

WIEN2k TiC Example

Ubuntu 20.04.3 LTS

WIEN2k_21.1 (Release 14/4/2021)

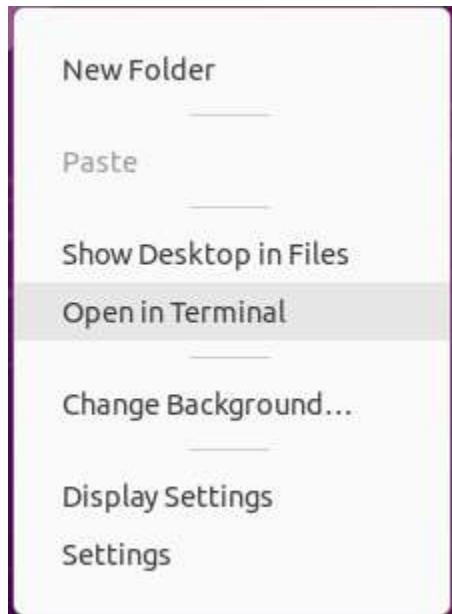
gfortran 9.3.0

WIEN2k patches [1]: Makefile.orig-lapw2.patch, Makefile.orig.patch,
analyse_phonon_lapw.patch, calLa_Pre_elast.patch, nn.patch, qdmft.patch, qtPara_lapw.patch,
x_lapw.patch

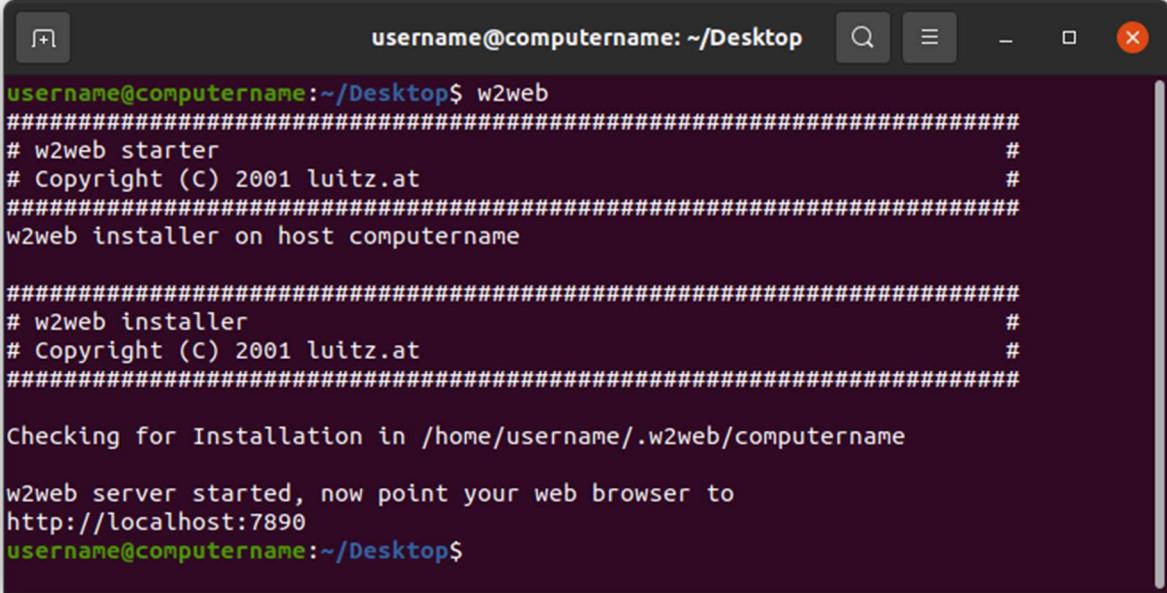
[1] <https://github.com/gsabo/WIEN2k-Patches/tree/master/21.1>

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:



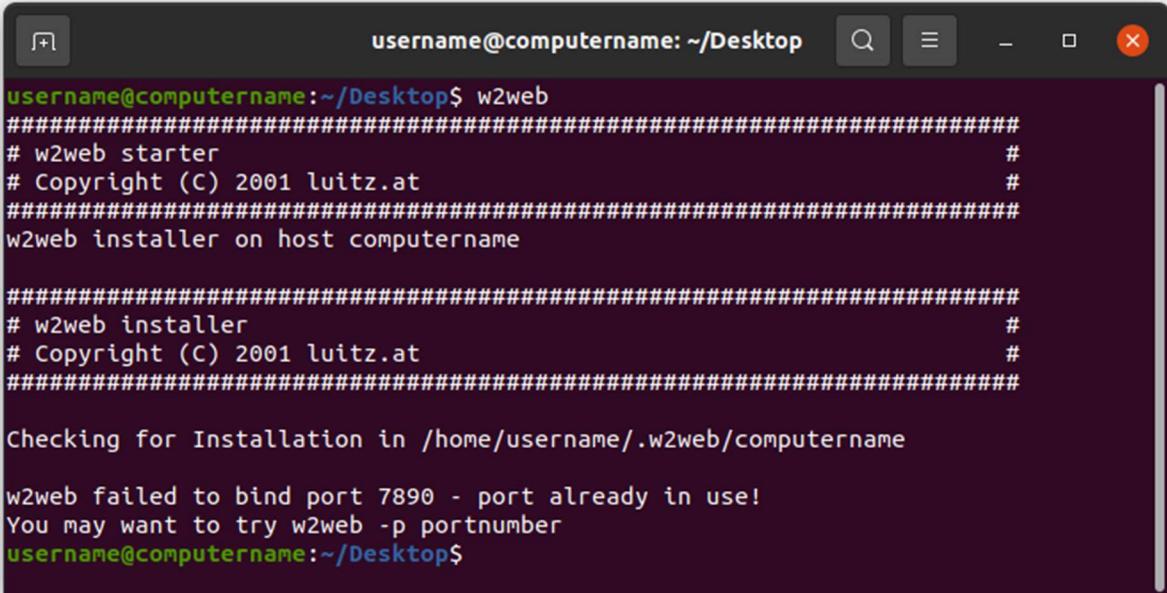
```
username@computername:~/Desktop$ w2web
#####
# w2web starter
# Copyright (C) 2001 luitz.at
#####
w2web installer on host computername

#####
# 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

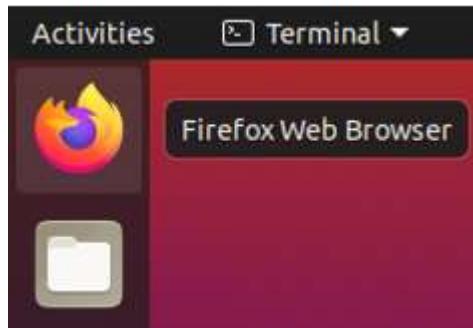
#####
# w2web installer
# Copyright (C) 2001 luitz.at
#####

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

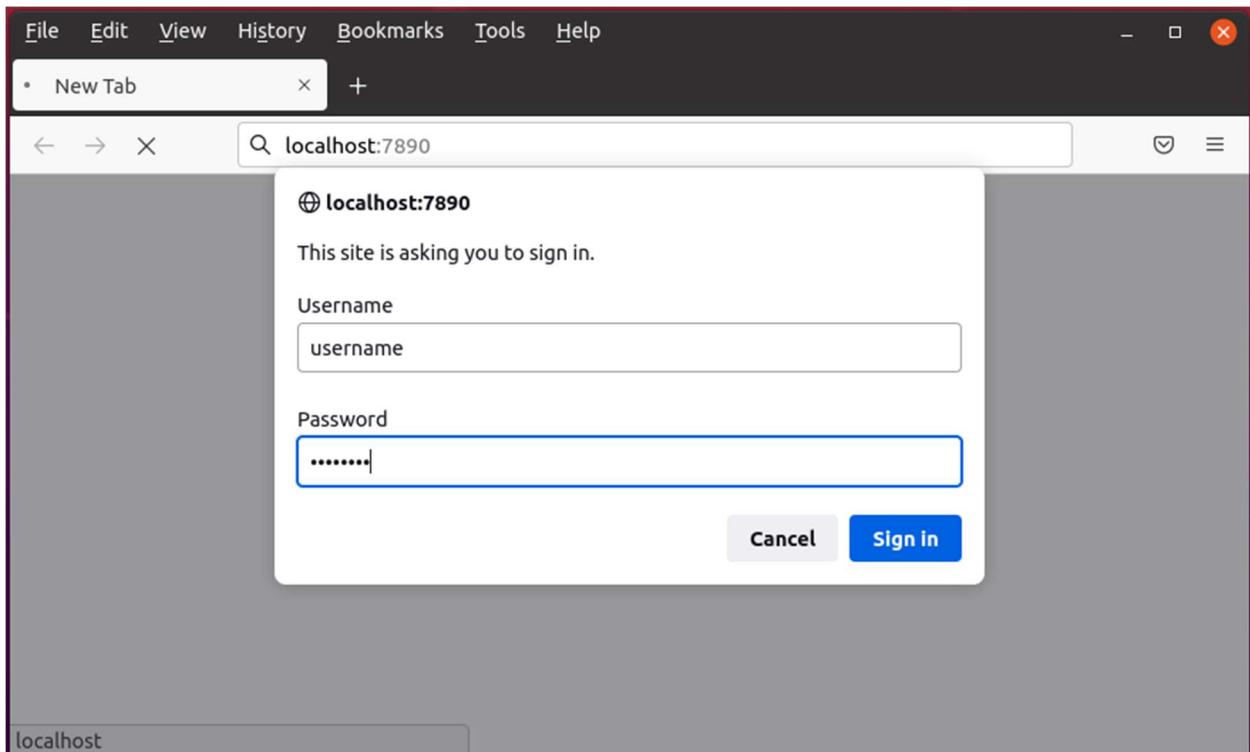
w2web failed to bind port 7890 - port already in use!
You may want to try w2web -p portnumber
username@computername:~/Desktop$
```

Open Firefox and login to w2web

3. Click on the Firefox icon to open Firefox:

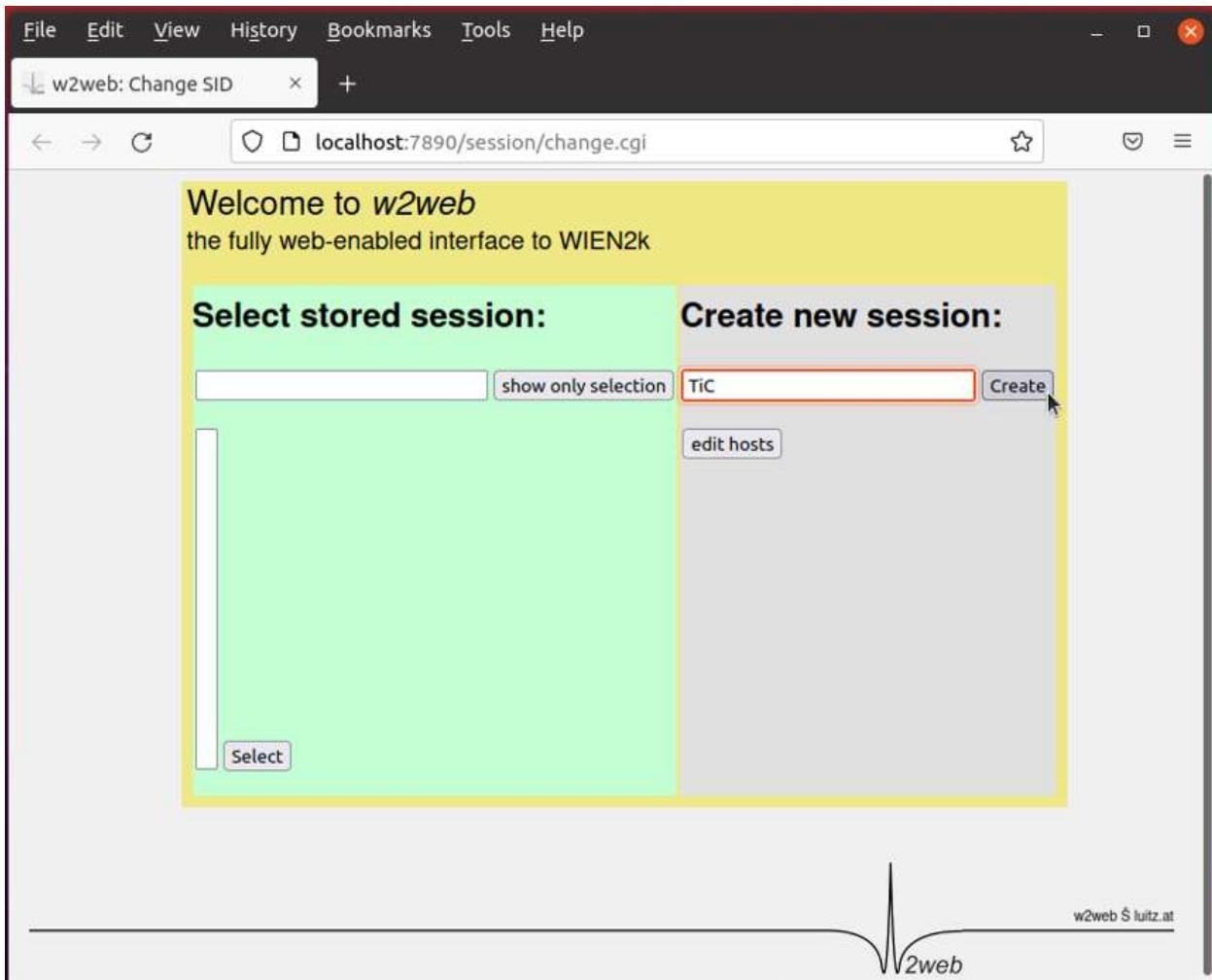


4. Enter url `http://localhost:7890`, type your w2web username and password, then click "Sign in" to login to w2web:

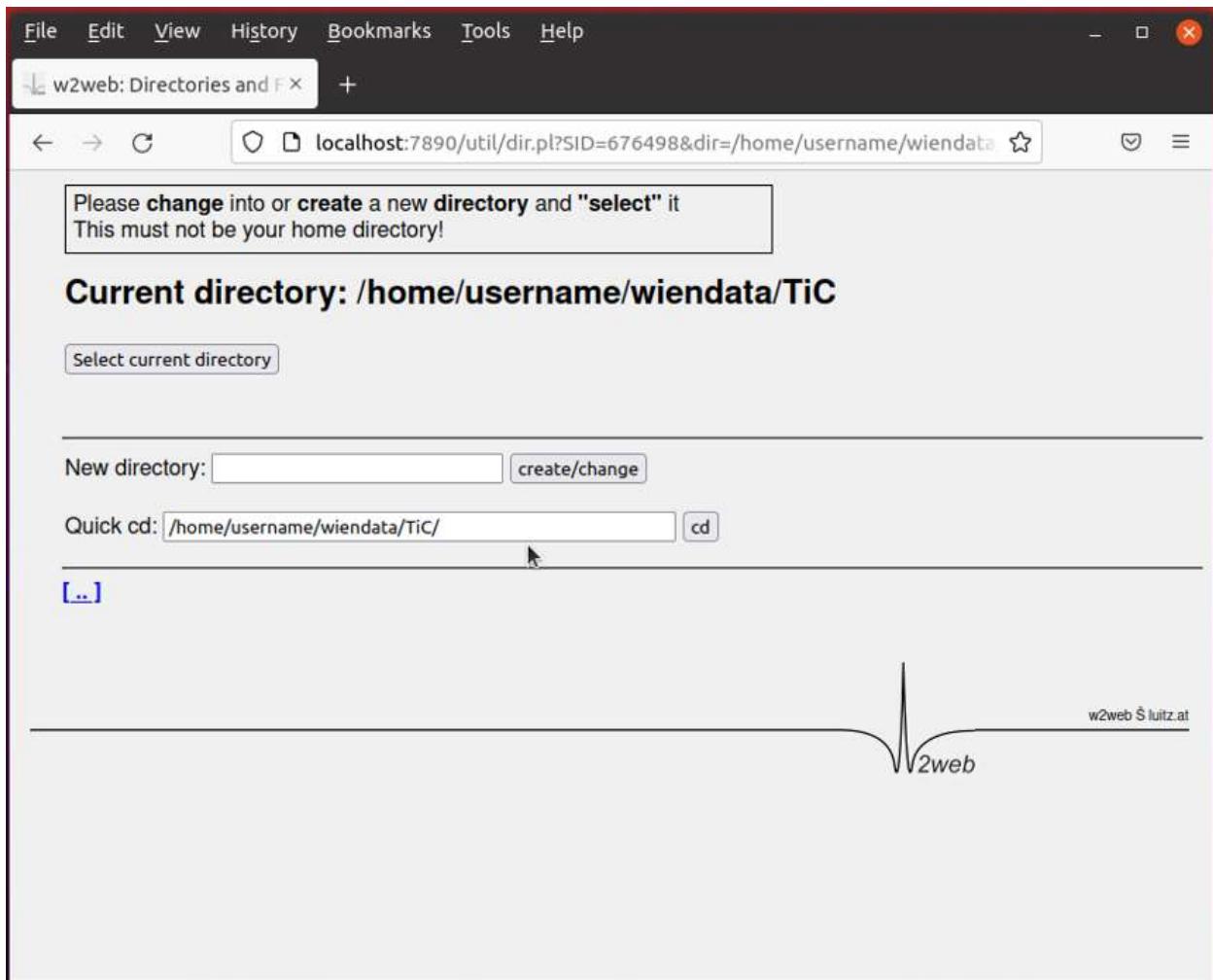


Create a new session (calculation)

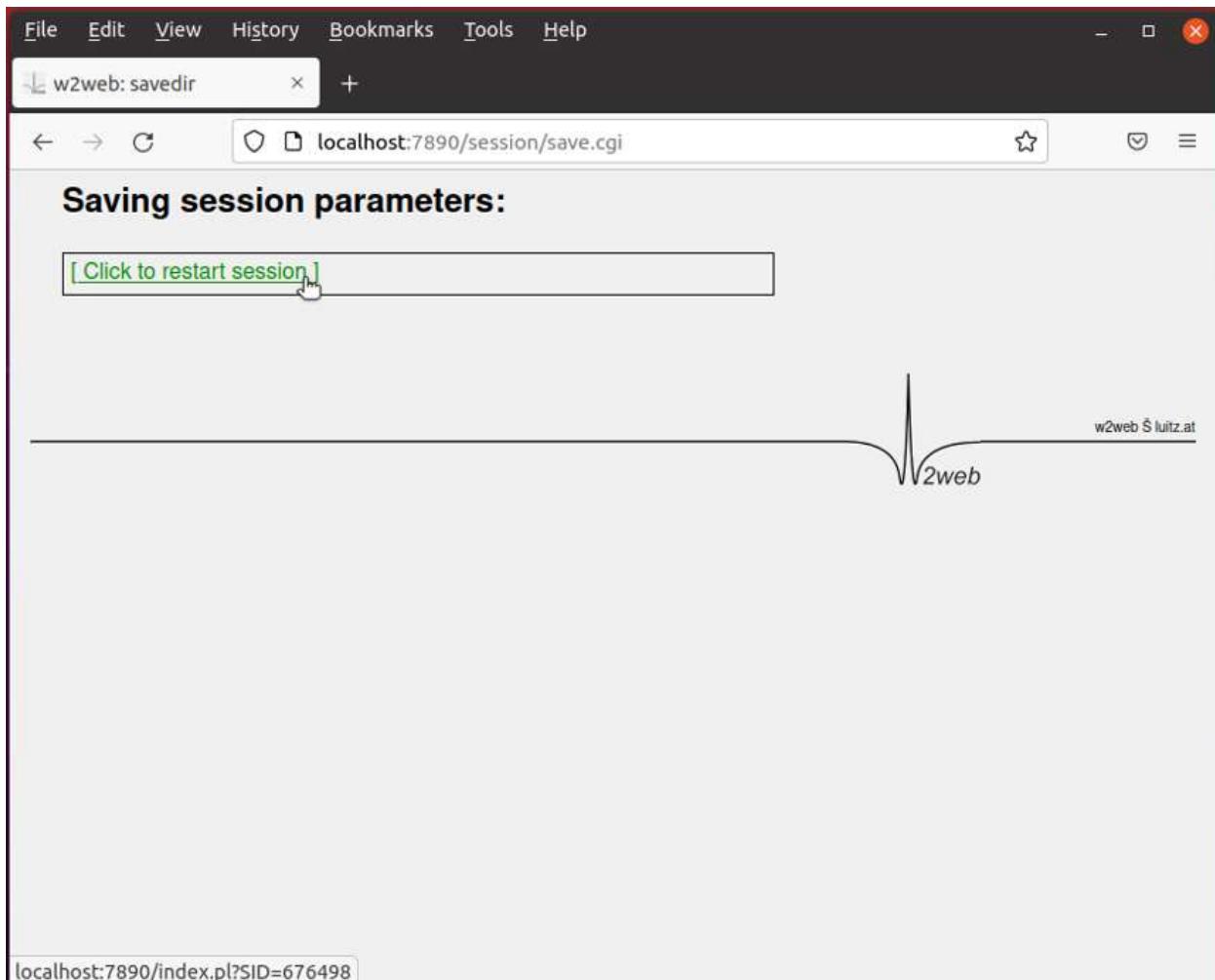
5. Enter “TiC” in the “Create new session:” box and then click the “Create” button:



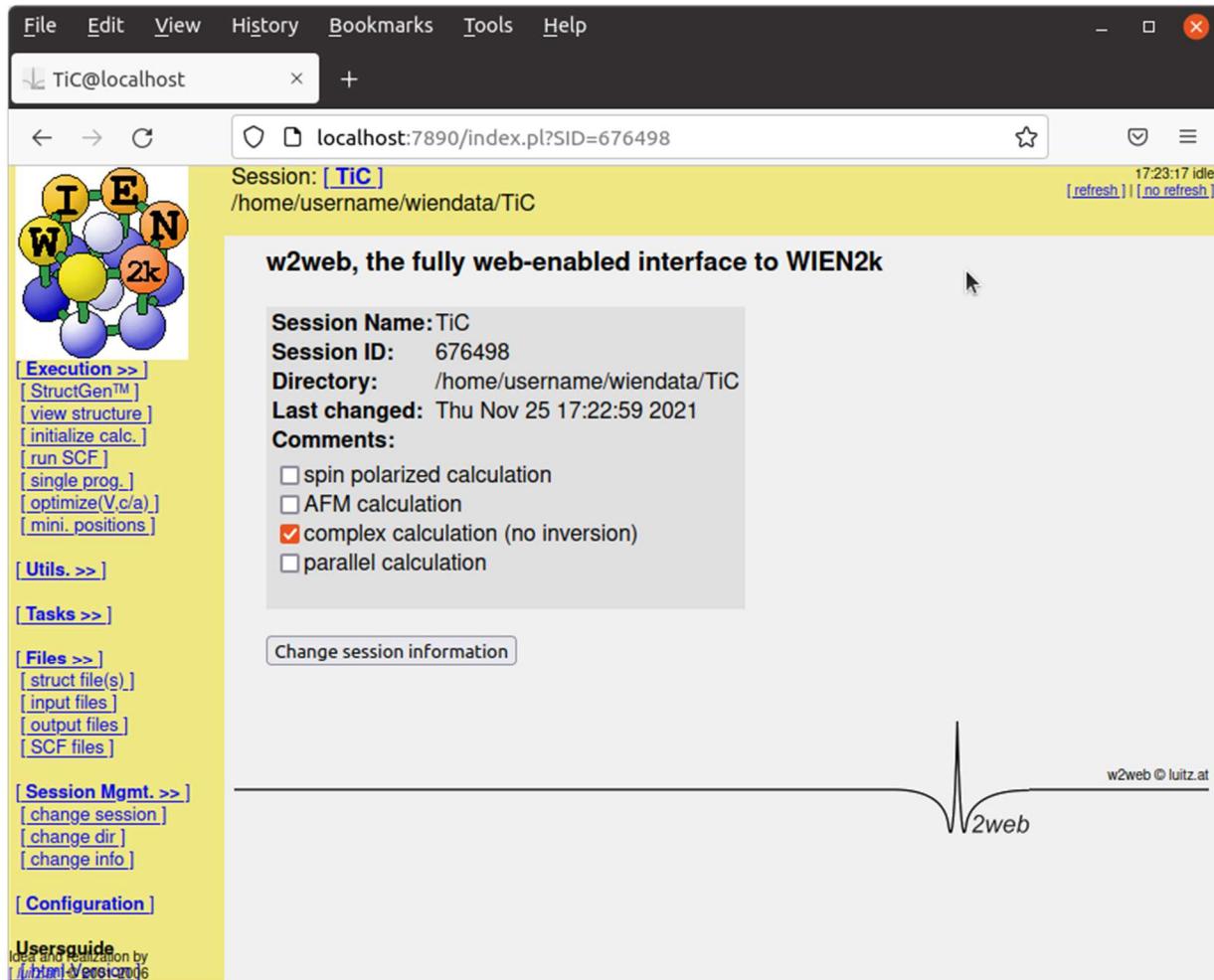
6. The “New directory” box will contain “TiC”, click the “create/change” button
7. The directory “TiC” is created and “TiC” will appear in the “Quick cd.” box:



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™ software interface. The main window title is "StructGen™". The left sidebar contains a navigation tree with sections such as Execution, Utils., Tasks, Files, Session Mgmt., Configuration, and Usersguide. The main content area displays a molecular model of TiC and a message: "You do not have a TiC.structure file yet." Below this, there is a section titled "Alternatively:" with instructions for using cif2struct and xyz2struct to convert files. A "Number of atoms:" input field is set to 2, and a "Generate template" button is visible. The status bar at the bottom indicates "17:24:18 idle".

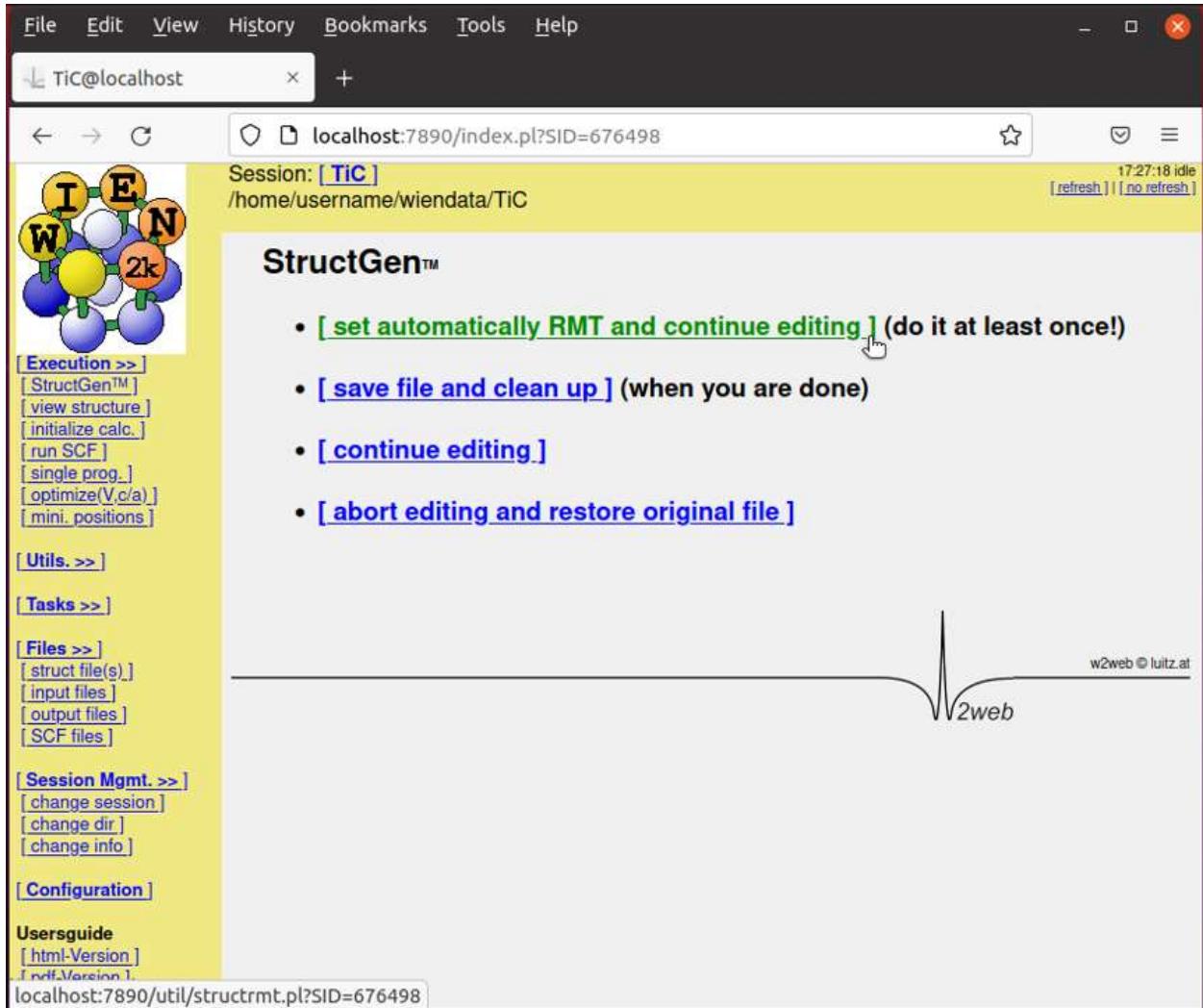
13. Type “TiC” in the “Title” box
14. Select “F” for the Lattice
15. Type 4.328 for a, b, and c for the Lattice parameters.
Note: Angstrom should be selected for the units and the angles α , β , and γ are 90 degrees by default.
16. Type “Ti” in the first box next to “Atom 1:”
Note: By default, x = 0, 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 web application interface. The left sidebar contains a navigation menu with links like Execution, Utilities, Tasks, Files, Session Management, Configuration, and Usersguide. A molecular model of TiC is displayed at the top. The main area shows a session titled 'TiC' with the path '/home/username/wiendata/TiC'. A dropdown menu for 'Lattice' is open, showing options P, F, B, CXY, CYZ, CXZ, R, H, and 1_P1. Below it, 'Spacegroups from Bilbao Cryst Server' is listed. The 'Lattice parameters in A' section shows $a=4.328$, $b=4.328$, $c=4.328$, $\alpha=90.000000$, $\beta=90.000000$, and $\gamma=90.000000$. The 'Inequivalent Atoms: 2' section lists two atoms: Atom 1 (Ti) at position $x=0.0000000$, $y=0.0000000$, $z=0.000$ with RMT=2.0000, and Atom 2 (C) at position $x=0.5$, $y=0.5$, $z=0.5$ with RMT=2.0000. Buttons for remove atom, remove, split, add position, and add an atom are available. A note at the bottom says 'You have to click "Save Structure" for changes to take effect!' and has a 'Save Structure' button.

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:

The screenshot shows a web browser window titled "TiC@localhost" at "localhost:7890/index.pl?SID=676498". The page header includes "Session: [TiC] /home/username/wiendata/TiC" and a timestamp "17:28:19 idle". The main content area is titled "Automatic determination of RMTs". It contains instructions: "Please specify the desired RMT reduction compared to almost touching spheres. Typically use:" followed by three examples: "for a single calculation: 0 %", "for force minimization: 1-5 %", and "for volume effects you may need even larger reductions.". Below this is a form with the text "Reduce RMTs by % using new or old scheme". A "do it" button is present. Further down, there's an alternative method: "Alternatively you can specify the sphere radii explicitly by element using a syntax like: Fe:2.0,C:1.77,...". It also includes a note: "Note: It is your responsibility that RMTs will not lead to overlapping spheres." and a text input field for specifying "name:radius". A watermark "w2web © luitz.at" and "2web" is visible in the bottom right corner.

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

The screenshot shows a web-based graphical user interface for a TiC session. The left sidebar contains various navigation links such as Execution, Utilities, Tasks, Files, Session Management, Configuration, and a Usersguide. The main area displays the following information:

- Title:** TiC
- Lattice:** F
- Type:** F
- Lattice parameters in A:**
 - $a = 4.328000038626$, $b = 4.328000038626$, $c = 4.328000038626$
 - $\alpha = 90.000000$, $\beta = 90.000000$, $\gamma = 90.000000$
- Inequivalent Atoms: 2**
 - Atom 1:** Ti (highlighted in green) with Z=22.000 and RMT=2.17. Position: x=0.0000000, y=0.0000000, z=0.0000000. Buttons: remove atom, remove, split, add position.
 - Atom 2:** C with Z=6.000 and RMT=1.77. Position: x=0.5000000, y=0.5000000, z=0.5000000. Buttons: remove atom, remove, split, add position.
- Number of symmetry operations:** generate
- Note:** You have to click "Save Structure" for changes to take effect!
- Buttons:** Save Structure

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:

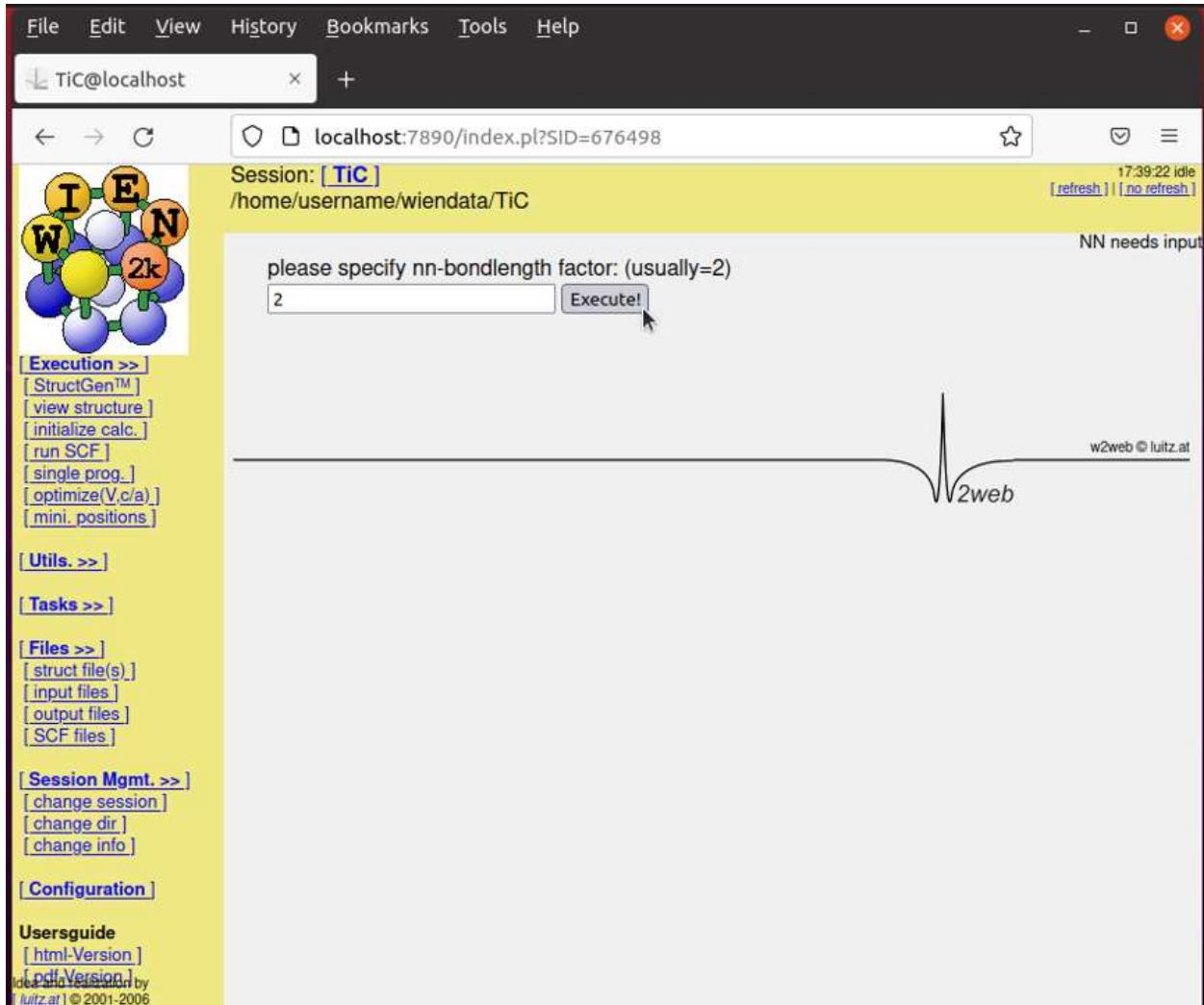
The screenshot shows a web browser window for 'TiC@localhost' at 'localhost:7890/index.pl?SID=676498'. The session title is 'TiC' and the path is '/home/username/wiendata/TiC'. The interface includes a navigation bar with File, Edit, View, History, Bookmarks, Tools, and Help. A sidebar on the left contains links for Execution, Utils, Tasks, Files, Session Mgmt., Configuration, and Usersguide. The main content area displays a crystal structure diagram with atoms labeled Ti, C, N, W, E, I, and 2k. A dropdown menu for 'Lattice' is open, showing options P, F, B, CXY, CYZ, CXZ, R, H, and 1_P1. Below the lattice dropdown are 'Lattice parameters' fields: $a = 4.328000038626$, $b = 4.328000038626$, $c = 4.328000038626$, $\alpha = 90.000000$, $\beta = 90.000000$, and $\gamma = 90.000000$. The section 'Inequivalent Atoms: 2' lists two atoms: Atom 1 (Ti) with Z=22.000 and Atom 2 (C) with Z=6.000. Both atoms have RMT values of 2.0000 and 1.9000 respectively. The 'Number of symmetry operations: generate' button is present. A note at the bottom says '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 TiC@localhost web interface. On the left, there's a sidebar with various links like 'Execution >>', 'StructGen™', 'view structure', etc. The main area is titled 'Session: [TiC]' and shows a molecular model of TiC. Below it, there's a form with several input fields and buttons. One button, 'x nn', is highlighted with a red box. To its right, there's a tooltip with instructions: 'check TiC.in1_st set RKmax (usually 5.0-9.0). [Click here for more info.]'. Further down, there are 'No' and 'Yes' buttons, and other buttons like 'x sgrou', 'x symmetry', 'x kgen', and 'x dstart'.

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



31. Click the “initlapw” button:

The screenshot shows a web browser window titled "TiC@localhost" displaying a session named "TiC". The URL is "localhost:7890/index.pl?SID=676498". The session area shows a 3D ball-and-stick model of a TiC structure with atoms labeled T, C, N, E, W, and 2x. Below the model is a command-line interface with the following text:

```

Session: [ TiC ]
/home/username/wiendata/TiC
17:39:52 idle
[refresh] | [no refresh]

Commandline: x nn
Program input is: "2"

specify nn-bondlength factor: (usually=2) [and optionally dlimit, dstmax (about 1.d-5, 20)]
DSTMAX: 20.00000000000000
iix,iiy,iiz      5      5      5  40.893689999999992      40.893689999999992

      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
0.008u 0.004s 0:00.01 0.0%      0+0k 0+32io 0pf+0w

Continue with
  initlapw

```

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]

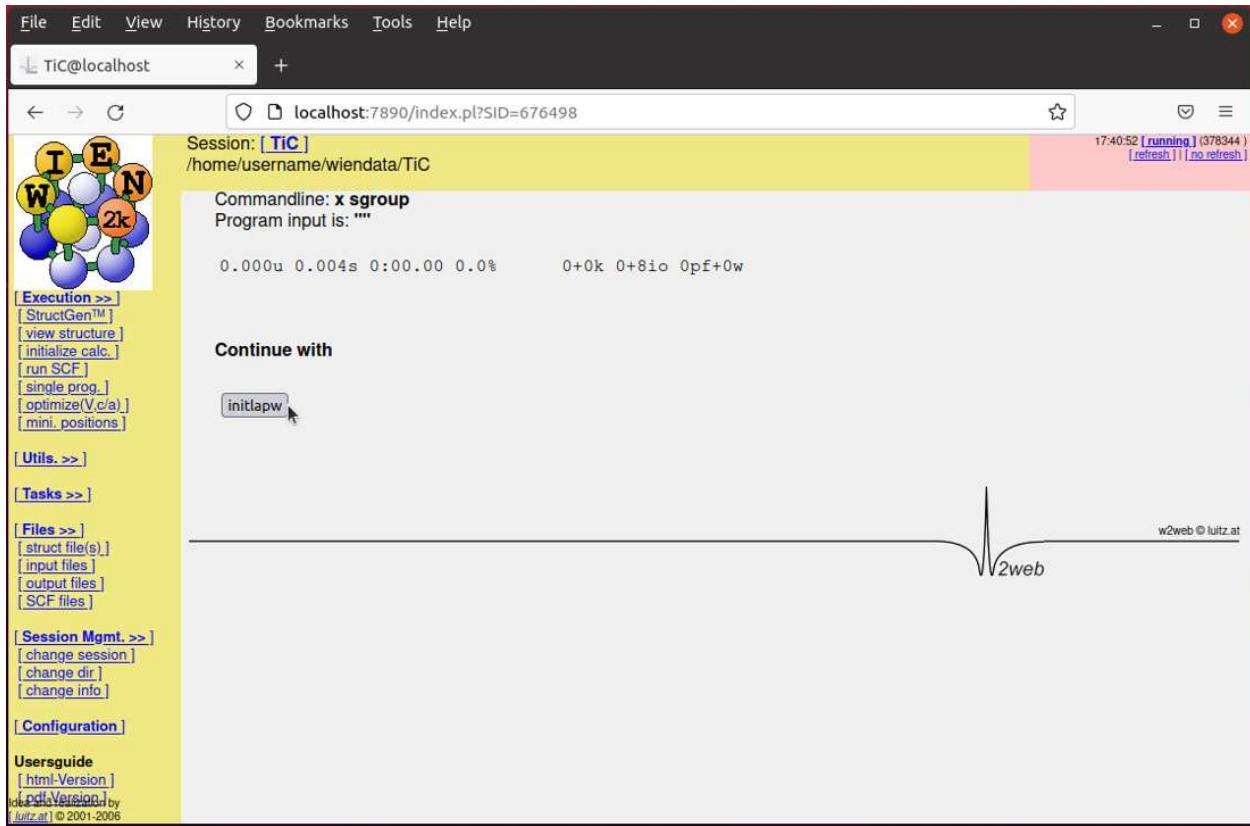
At the bottom left, it says "Icons provided by iulitz.at © 2001-2006". At the bottom right, it says "w2web © iulitz.at".

