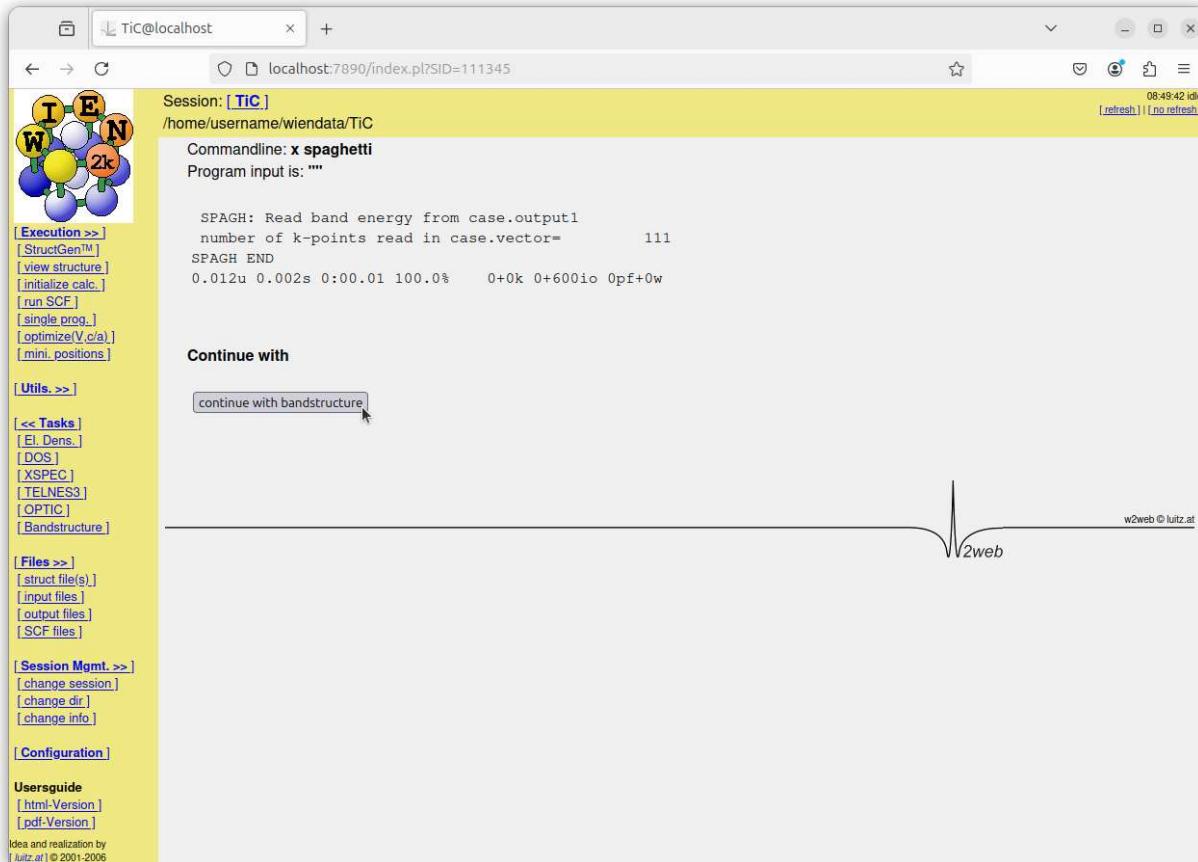
Fermi switch:

- 0...no line
- 1...solid line
- 2...dashed line
- 3...dotted line

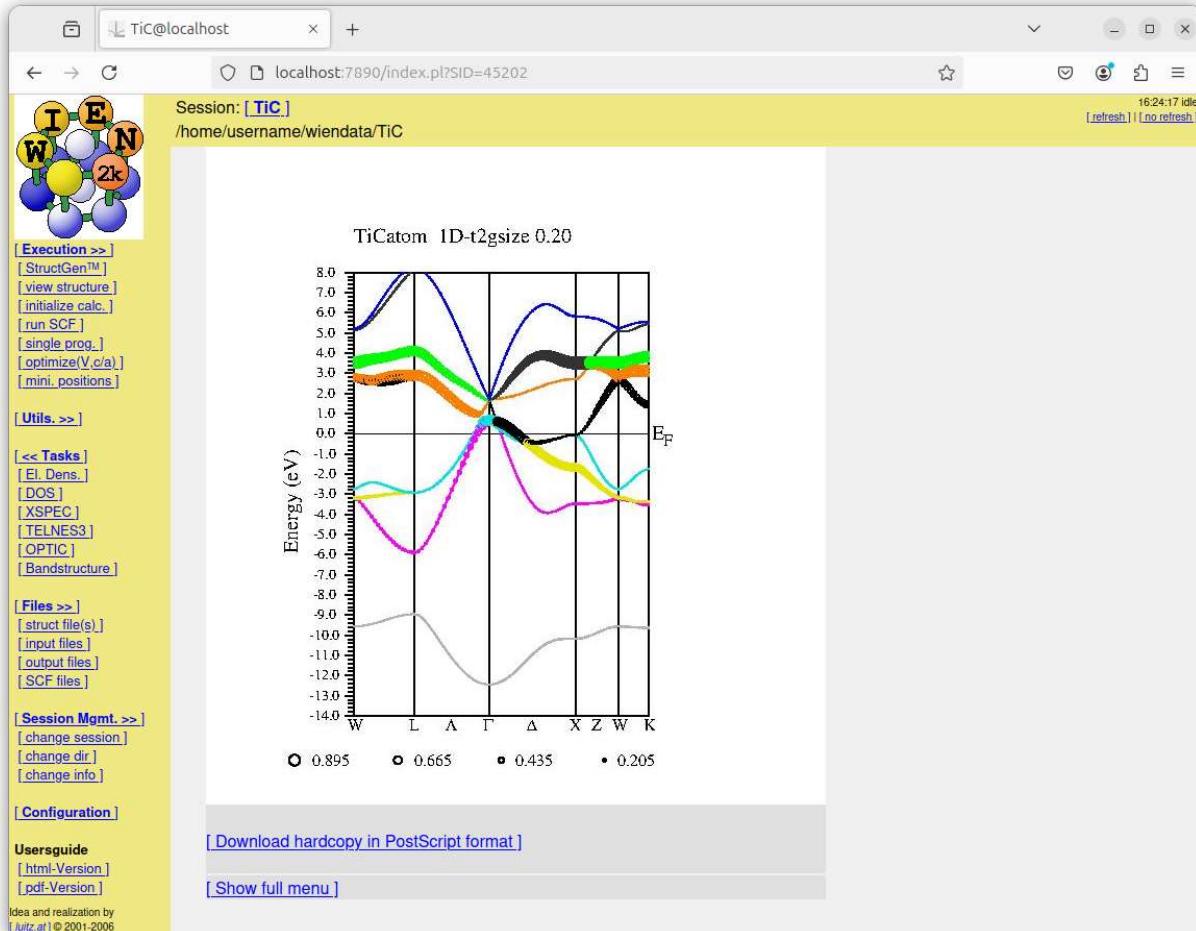