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

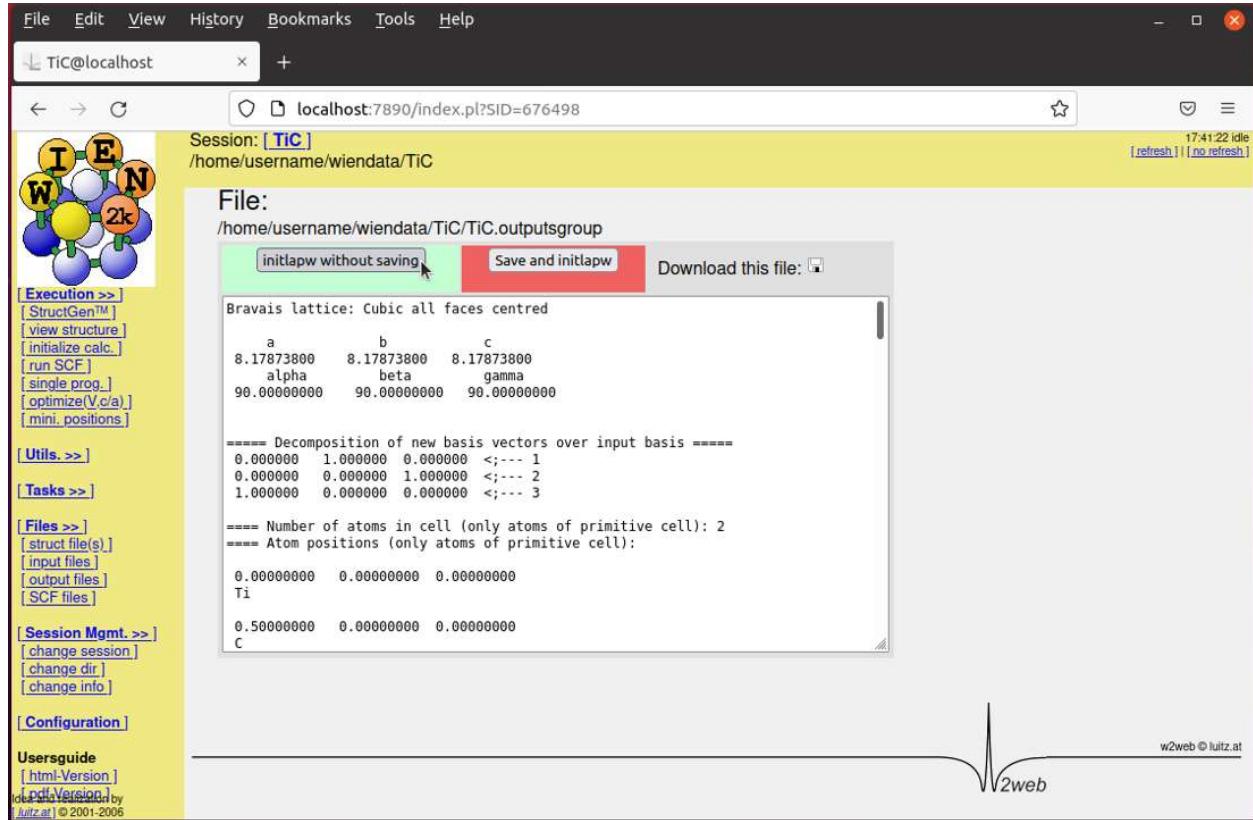
The figure shows a screenshot of the TiC@localhost web application. The top navigation bar includes File, Edit, View, History, Bookmarks, Tools, and Help. The main window displays a molecular structure with atoms labeled I, E, W, N, and 2k. Below the structure, a session summary shows "Session: [TiC]" and the path "/home/username/wiendata/TiC". A status bar at the top right indicates "17:40:22 idle" with refresh/no refresh buttons. On the left, a sidebar lists various menu items under Execution, Utilities, Tasks, Files, and Session Management. The central content area is titled "File:" and shows the output file "TiC.outputnn". It contains several tables of data, including atomic coordinates and Bravais Matrix values.

TiC					
F					
	RELA				
8.178738	8.178738	8.178738	90.000000	90.000000	90.000000
-1	0.00000000	0.00000000	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		

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 for the TiC@localhost application. The URL is `localhost:7890/index.pl?SID=676498`. The session name is **TiC**, located at `/home/username/wiendata/TiC`. The status bar indicates it's 17:41:22 idle with refresh and no refresh options.

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

Buttons in the toolbar: **initlapw without saving** (highlighted), **Save and initlapw**, and **Download this file:**

```

Bravais lattice: Cubic all faces centred

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
C
  
```

Execution >>: [StructGen™], [view structure], [initialize calc.], [run SCF], [single prog.], [optimize(Vc/a.)], [mini_positions]

Utils. >>: [Session Mgmt. >>]

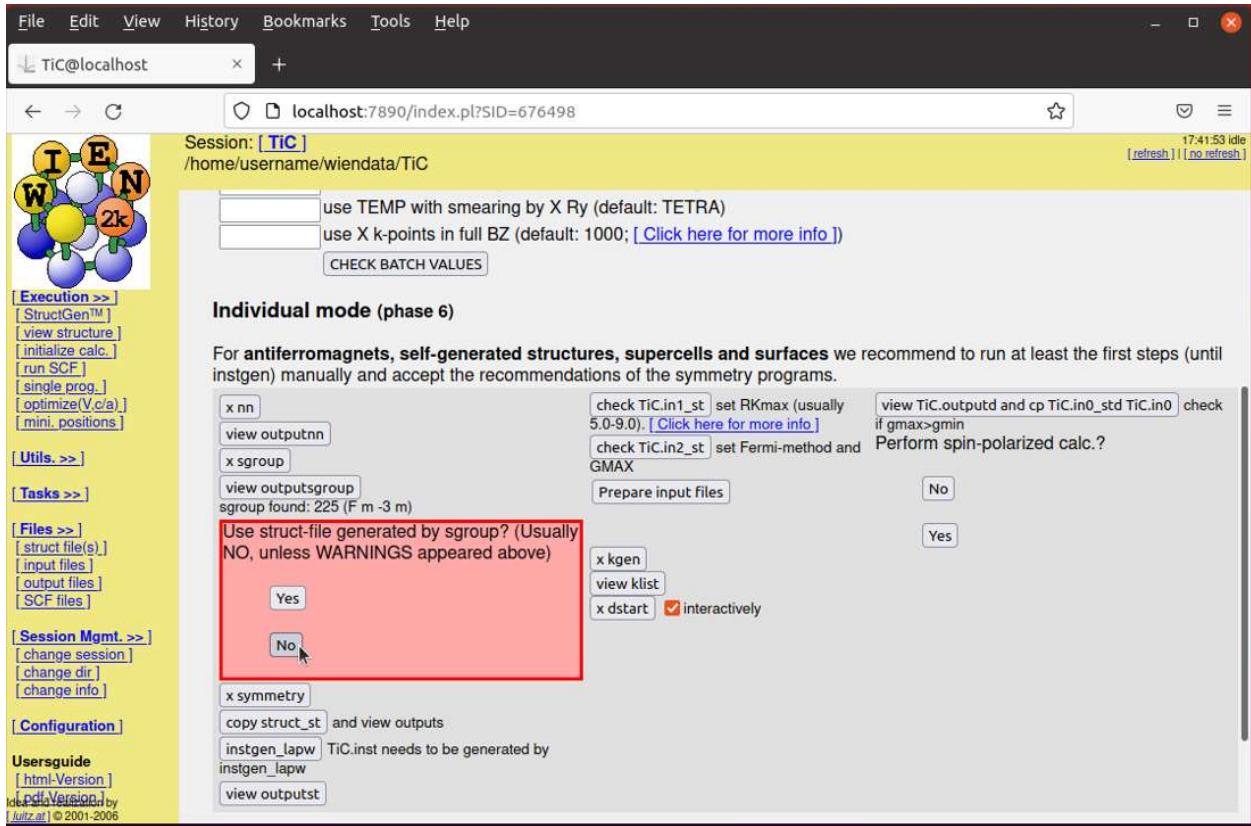
Tasks >>: [Files >>], [struct file(s)], [input files], [output files], [SCF files]

Session Mgmt. >>: [change session], [change dir.], [change info]

Configuration: [Usersguide], [html-Version], [pdf-Version], by kult.at © 2001-2006

w2web © kult.at

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

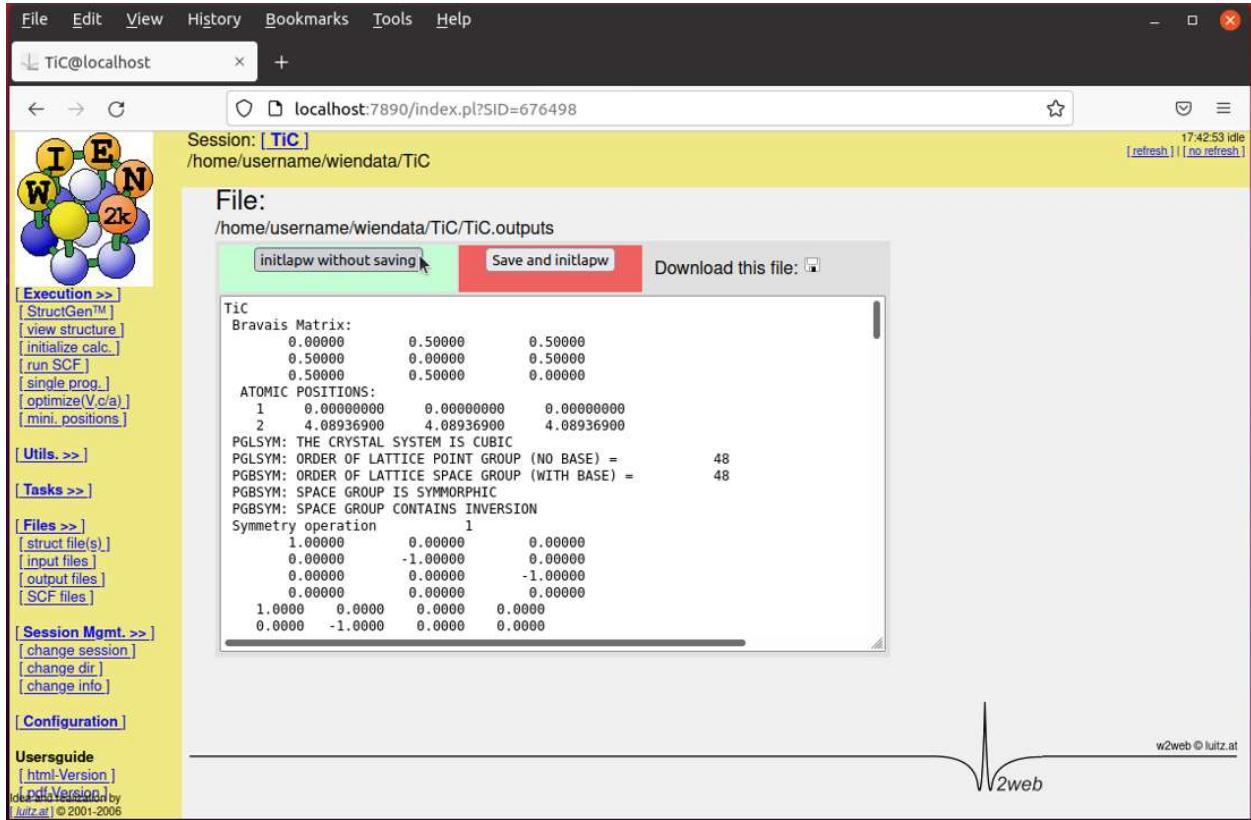


39. Click the “x symmetry” button

40. Click the “initlapw” button:

The screenshot shows a web browser window for the TiC@localhost application. The URL is `localhost:7890/index.pl?SID=676498`. The page displays a molecular structure with atoms labeled I, E, N, W, and 2k. A yellow sidebar on the left contains various navigation links such as Execution, Utils, Tasks, Files, Session Mgmt., and Configuration. The main content area shows session details: "Session: [TIC] /home/username/wiendata/TiC". It also displays commandline output: "Commandline: x symmetry" and "Program input is: ''". Below this, it shows "SPACE GROUP CONTAINS INVERSION" followed by a series of numerical values. A "Continue with" section contains a button labeled "initlapw", which is highlighted with a mouse cursor. At the bottom right, there is a small logo for "w2web © iulz.at" and the text "2web".

41. Click the “copy struct_st” button
 42. Click the “initlapw without saving” button:



The screenshot shows a web-based graphical user interface for a crystal structure analysis. On the left, there is a molecular model of a TiC unit cell with atoms labeled T, C, Ti, and N. A sidebar on the left contains various navigation links such as Execution, Utils, Tasks, Files, Session Mgmt., and Configuration. The main area displays session details for 'Session: [TiC]' at '/home/username/wiendata/TiC'. It shows the output of a calculation, including the Bravais Matrix and ATOMIC POSITIONS. At the bottom of the output window, there are three buttons: 'initlapw without saving' (highlighted with a cursor), 'Save and initlapw', and 'Download this file:'. The right side of the interface includes a status bar with '17:42:53 idle' and refresh/no-refresh buttons, and a footer with 'w2web © iuitz.at'.

```

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

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  0.00000000   0.00000000   0.00000000
  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

```

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

The screenshot shows a web browser window with the URL `localhost:7890/index.pl?SID=676498`. The title bar says "TiC@localhost". The main content area is titled "Session: [TiC] /home/username/wiendata/TiC". It displays a molecular structure of TiC with atoms labeled Ti, C, E, W, N, and 2k. On the left, there's a sidebar with various menu items like "Execution >>", "Tasks >>", "Files >>", "Session Mgmt. >>", and "Configuration". The main panel has the following text:
Specify options for instgen_lapw
Choose atomic configurations as:
 spin up (default)
 spin dn
 no spin-polarization
 selected below: chose u,d,n for each atom. (For AFM calculations you must define the proper magnetic order here !!!)
atom 1: Ti
atom 2: C
A button labeled "Execute!" is highlighted with a mouse cursor. In the top right corner, it says "17:43:23 idle" and "[refresh] | [no refresh]". In the bottom right corner, there's a small logo with the text "w2web © luitz.at" and "2web".

45. Click the “initlapw” button:

File Edit View History Bookmarks Tools Help

TiC@localhost

localhost:7890/index.pl?SID=676498

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

17:43:23 idle
[refresh] | [no refresh]

Commandline: **instgen_lapw -s -nm**
Program input is: " u u "

2 Atoms found: with labels Ti C
generate atomic configuration for atom 1 : Ti
generate atomic configuration for atom 2 : C

Continue with

initlapw

w2web © iuitz.at
2web

[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]
iuitz.at © 2001-2006

46. Click the “x lstart” button

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

File Edit View History Bookmarks Tools Help

localhost:7890/index.pl?SID=676498

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

17:43:53 idle
[refresh] | [no refresh]

LSTART needs input

Select Exchange Correlation Potential:
PBE-GGA (Perdew-Burke-Ernzerhof 96)

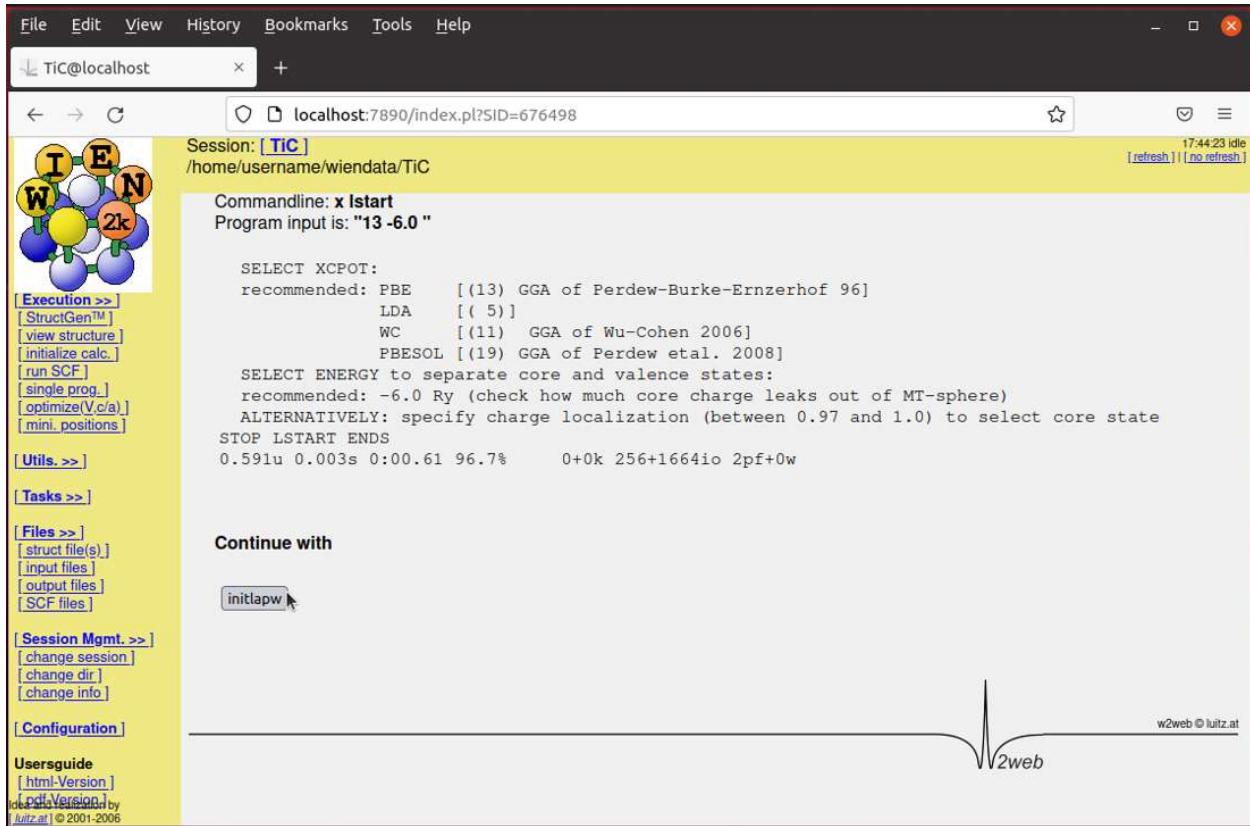
ENERGY to separate core and valence states:
ALTERNATIVELY: specify charge localization (between 0.97 and 1.0) to select core state
-6.0 (recommended: -6.0 Ry)
(check how much core charge leaks out of MT-sphere)

Execution >>
StructGen™
view structure
initialize calc.
run SCF
single prog.
optimize(V,c/a)
mini_positions

Utils. >>
Tasks >>
Files >>
Session Mgmt. >>
Configuration
Usersguide
HTML-Version
PDF-Version
by
w2web © iuitz.at

2web

48. Click the “initlapw” button:



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 URL is `localhost:7890/index.pl?SID=676498`. The page title is "Session: [TiC] /home/username/wiendata/TiC". On the left, there is a sidebar with various links for execution, tasks, files, and session management. The main content area displays a molecular structure of TiC and a session log. The session log includes the following text:

```
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         -1.210000E+02
1S          1.000         -1.210000E+02
```

At the bottom right of the log area, there is a logo for "2web".

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:

File Edit View History Bookmarks Tools Help

TiC@localhost

localhost:7890/index.pl?SID=676498

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

17:45 24 idle
[refresh] | [no refresh]

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

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

```
WEFFIL EE= 0.50000 (WEFFIL, WEPRIT, ENFIL, SUPWF)
 7.00   10   4 ELPB pxa BL 64 (R-MT*K-MAX,MAX L IN WE,V,NFT,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    37  emin / de (emax=Ef+de) / oband
```

w2web © luitz.at

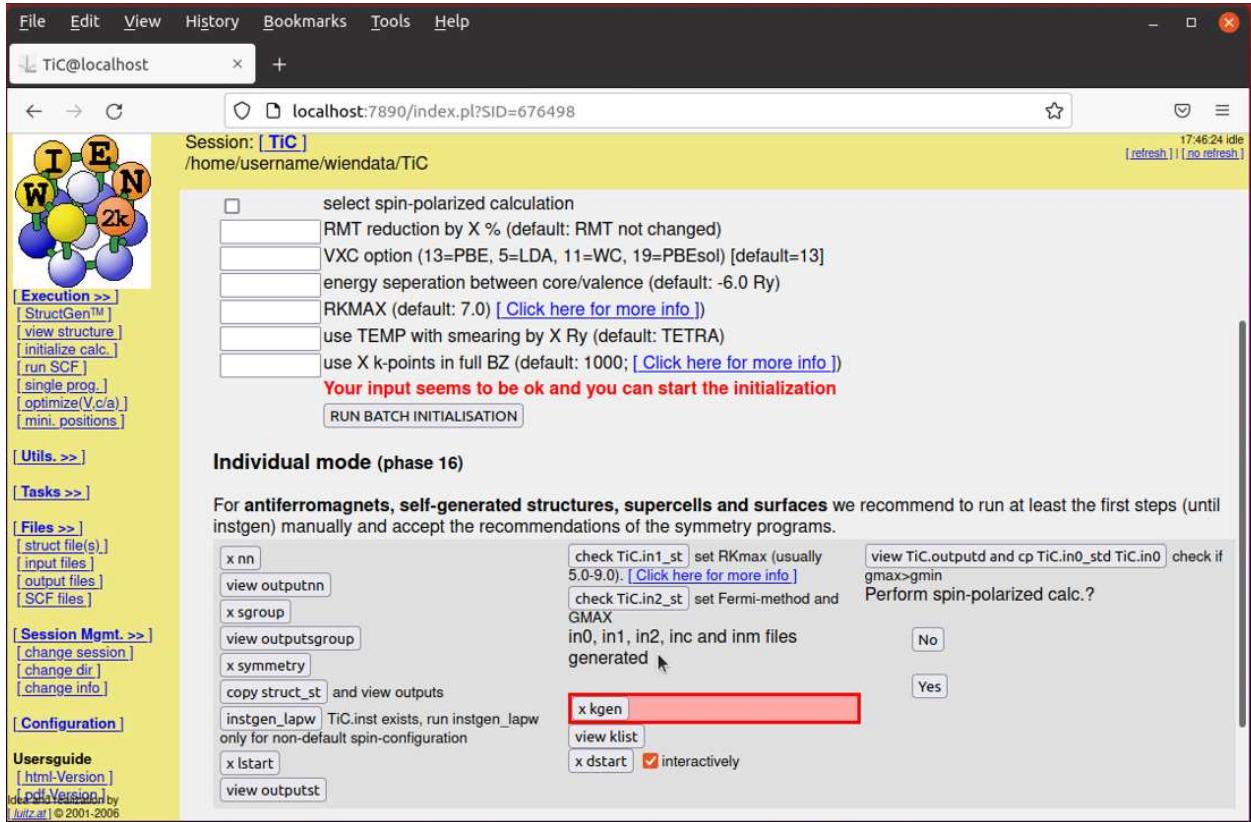
54. Click the “check TiC.in2_st” button
55. Click the “initlapw without saving” button:

The screenshot shows a web browser window with the URL `localhost:7890/index.pl?SID=676498`. The title bar says "TiC@localhost". The main content area displays a session titled "Session: [TIC] /home/username/wiendata/TiC". On the left, there is a sidebar with various menu options under categories like "Execution >>", "Tasks >>", "Files >>", "Session Mgmt. >>", and "Configuration". A molecular model of TiC is shown at the top left. The central area contains a text box with the following content:

```
File: /home/username/wiendata/TiC/TiC.in2_st
initlapw without saving Save and initlapw Download this file: [ ]
TOT (TOT,FOR,OTL,EFG,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 reciprlist
```

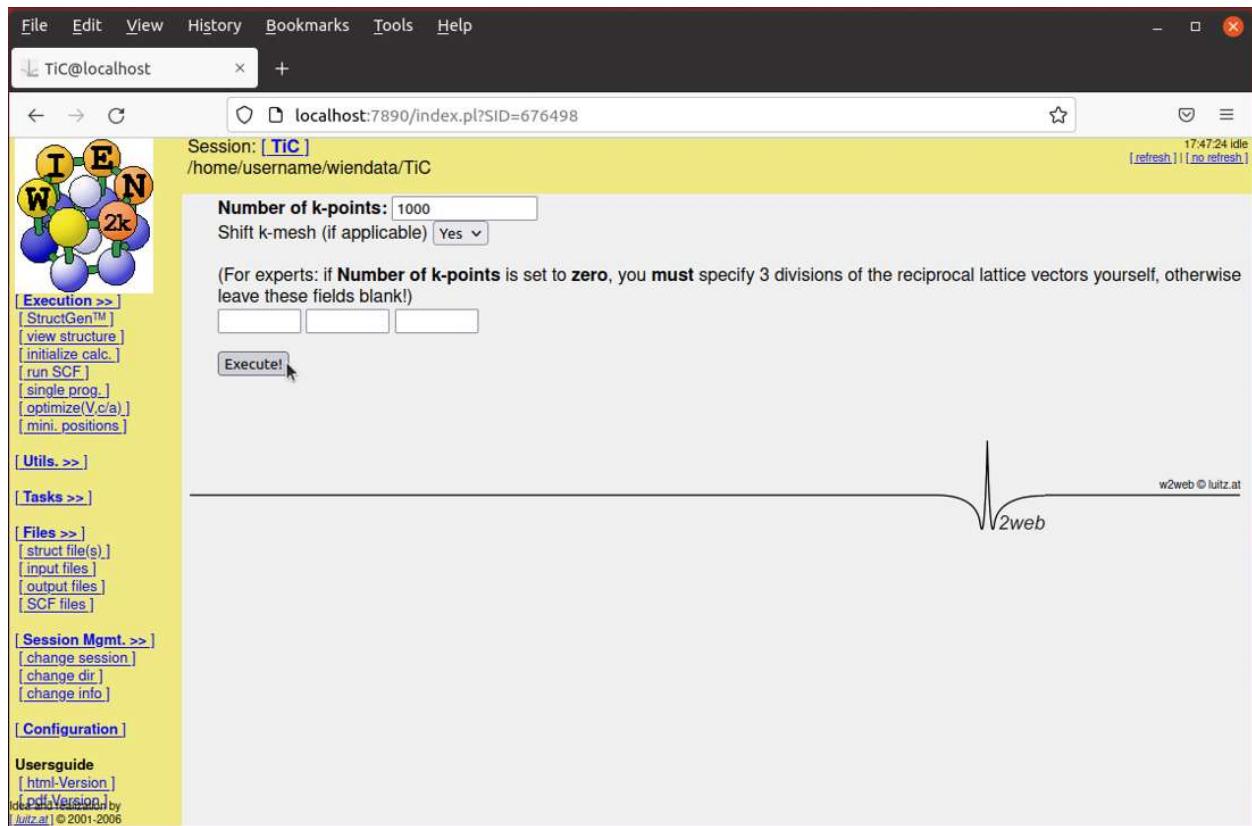
At the bottom right of the window, there is a logo for "2web" and the text "w2web © iulitz.at".

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 browser window titled "TiC@localhost". The address bar displays "localhost:7890/index.pl?SID=676498". The main content area shows a session named "TiC" with the path "/home/username/wiendata/TiC". The session status is "idle". The commandline is "x kgen" and the program input is "1000 1". The log output includes:
NUMBER OF K-POINTS IN WHOLE CELL: (0 allows to specify 3 divisions of G)
length of reciprocal lattice vectors: 1.331 1.331 1.331 10.000 10.000 10.000
47 k-points generated, ndiv= 10 10 10
STOP KGEN ENDS
0.046u 0.004s 0:00.05 80.0% 0+0k 0+192io 0pf+0w

On the left, there is a sidebar with various links:

- [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]

A large molecular model of TiC is displayed at the top left. At the bottom right, there is a logo for "w2web © iuitz.at".

60. Click the “view klist” button

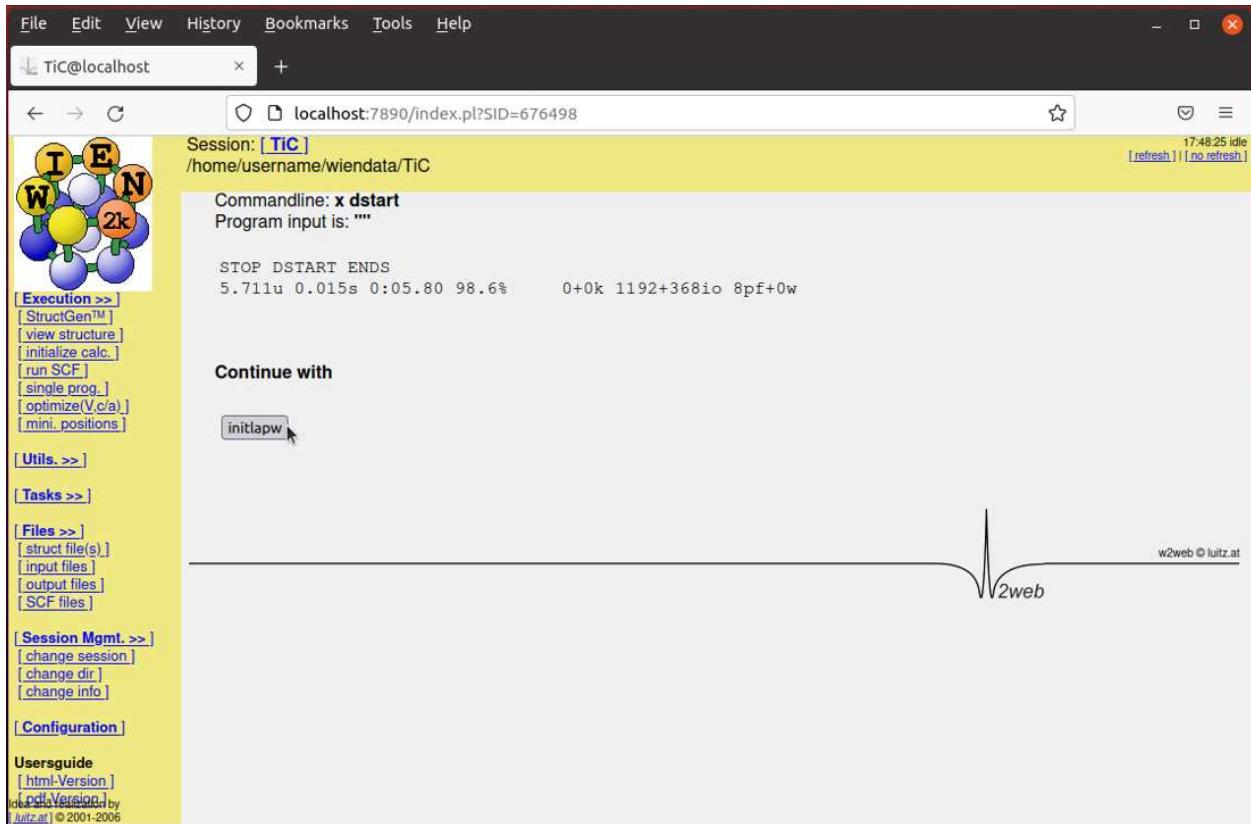
61. Click the “initlapw without saving” button:

The screenshot shows a web browser window with the URL `localhost:7890/index.pl?SID=676498`. The page title is "Session: [TiC] /home/username/wiendata/TiC". The main content area displays a molecular structure of TiC with atoms labeled T, E, N, W, and 2k. Below the structure is a table titled "File: /home/username/wiendata/TiC/TiC.klist". The table contains 20 rows of data, each representing a k-vector. The columns are labeled 1 through 10, followed by 1.0, -7.0, 1.5, and 1000 k, d. The data is as follows:

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

The interface includes a sidebar with various menu items such as Execution, Utils, Tasks, Files, Session Mgmt., Configuration, and Usersguide. The bottom right corner features a logo for "2web" and the text "w2web © iulitz.at".

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:

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

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

initlapw without saving Save and initlapw Download this file:

```
rmt(min)*kmax = 7.00000
9         9         9       7       7       7
rmin = 7.36842
rmax = 12.80000

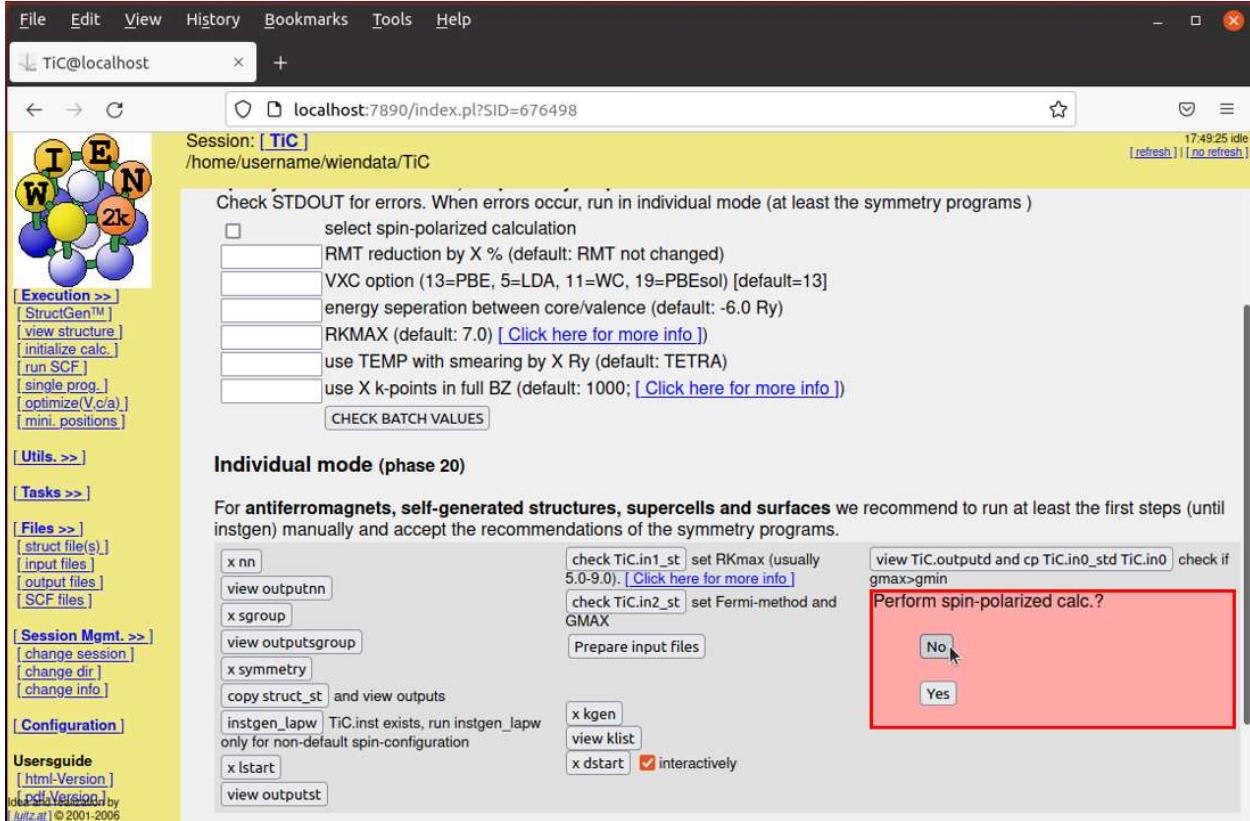
cutoff distance for superposition: 16.205
unitsell range: 4 4 4

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
```

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



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

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

energy seperation between core/valence (default: -6.0 Ry)

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

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

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

[CHECK BATCH VALUES](#)

Individual mode (phase 21)

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.

x nn
view outputnn
x sgroup
view outputsgroup
x symmetry
copy struct_st and view outputs
instgen_lapw TiC.inst exists, run instgen_lapw only for non-default spin-configuration
x lstart
view outputst

check TiC.in1_st set RKmax (usually 5.0-9.0). [\[Click here for more info.\]](#)
check TiC.in2_st set Fermi-method and GMAX
Prepare input files

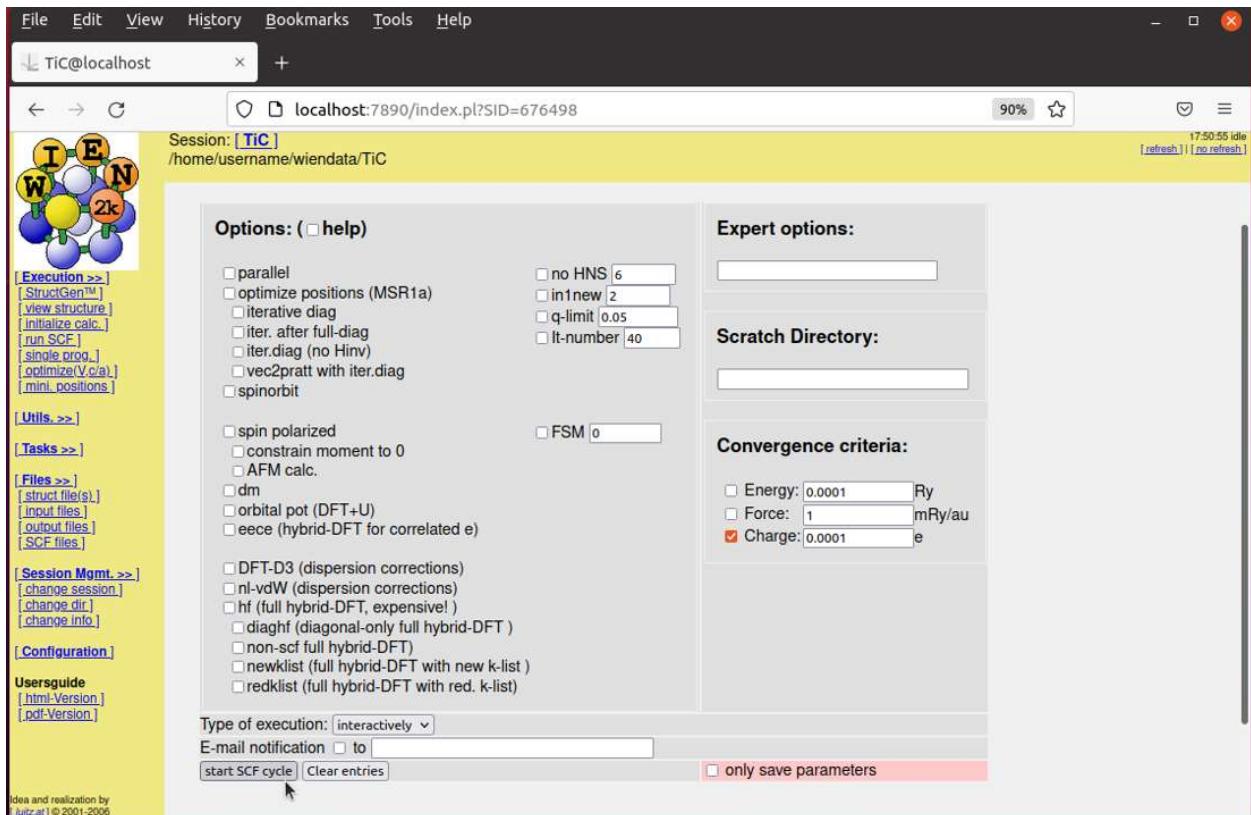
x kgen
view klist
x dstart interactively

Initialization done

[\[Continue with run SCF\]](#)

Run the calculation

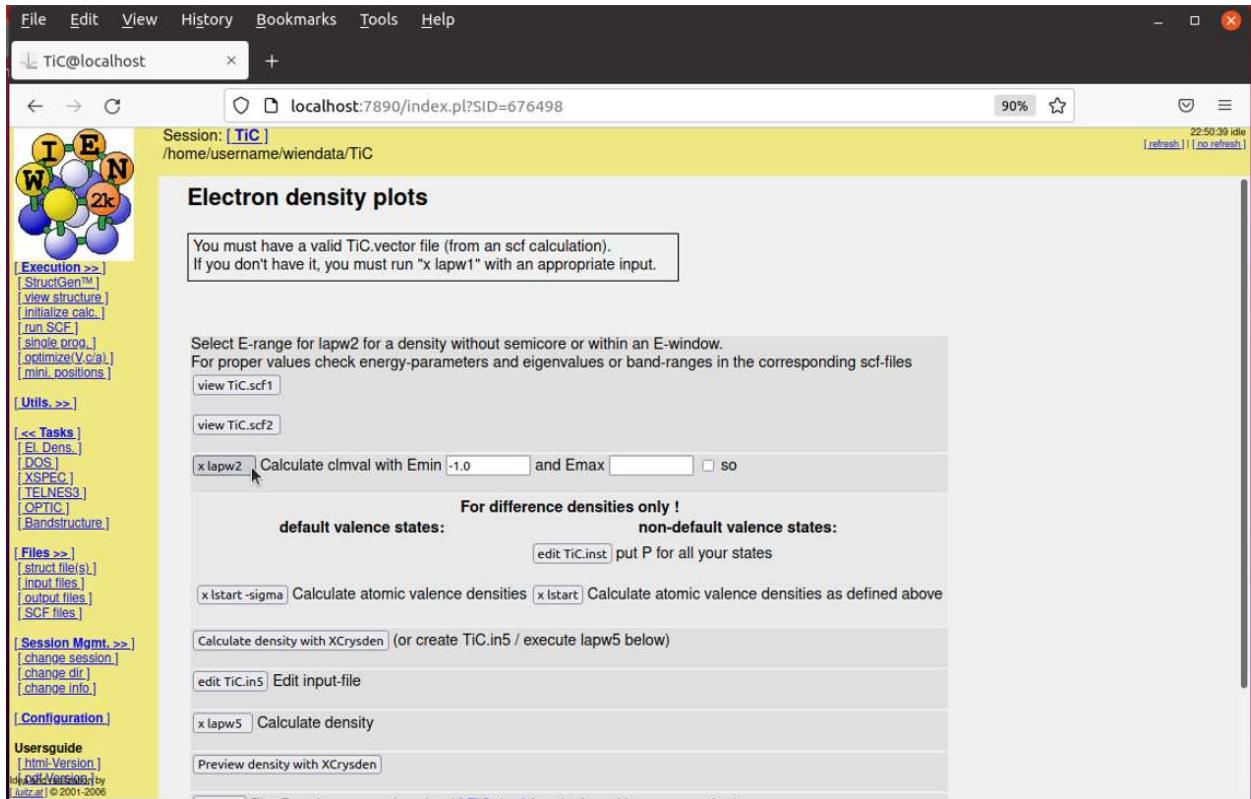
68. Uncheck the “Energy” box, check the “Charge” box, and type 0.0001 into the box next to it.
 69. Select “interactively” for the “Type of execution”, then click the “start SCF cycle” to perform the calculation:



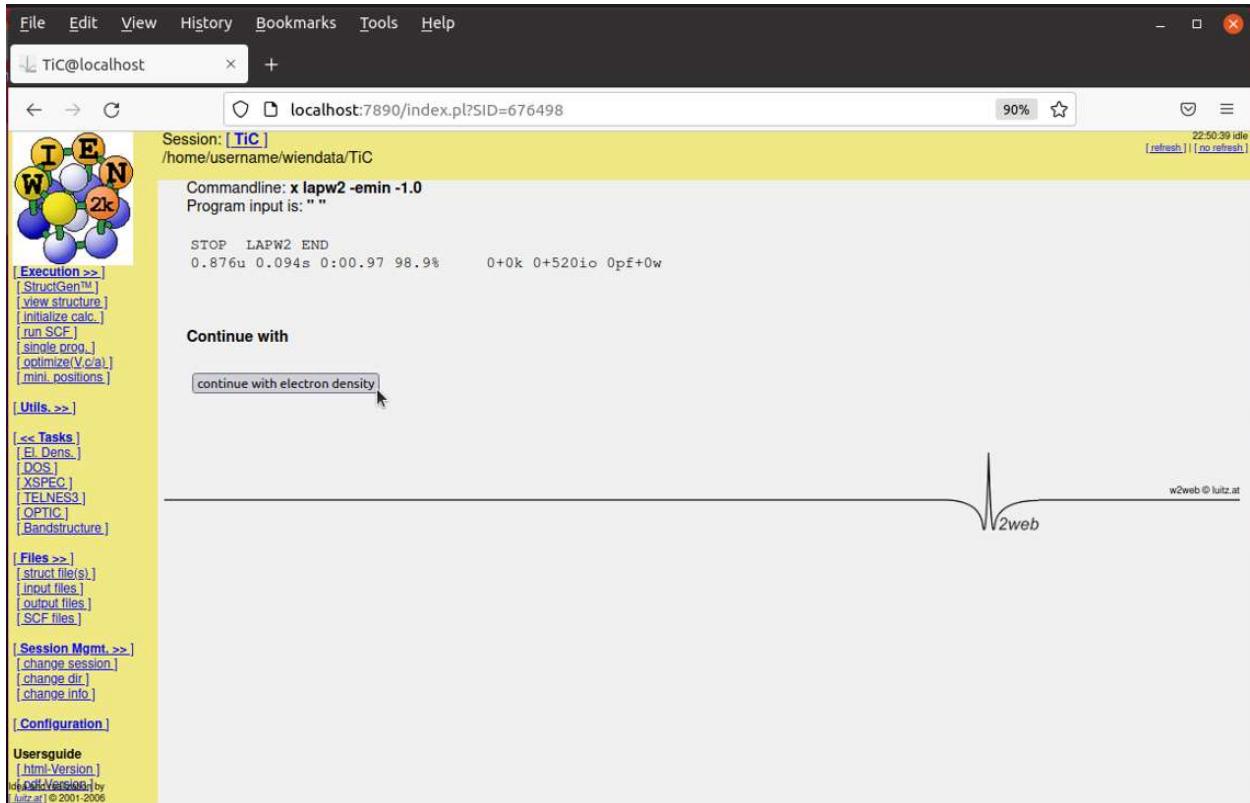
70. As shown, this calculation converges after 10 cycles:

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):

The screenshot shows the WIEN2k web interface with a session titled "TiC". The left sidebar contains various menu items and links related to the session management and tools. The main area is a code editor showing the input file "TiC.in5". The first three lines of the file are highlighted with a red box:

```

-1 -1 0 4      # x, y, z, divisor of origin
-1 3 0 4      # x, y, z, divisor of x-end
3 -1 0 4      # x, y, z, divisor of y-end

```

Below these lines, the rest of the file includes comments about point density, RHO parameters, and plotting directions. At the bottom right of the code editor, there is a small logo for "w2web" with the text "w2web © lutz.at".

First three lines in TiC.in5 were changed to:

-1 -1 0 4 #origin of plot

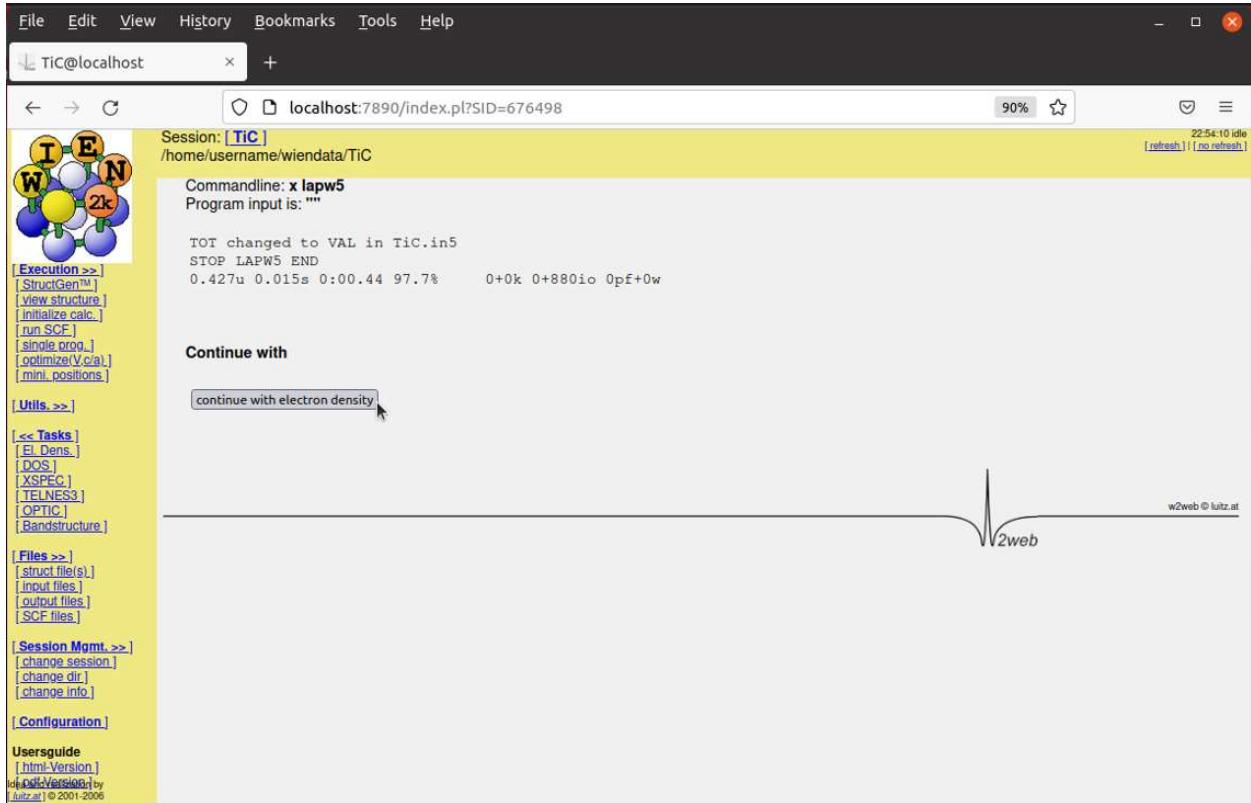
-1 3 0 4 #x-end of plot

3 -1 0 4 #y-end of plot

ADD was removed

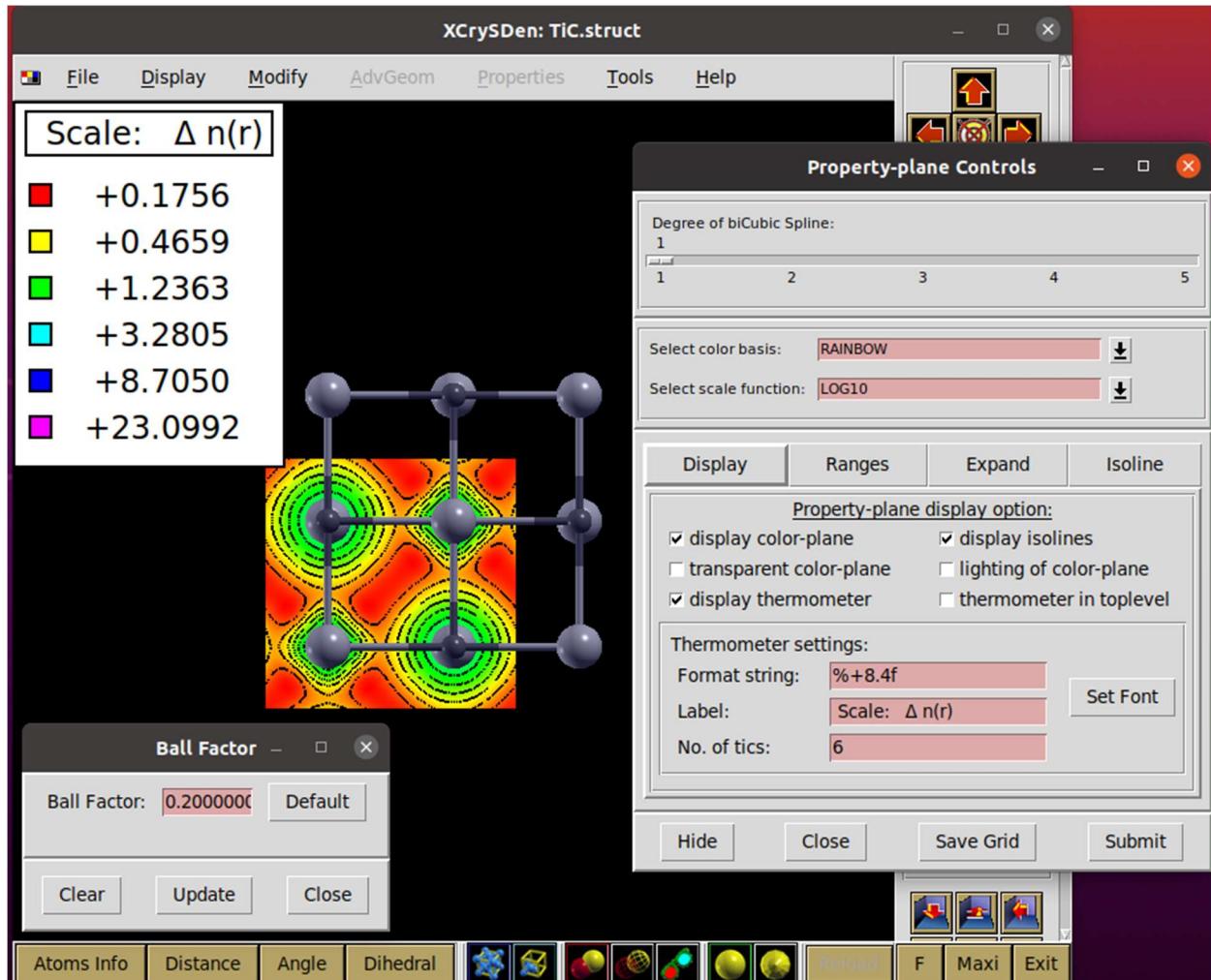
76. Click the “Save and continue with electron density” button

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



9. Click the “Preview density with XCrysden” button
10. Select “RAINBOW” for “Select color basis”
11. Select “LOG10” for “Select scale function:”
12. Check “display thermometer”
13. Click the “Submit” button
14. Click “Modify”, then click “Ball Factor”
15. Change Factor to 0.2 and click the “Update” button
16. Can rotate the structure by left clicking in the black widow and then moving the mouse

79. The following results (compare to Figure 3.7 in the Wien2k usersguide):

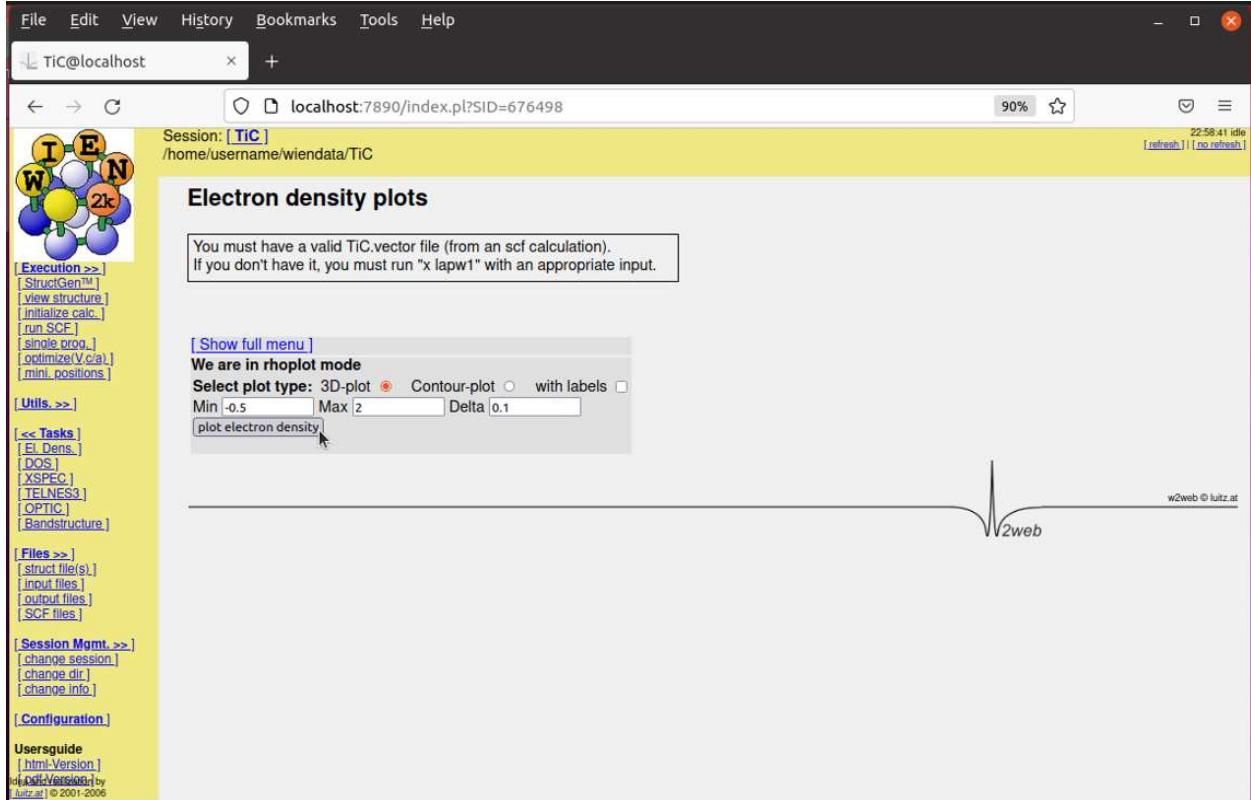


80. Click the “x” in the top right corner to close XCrySDen

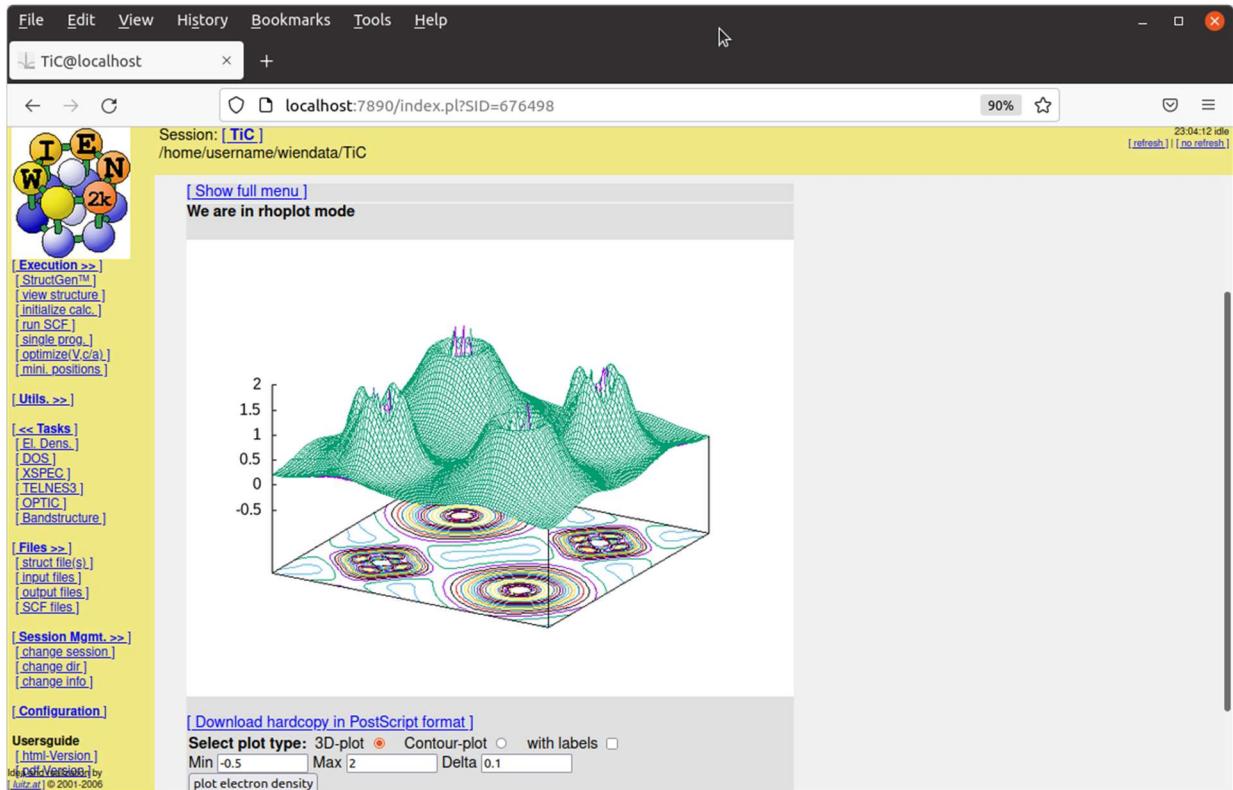
81. In the left menu, click “El. Dens.” under “Tasks”