Line switch:

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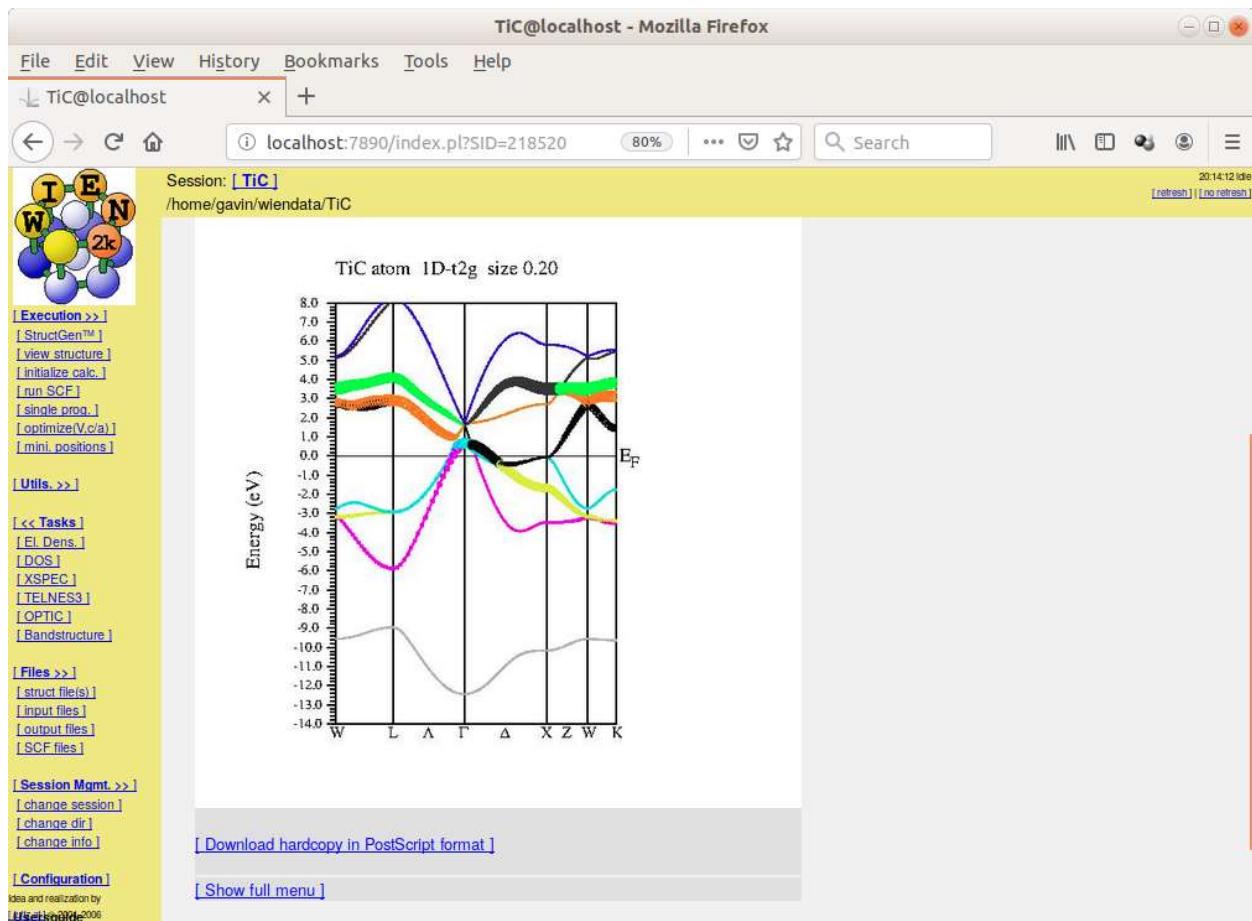
119. Click “Save and continue with bandstructure”
120. Click “x spaghetti”
121. Click “continue with bandstructure”:



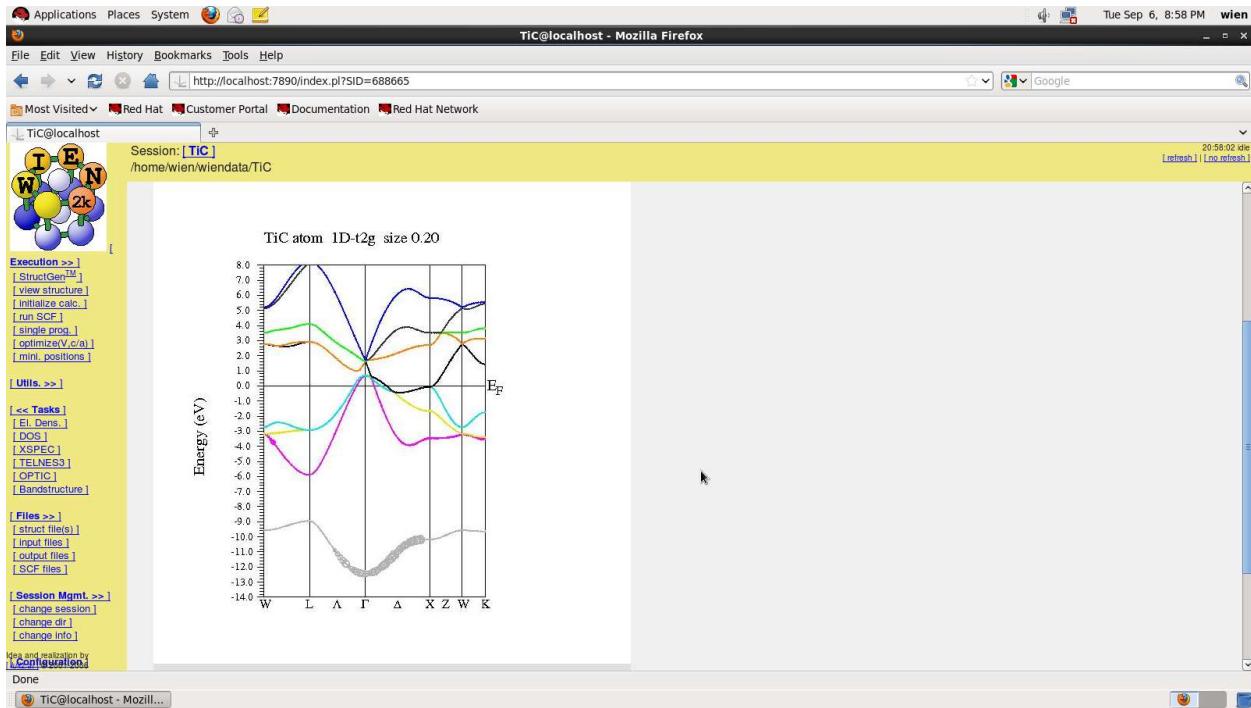
122. Click “plot bandstructure”, the creates