82. Click the “rhoplot” button

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

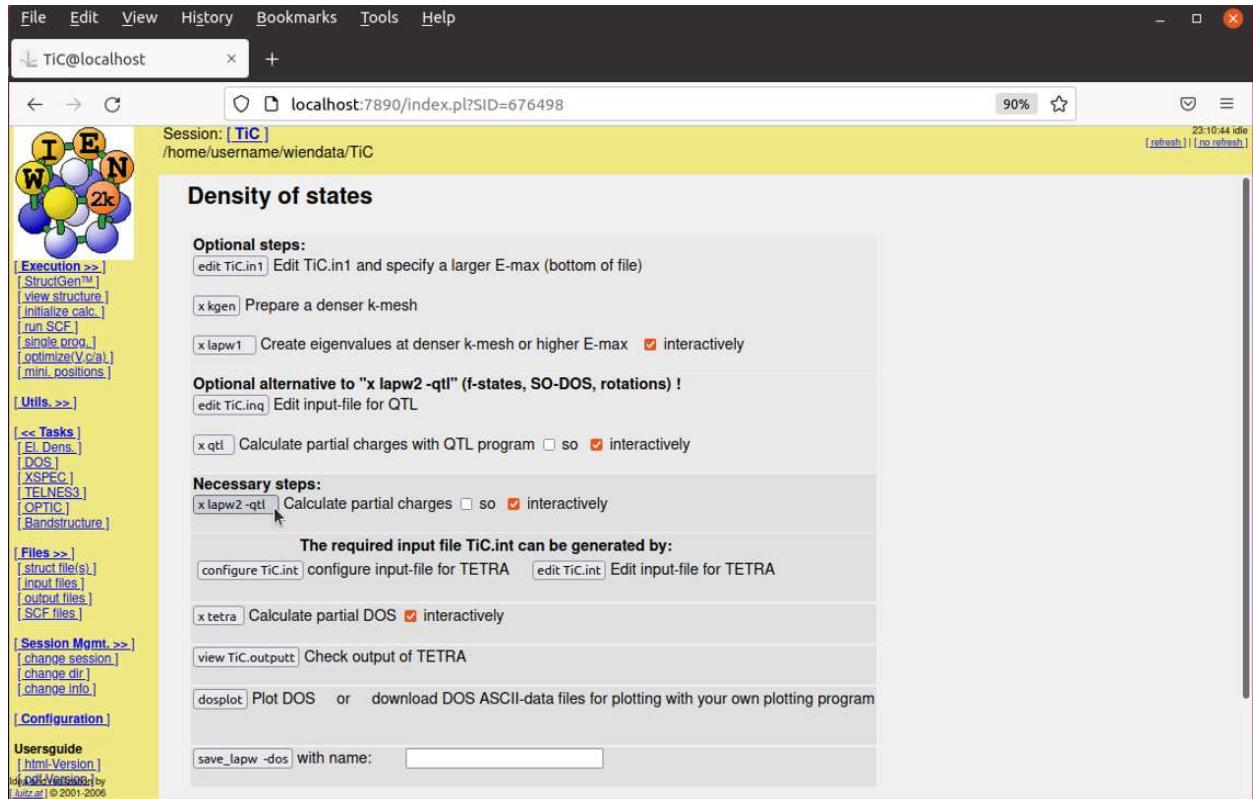


84. This gives us the following plot (compare to Figure 3.8 in the WIEN2k usersguide):

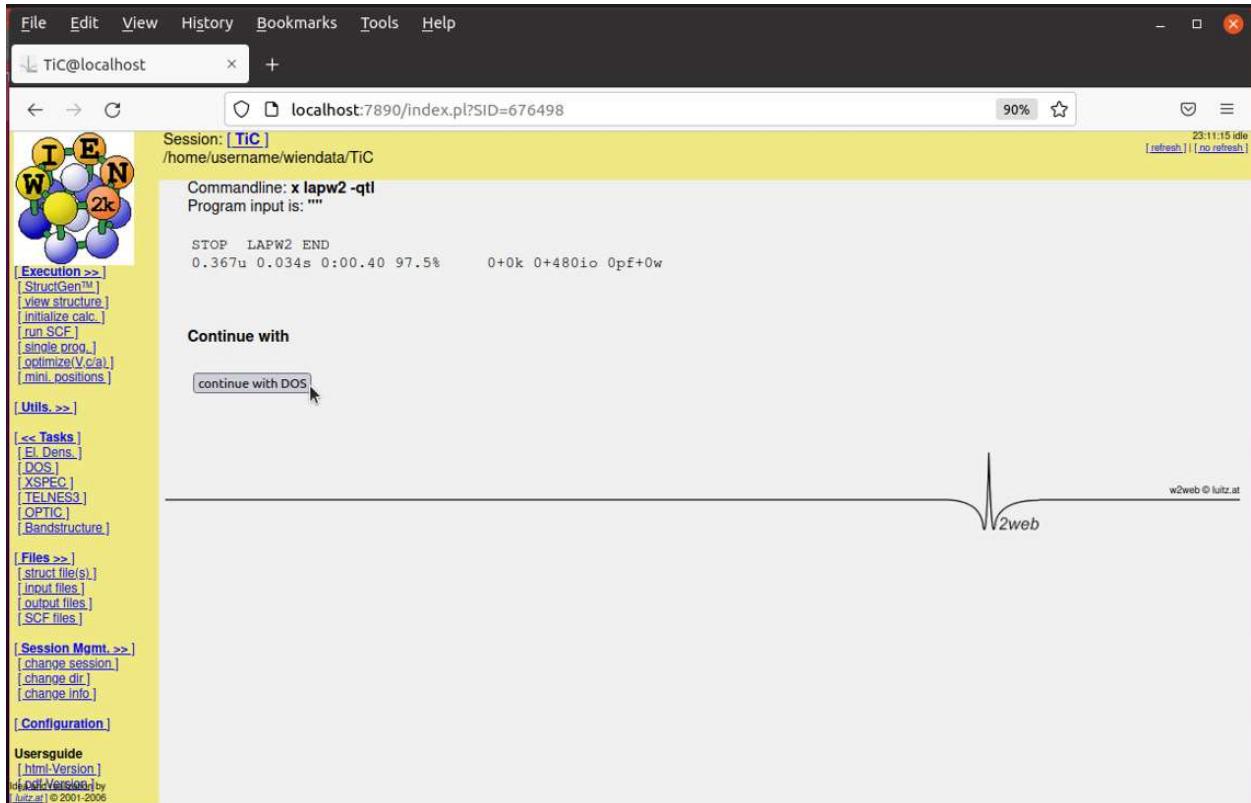


Plot density of states (DOS)

85. In the left menu, click on “DOS” under “Tasks”
 86. Click on “x lapw2 -qtl”:



87. Click on “continue with DOS”:



88. Click “edit TiC.int”

89. 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 #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.qli:

```
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).KSEL
0 1 to # 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, MAX_OF_SUMMANDS
2 5          # this sums dos-cases 2+5 from the input above
```

90. Click “Save and continue with DOS”

91. Click “x tetra”

92. Click “continue with DOS”:

The screenshot shows a web browser window titled "TiC@localhost". The URL is "localhost:7890/index.pl?SID=676498". The session name is "TIC". The main content area displays a 3D molecular model with atoms labeled I, E, N, W, and 2k. Below the model, there is a commandline output:
STOP LEGAL END TETRA
0.136u 0.008s 0:00.14 92.8% 0+0k 0+624io 0pf+0w

Below the commandline, there is a "Continue with" section containing a button labeled "continue with DOS".

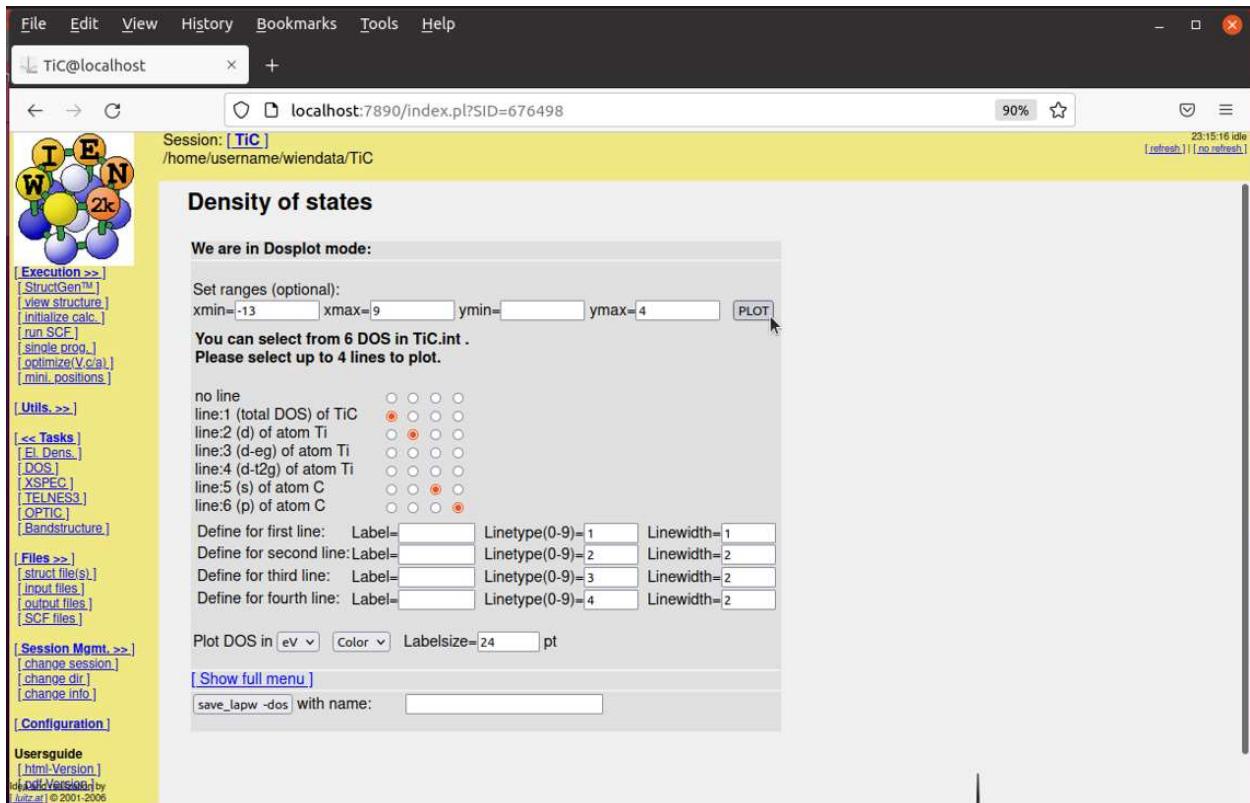
The left sidebar contains a vertical menu with the following items:

- [Execution >>]
 - [StructGen™]
 - [view structure]
 - [initialize calc.]
 - [run SCF]
 - [single prop.]
 - [optimizeV/c/a]
 - [mini_positions]
- [Utils. >>]
 - [<< Tasks]
 - [El Dens.]
 - [DOS]
 - [XSPEC]
 - [TELNESS3]
 - [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]
- Info [pdf-Version] by Lutz

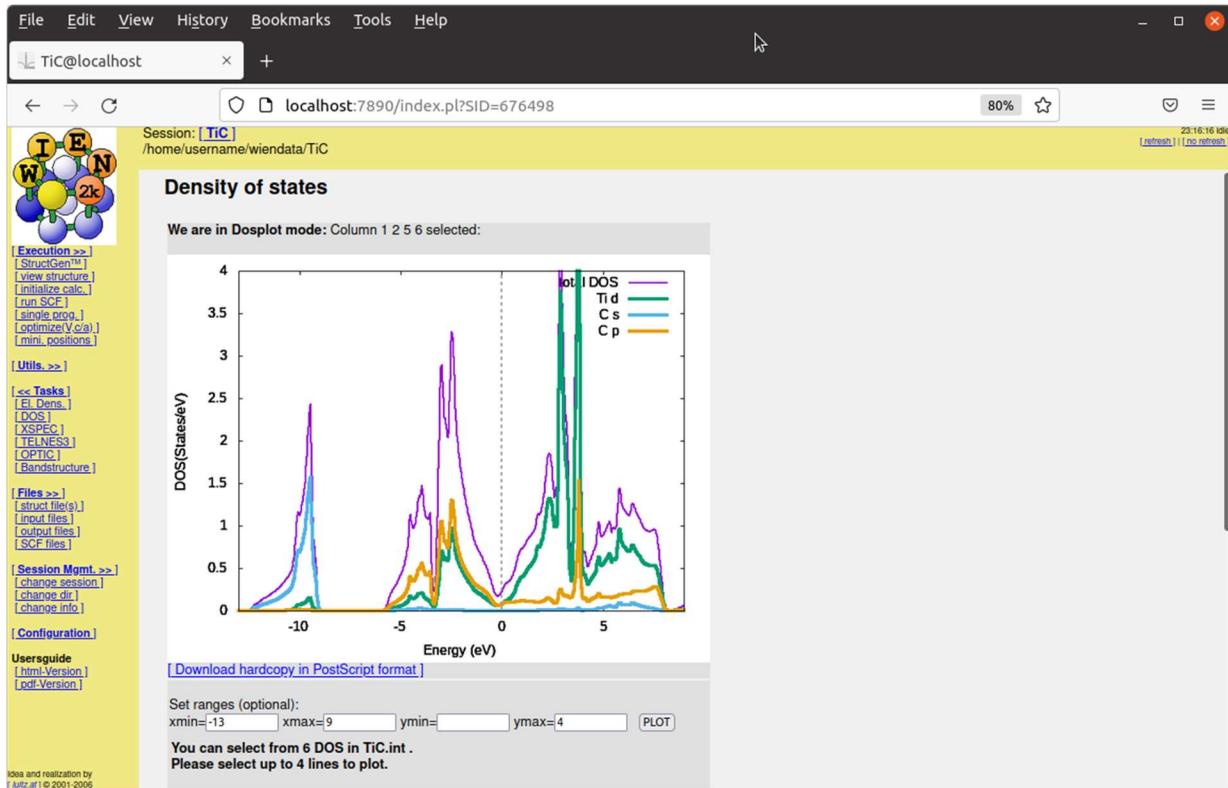
At the bottom right of the main content area, there is a small logo with the text "w2web © lutz.at" and a stylized wave graphic.