the following plot (version 24.1-23.2):



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:

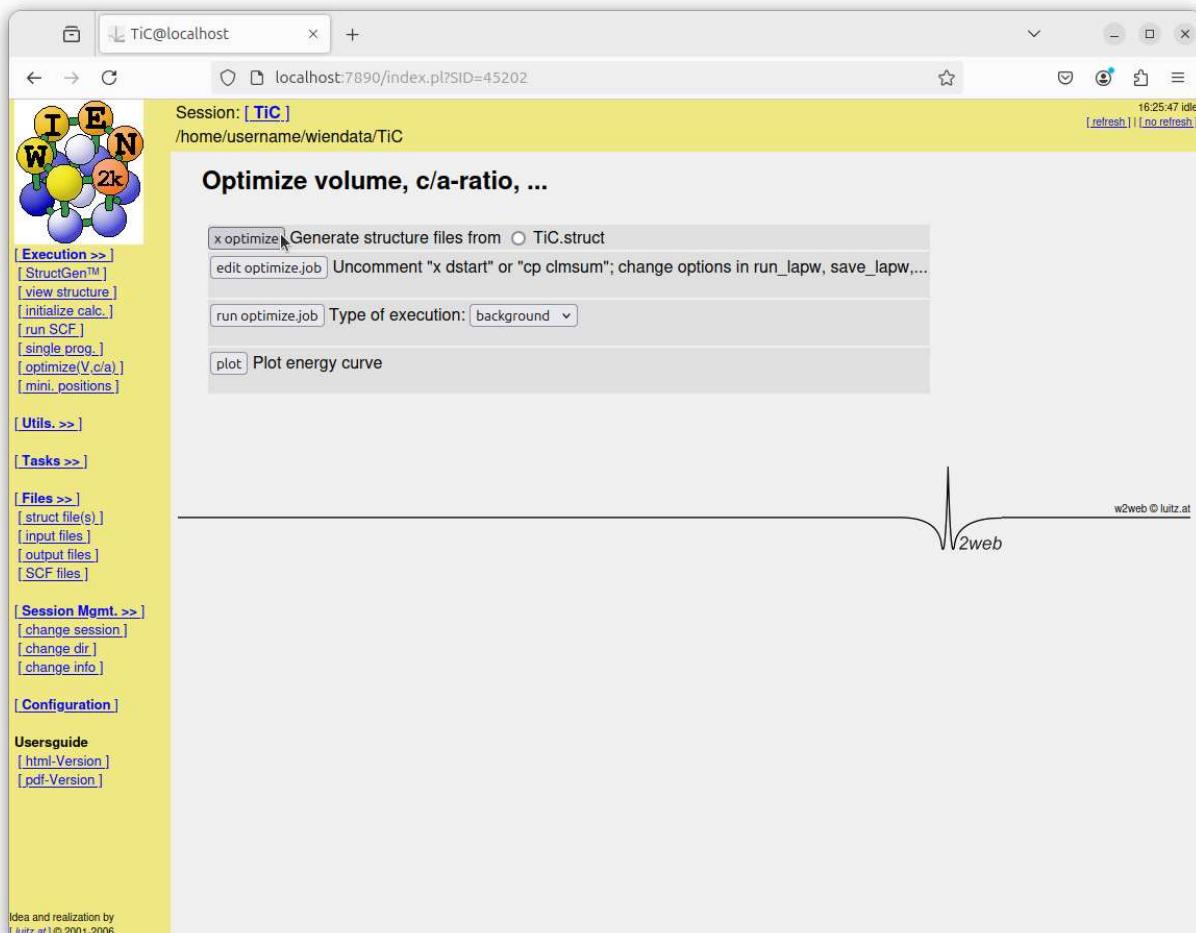


## Plot volume optimization

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

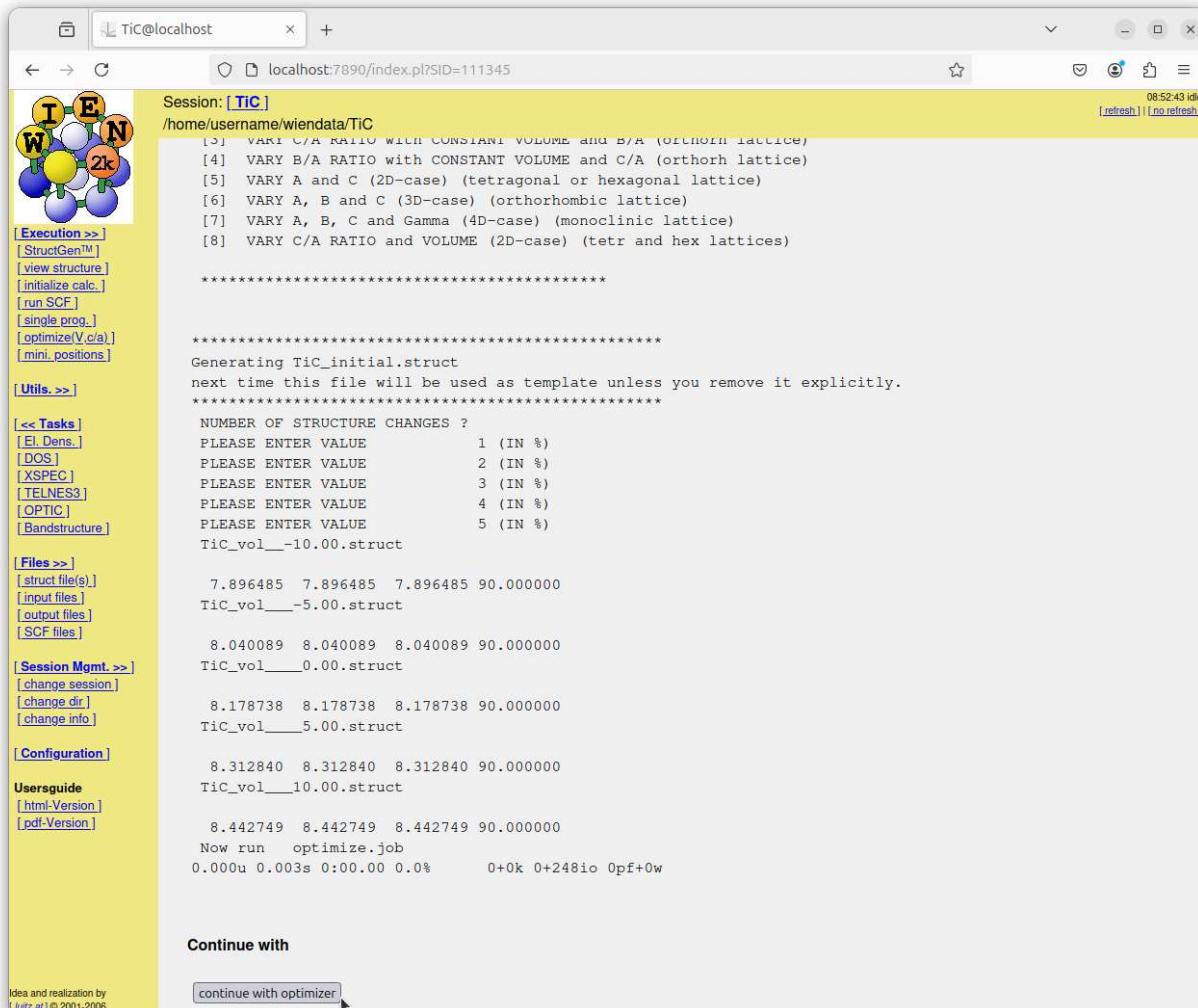
For option 6: specify number of structures: 10, 