93. Click “dosplot”

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

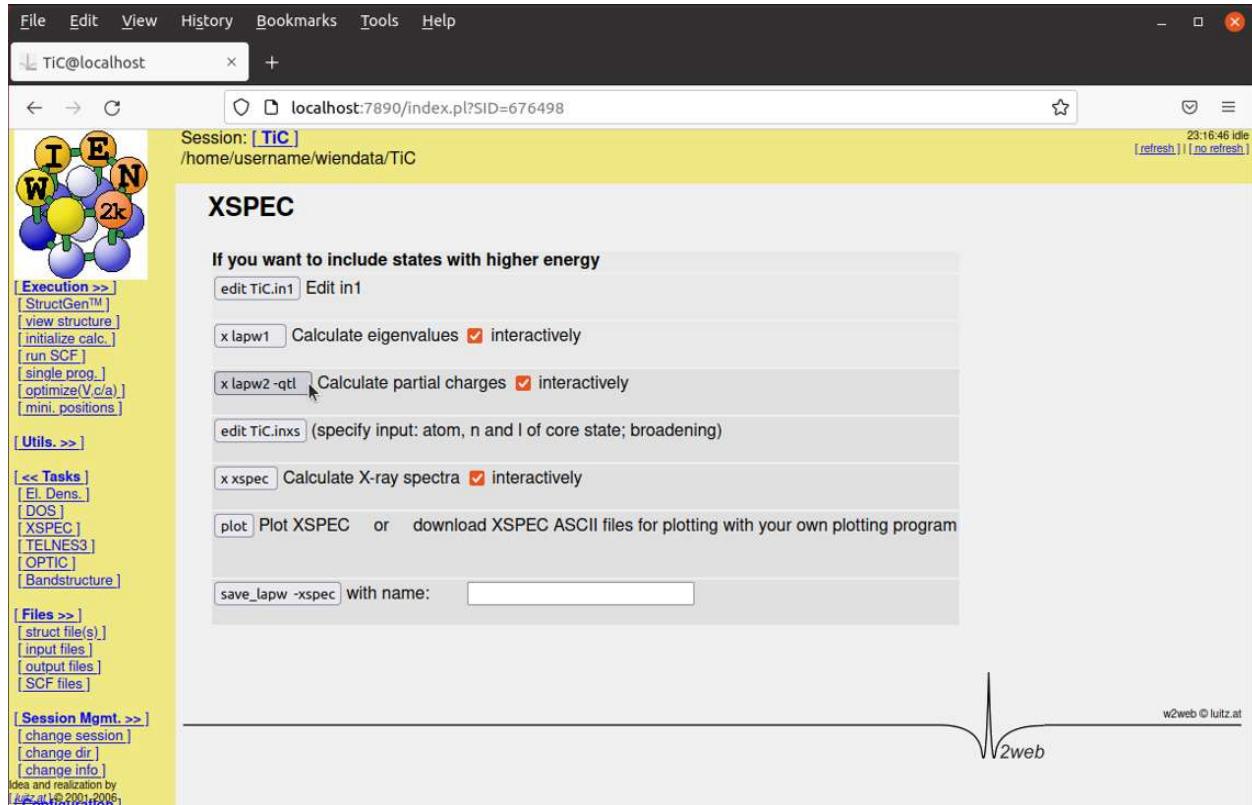


95. The resulting plot is (this is similar to Figure 3.9 in the user guide):

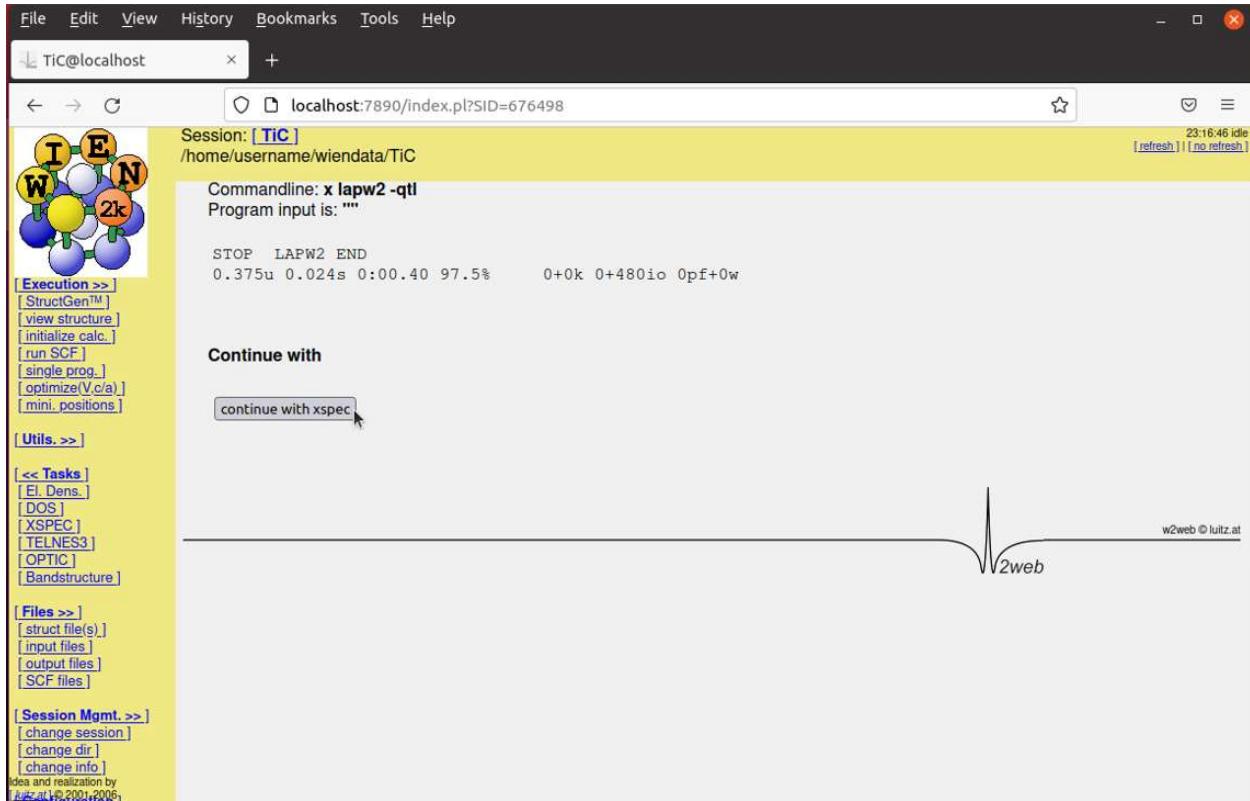


Plot x-ray spectra

96. In the left menu, click on “XPEC” under “Tasks”
 97. Click “x lapw2 -qtl”:

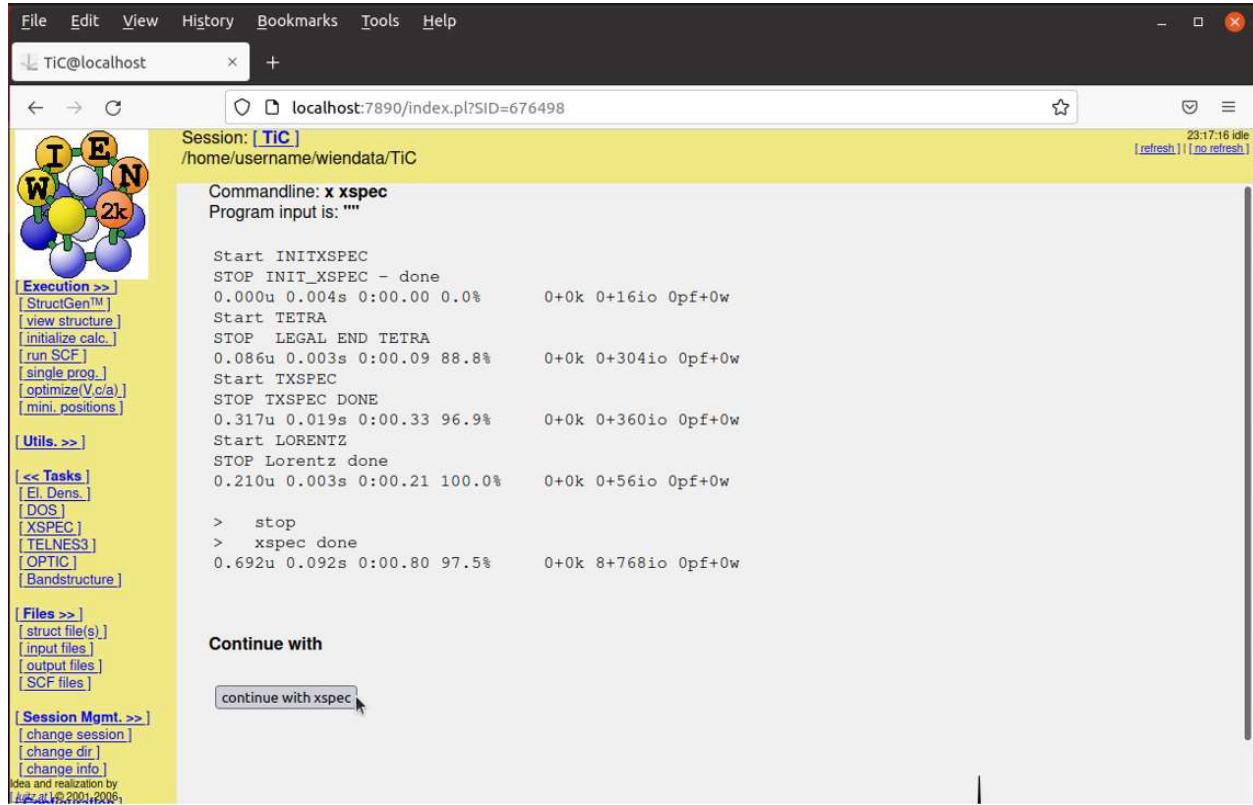


98. Click “continue with xspec”:



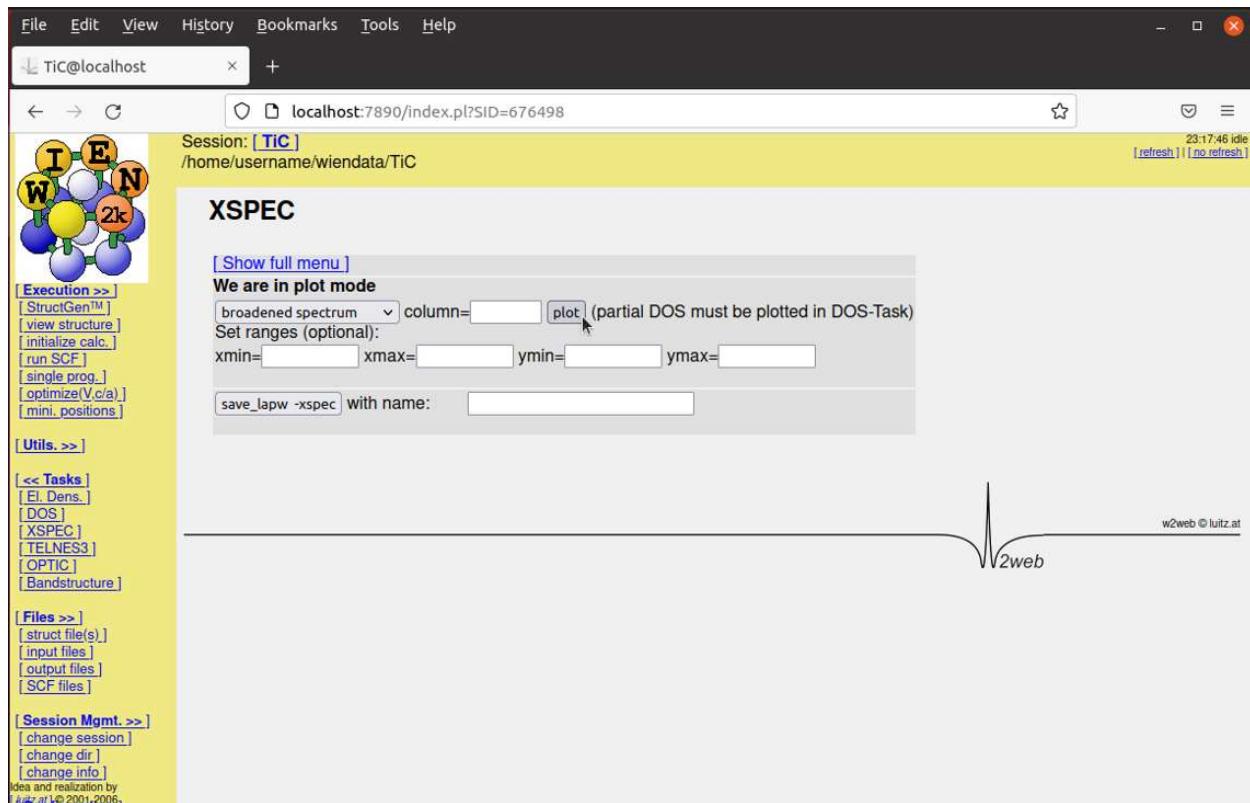
99. Click “x xspec”

100. Click “continue with xspec”:

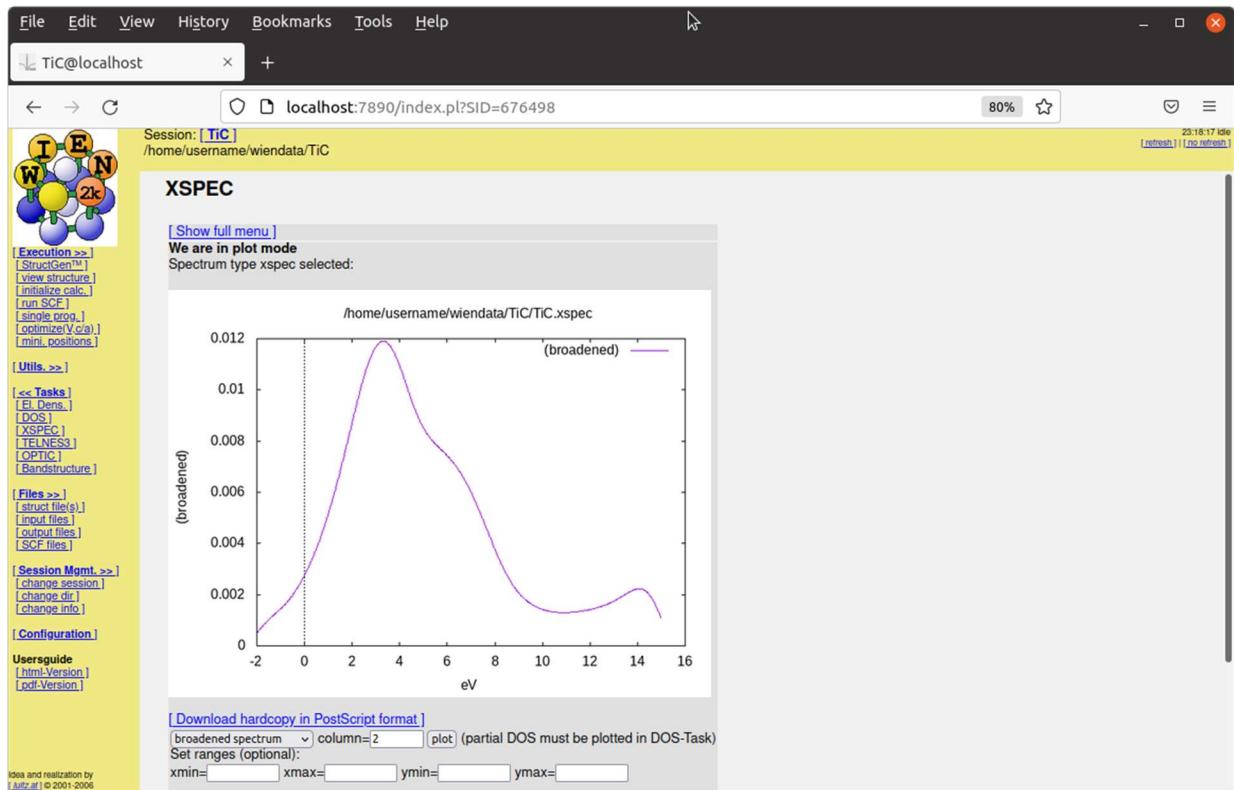


101. Click “plot”

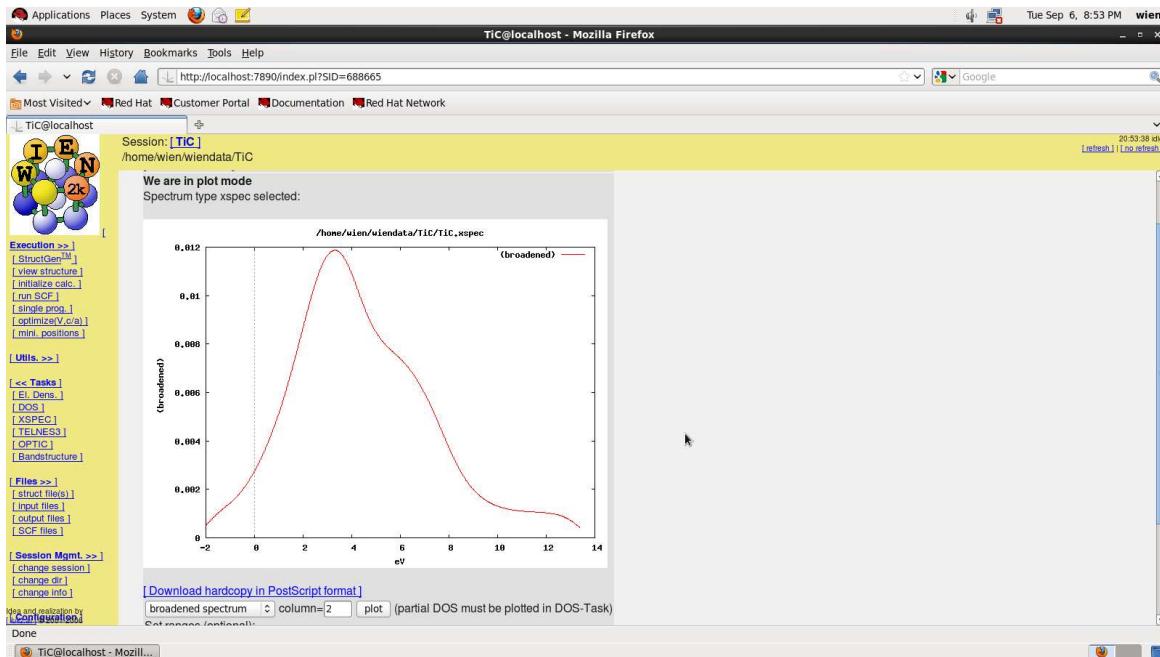
102. Click “plot”:



103. The resulting plot (versions 14.1-21.1) is shown below (this is similar to Figure 3.11 in the user guide):

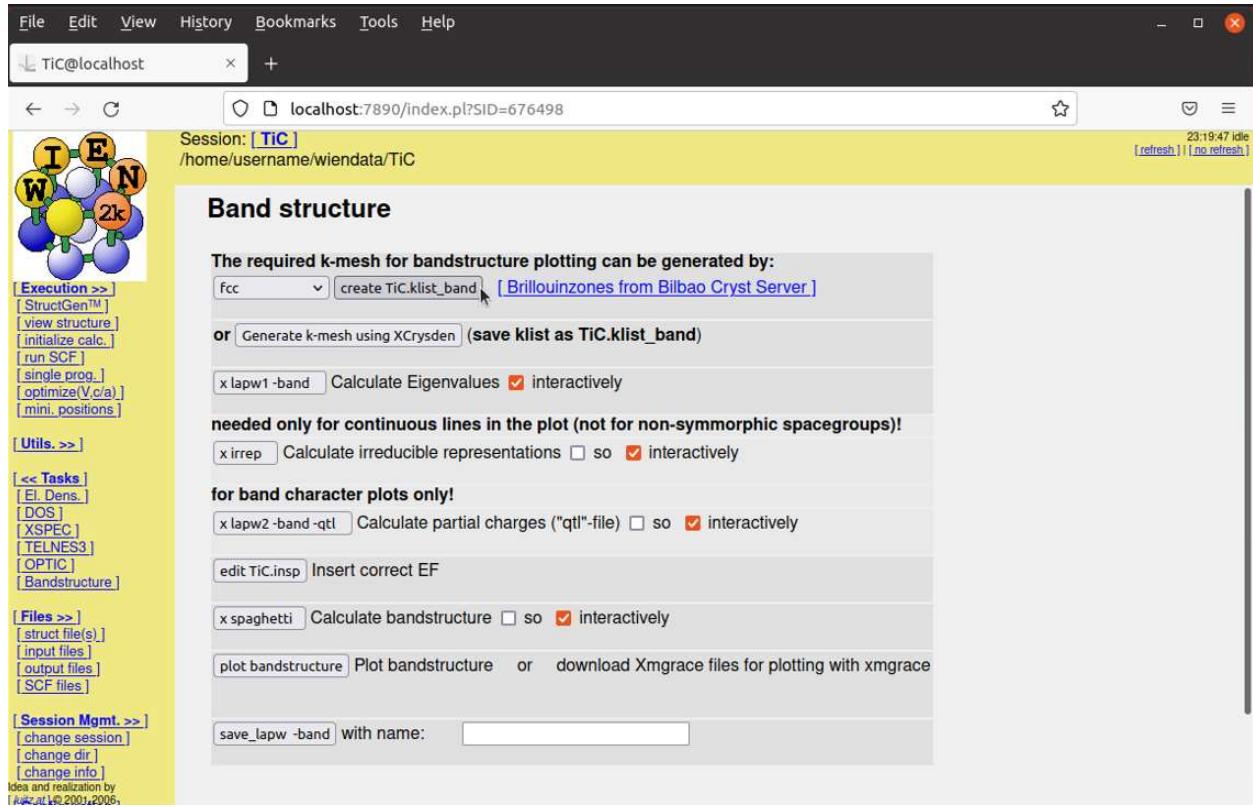


However, there seems to be some difference in the eV axis compared to WIEN2k versions 11.1-13.1:



Plot bandstructure

104. In the left menu, click on “Bandstructure” under “Tasks”
105. Click on “create TiC.klist_band” with fcc selected:



106. Click on “x lapw1 -band”
107. Click “continue with bandstructure”:

The screenshot shows a web browser window titled "TiC@localhost" at "localhost:7890/index.pl?SID=676498". The session is named "TiC" and is located at "/home/username/wiendata/TiC". The status bar indicates "23:20:17 [running] (lapw1) [refresh] || [no refresh]".
The main content area displays the commandline: "Commandline: x lapw1 -band" and "Program input is: '". Below this, there is a log output:

```
STOP LAPW1 END
10.036u 0.414s 0:10.46 99.8% 0+0k 0+5992io 0pf+0w
```

Below the log, there is a section titled "Continue with" containing a button labeled "continue with bandstructure". To the right of this button is a small logo consisting of a vertical line with a dip and the text "2web".
On the left side of the interface, there is a sidebar with various links:

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

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108. Click on “x lapw2 -band -qtl”
109. Click “continue with bandstructure”:



110. Edit TiC.insp by clicking “edit TiC.insp”, change jatom to 1, jtype to 6 , Fermi energy to 0.7425 (or could enter 0.7429194506 shown on the screen):

File Edit View History Bookmarks Tools Help

TiC@localhost

localhost:7890/index.pl?SID=676498

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

23:22:41 idle
[refresh] | [no refresh]

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.)= 0.7429194506
```

Execution >>

- [StructGen™]
- [view structure]
- [initialize calc.]
- [run SCF]
- [single proc.]
- [optimize(V/c/a)]
- [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]

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Wien2k © 2001-2006

Save and continue with bandstructure

Header from TiC.qtl and possible FERMI energies:

```
## Figure configuration
5.0 3.0          # paper offset of plot
10.0 15.0 3.0    # xsize,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

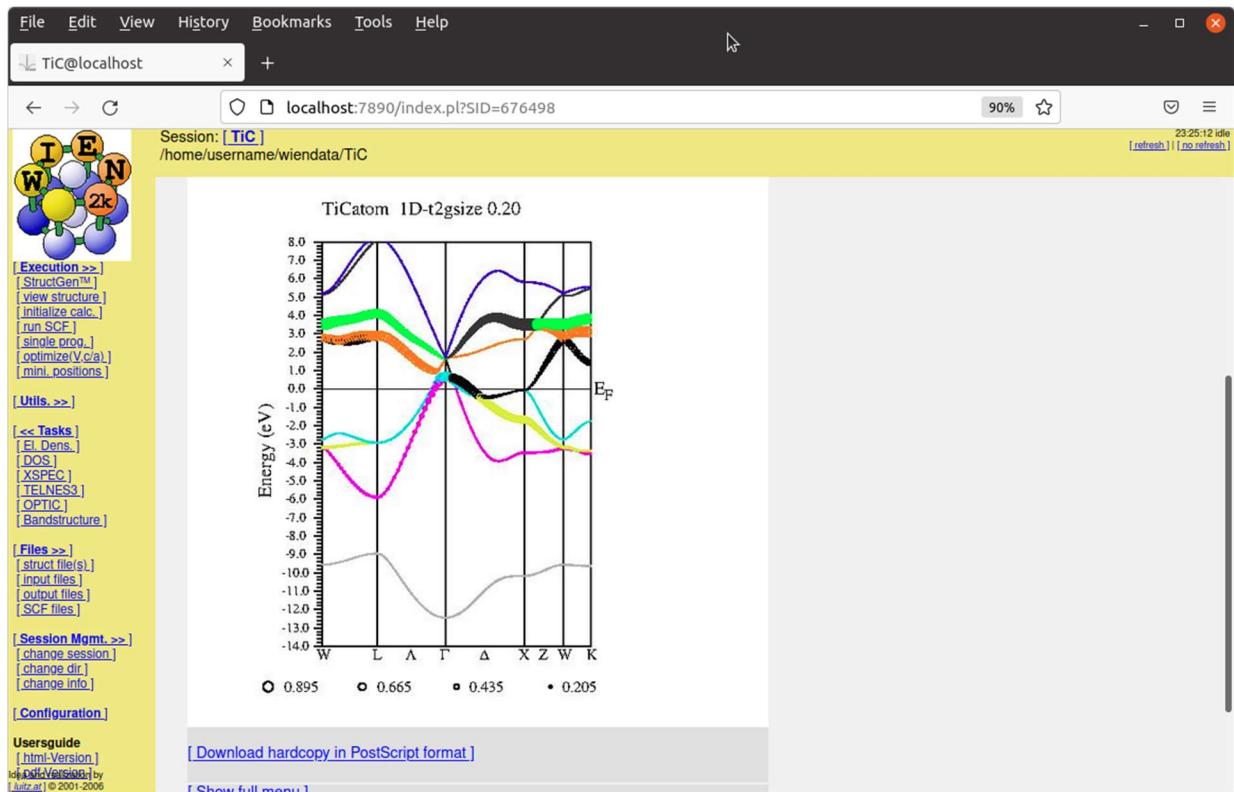
Fermi switch:
0...no line
1...solid line
2...dashed line
3...dotted line