27 (3x3x3), 64 (4x4x4), 125 (5x5x5) 16 specify the % change: 1.0

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

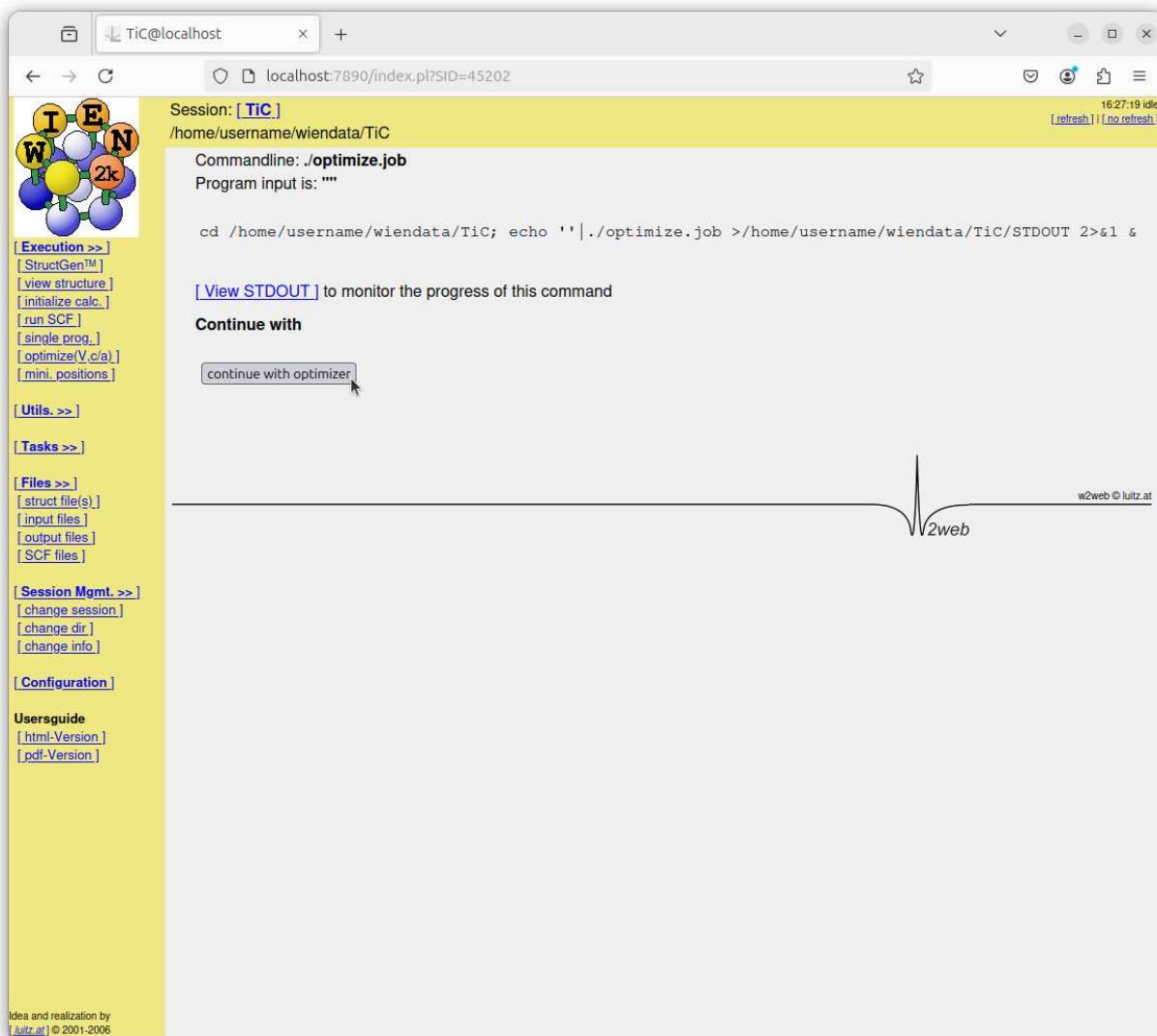