Line switch:
0...dots
```

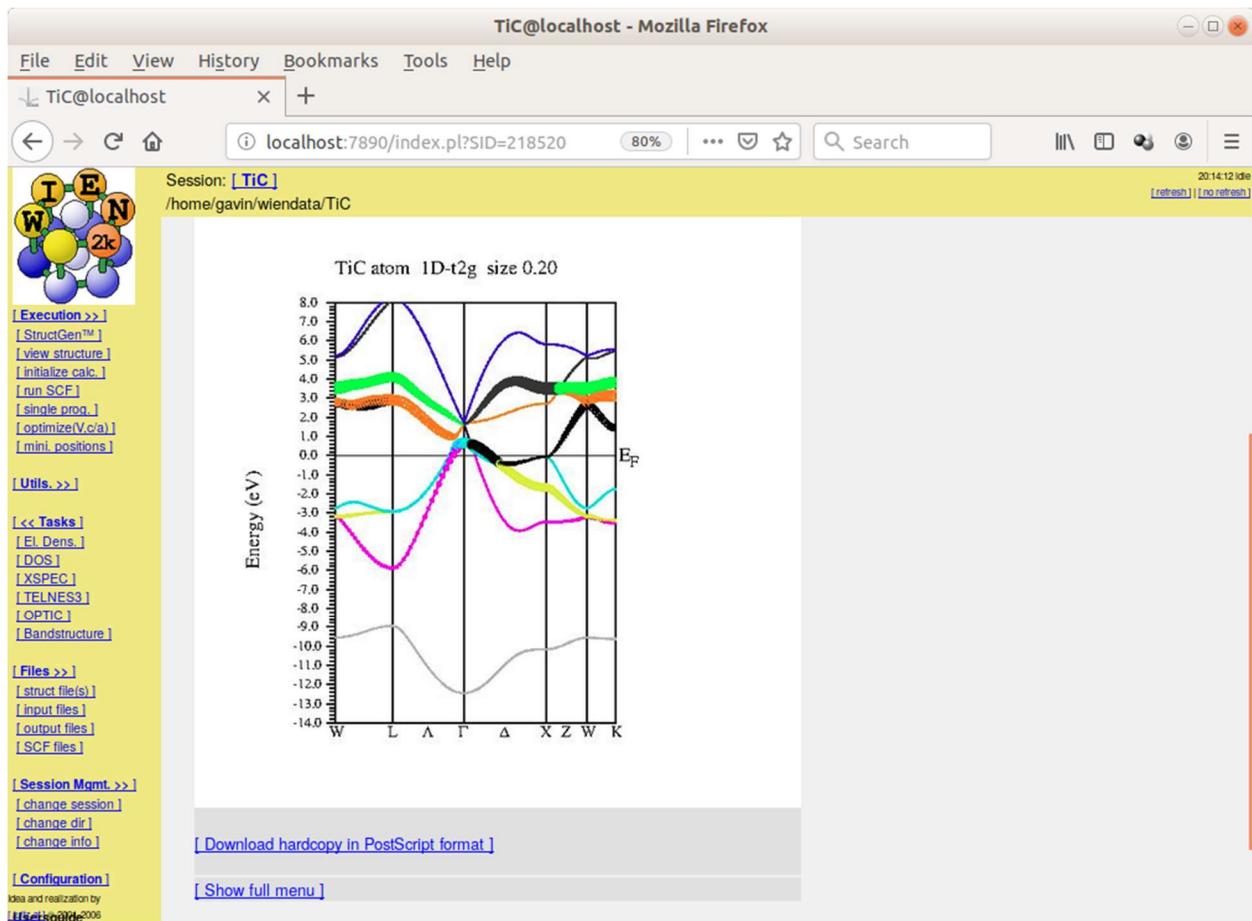
111. Click “Save and continue with bandstructure”
112. Click “x spaghetti”
113. Click “continue with bandstructure”:



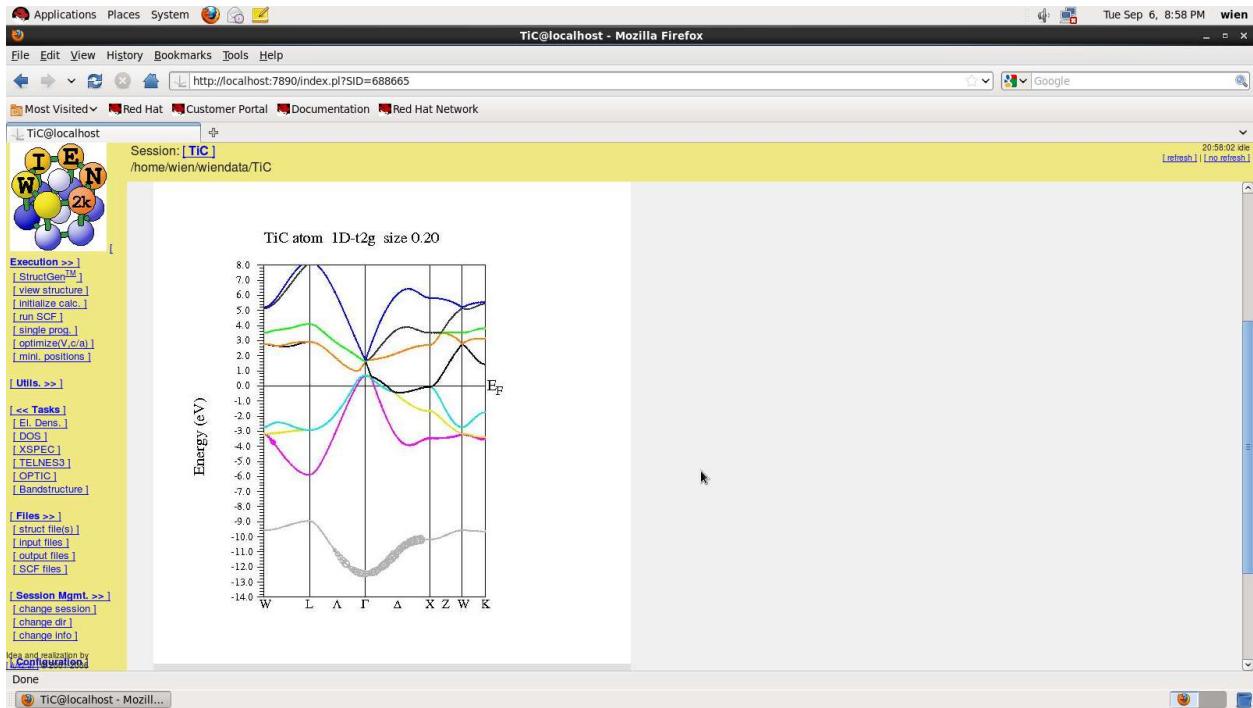
114. Click “plot bandstructure”, the creates the following plot (version 21.1):



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

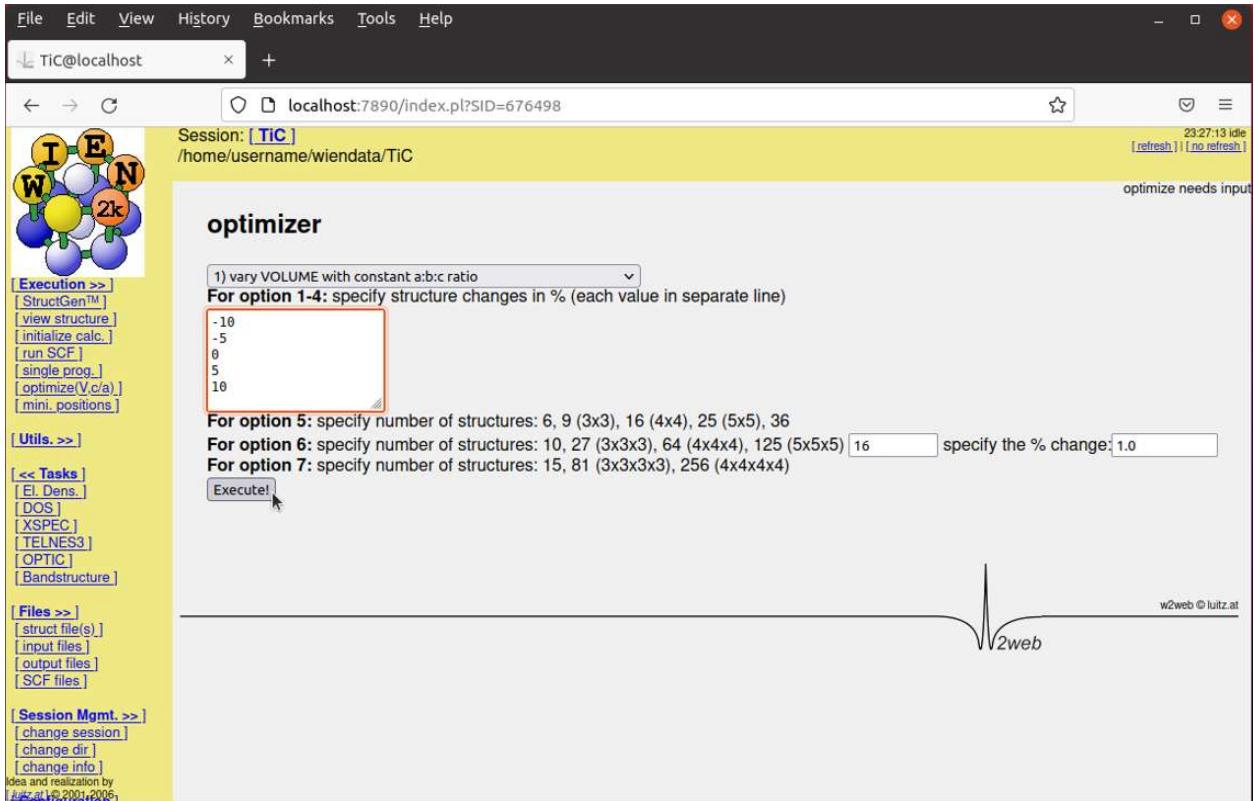
115. In the left menu, click on “optimize(V,c/a)” under “Execution”

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.

116. Click “x optimize”:

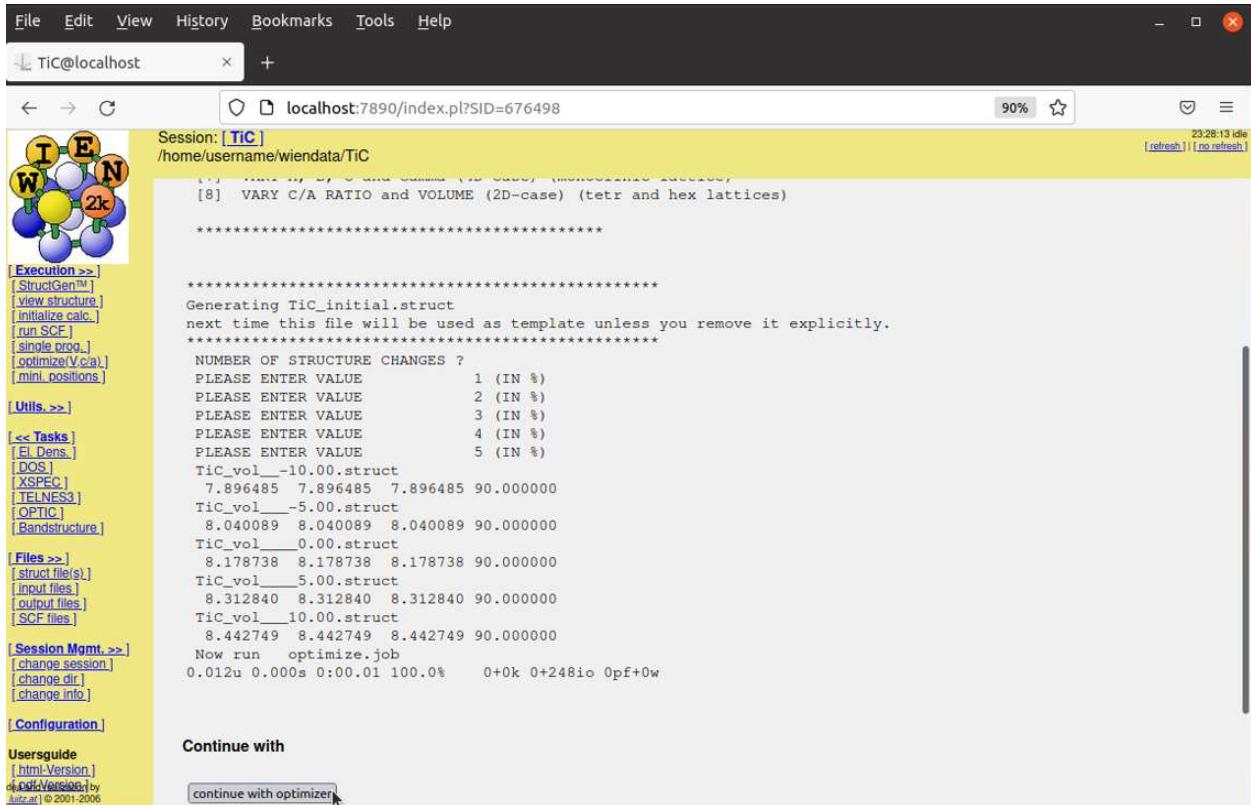
The screenshot shows the w2web interface for a TiC session. The left sidebar contains a molecular structure of TiC and a list of execution options: Execution >> (StructGen™, view structure, initialize calc., run SCF, single proc., optimize(V,c/a), mini_positions); Utils. >> (<< Tasks, El Dens., DOS, XSPEC, TELNES3, OPTIC, Bandstructure); Files >> (struct file(s), input files, output files, SCF files); Session Mgmt. >> (change session, change dir, change info). The main content area shows the title "Optimize volume, c/a-ratio, ..." and a form with fields for "x optimize" (radio button selected), "Generate structure files from" (radio button selected for TiC.struct), "edit optimize.job" (link to uncomment x dstart or cp clmsum), "run optimize.job" (Type of execution: background dropdown), and "plot" (link to Plot energy curve). Below the form is a plot of energy (y-axis) versus volume (x-axis), showing a single sharp minimum. The URL in the browser is localhost:7890/index.pl?SID=676498. The top status bar shows the session name [TiC] and path /home/username/wiendata/TiC, along with a timestamp 23:26:42 idle and refresh/no refresh buttons.

117. 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
 118. Click “Execute!”:

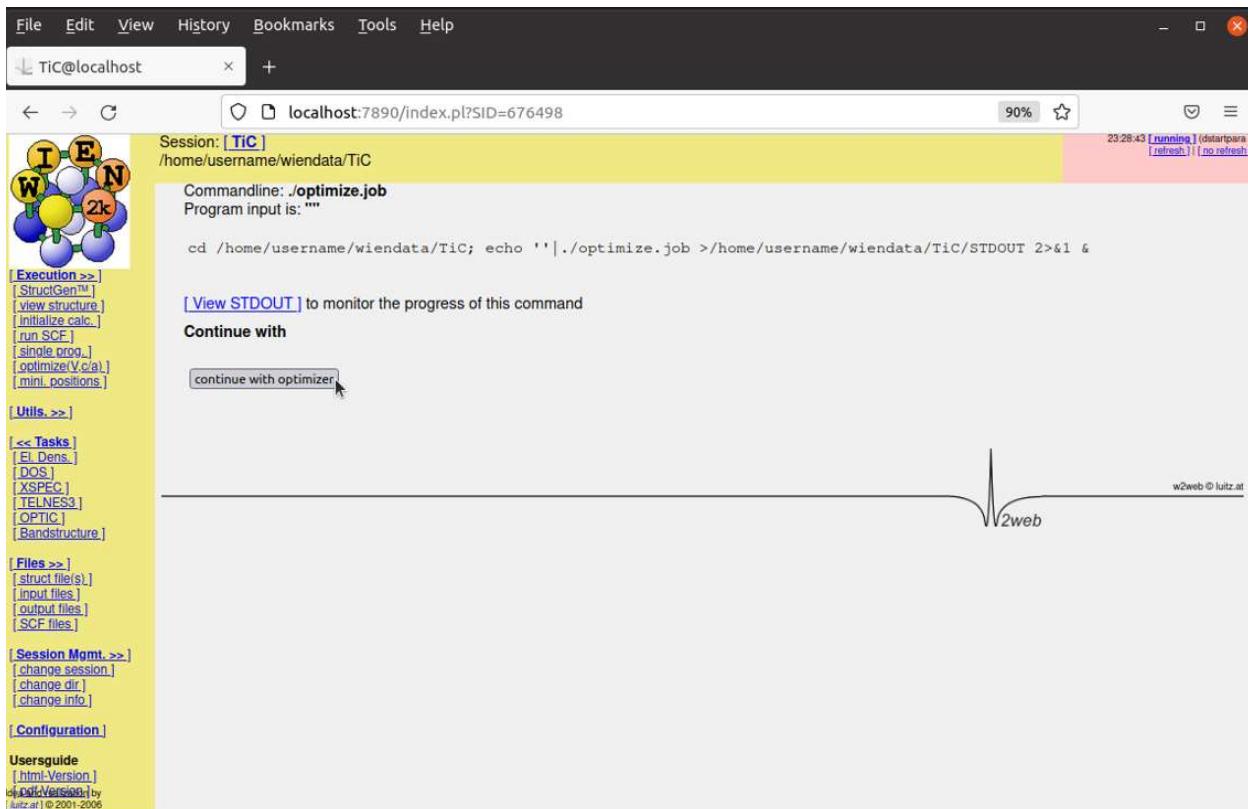


The screenshot shows the TiC web interface for the optimizer. On the left, there's a sidebar with various buttons like 'Execution >>', 'StructGen™', 'view structure', etc. The main area has a yellow header bar with 'Session: TiC' and the URL 'localhost:7890/index.pl?SID=676498'. Below the header, the title 'optimizer' is displayed. A dropdown menu is open under the heading '1) vary VOLUME with constant a:b:c ratio'. Inside the dropdown, five values are listed: -10, -5, 0, 5, and 10. At the bottom of the dropdown menu, there are instructions for options 5, 6, and 7, followed by a large 'Execute!' button which is highlighted with a red box.

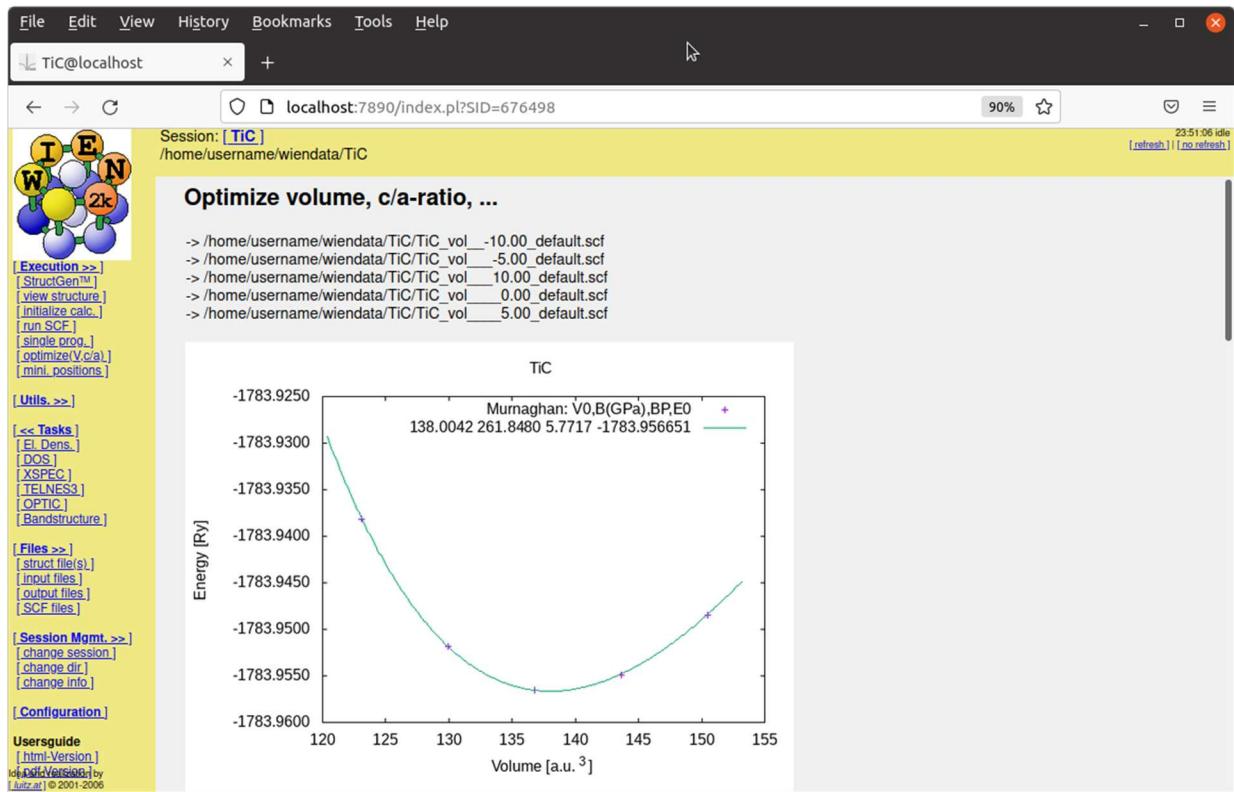
119. Click “continue with optimizer”:



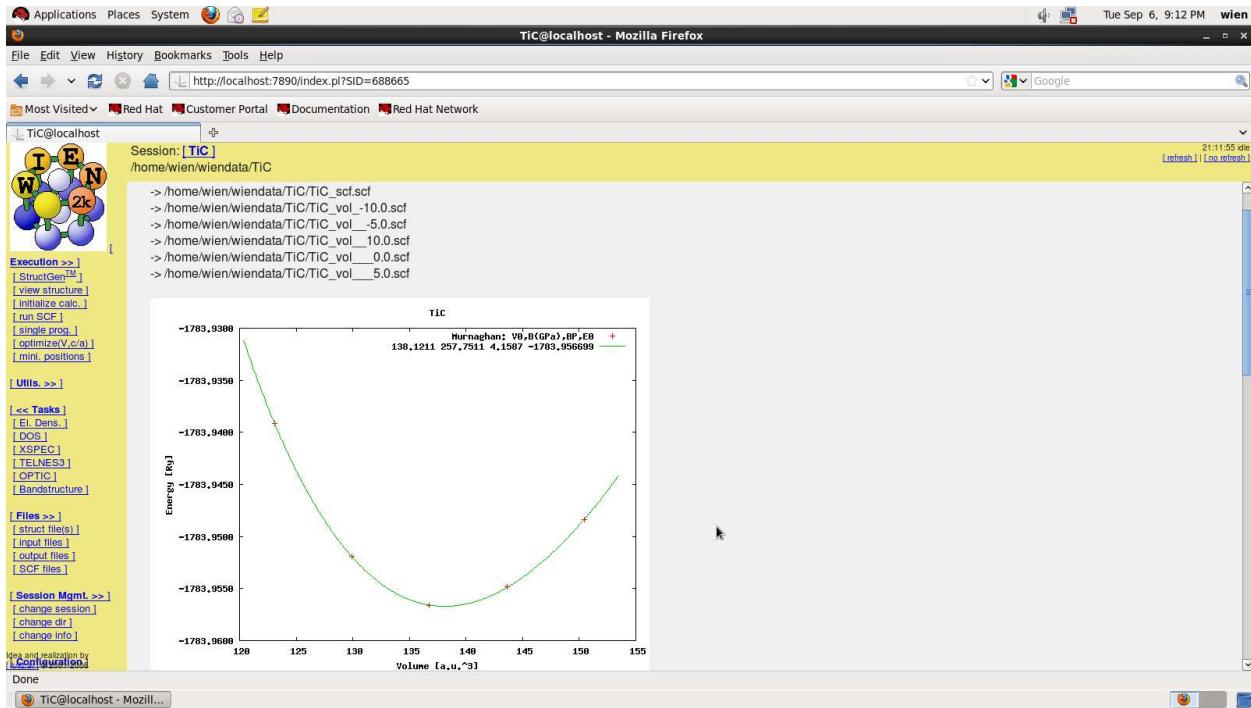
120. Click “run optimize.job”
121. Click “continue with optimizer”:



122. Wait for job to finish, then click “plot”
123. Click “plot” with E vs. volume selected (versions 19.1-21.1):



Could compared to the differences in versions 11.1-13.1:



TiC example has been completed.