**Execute!**

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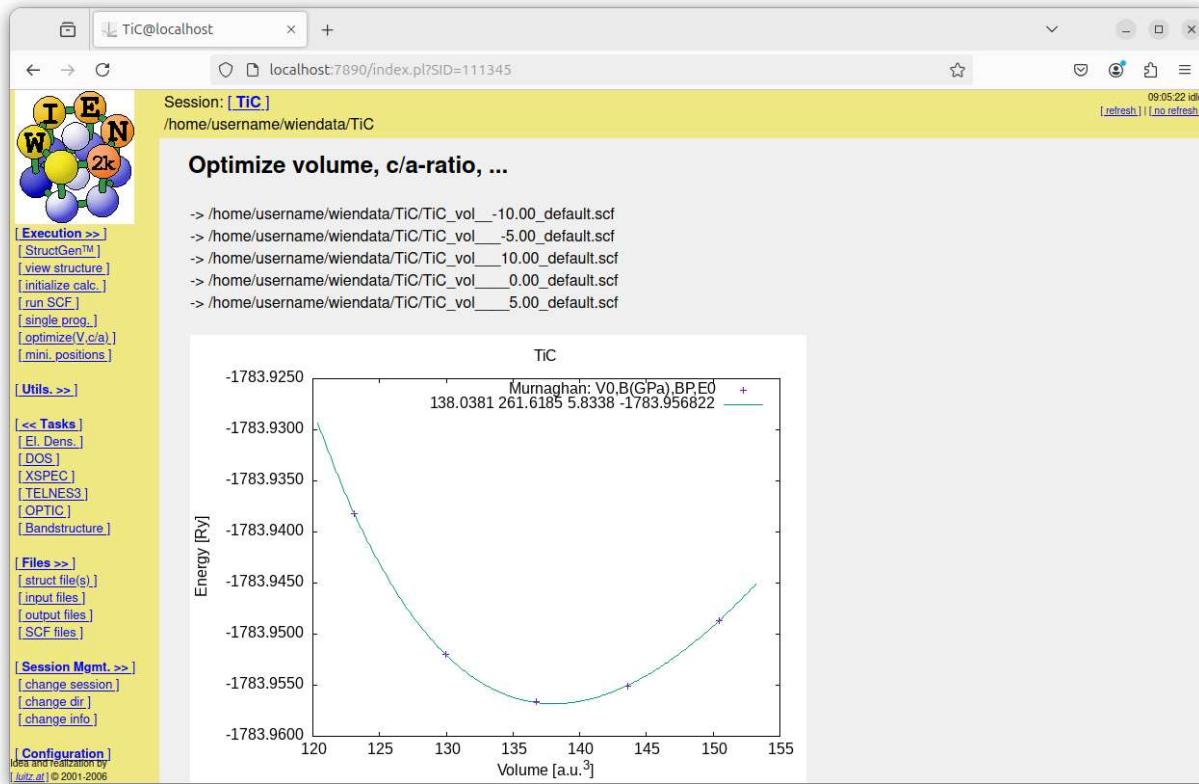
127. Click “continue with optimizer”:



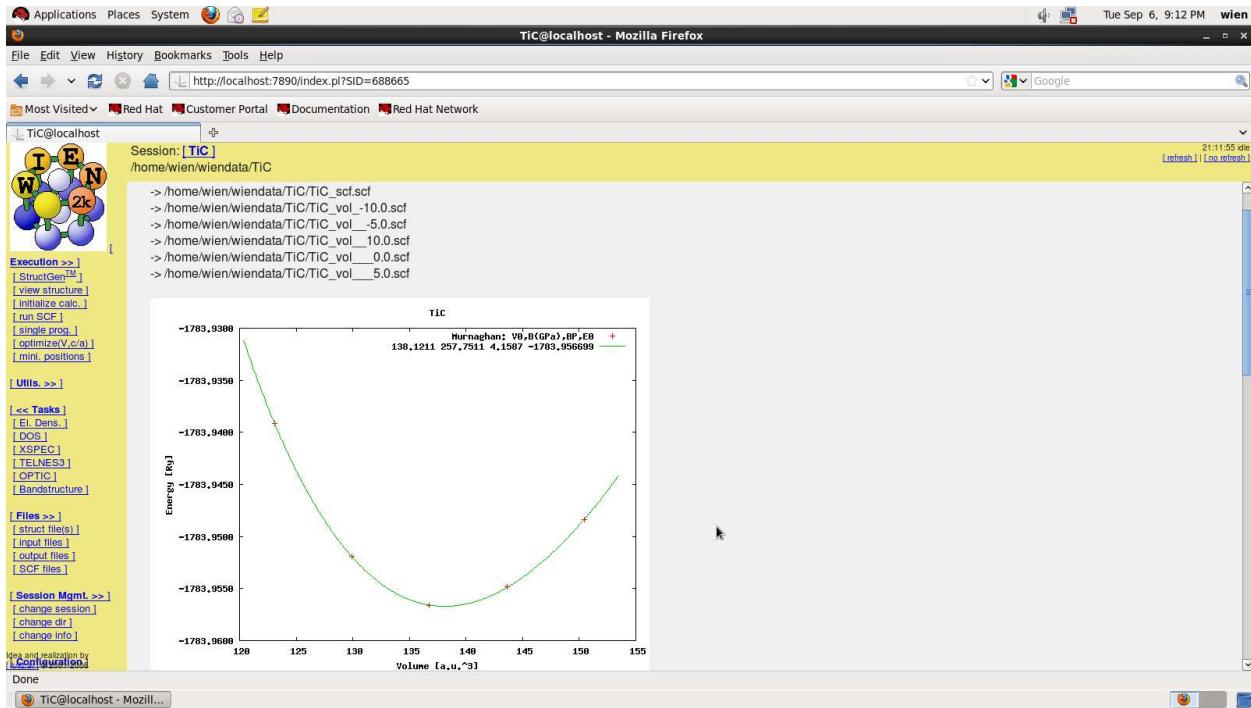
128. Click “run optimize.job”
129. Click “continue with optimizer”:



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.