

WIEN2k TiC Example

Ubuntu 24.04.3 LTS

WIEN2k_24.1 (Release 1/8/2024)

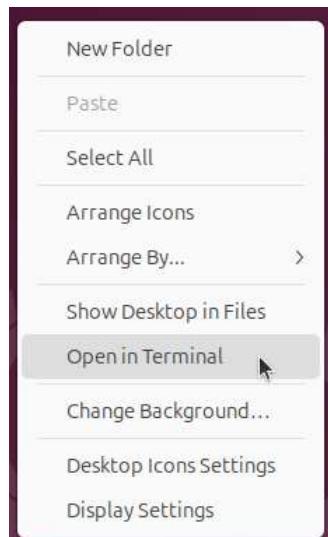
ifx version 2025.3.2

WIEN2k patches [1]: Makefile.orig.patch, SearchZ.patch, StorePot.patch, angle.patch, atom_read.patch, atom_write.patch, charge.patch, executor.patch, find_nfloat.patch, init_elast_lapw.patch, init_orb_lapw.patch, l2main.patch, lapw0.patch, make.sys.patch, and x_lapw.patch.

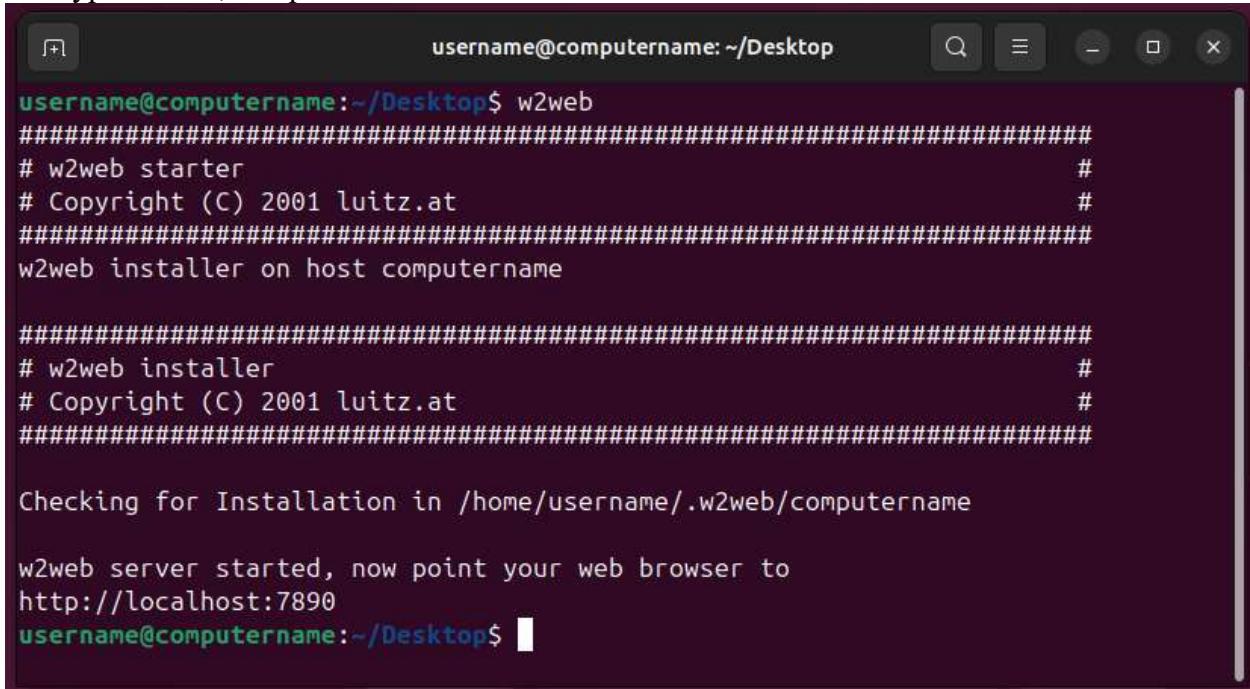
[1] <https://github.com/gsabo/WIEN2k-Patches/tree/master/24.1>

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:



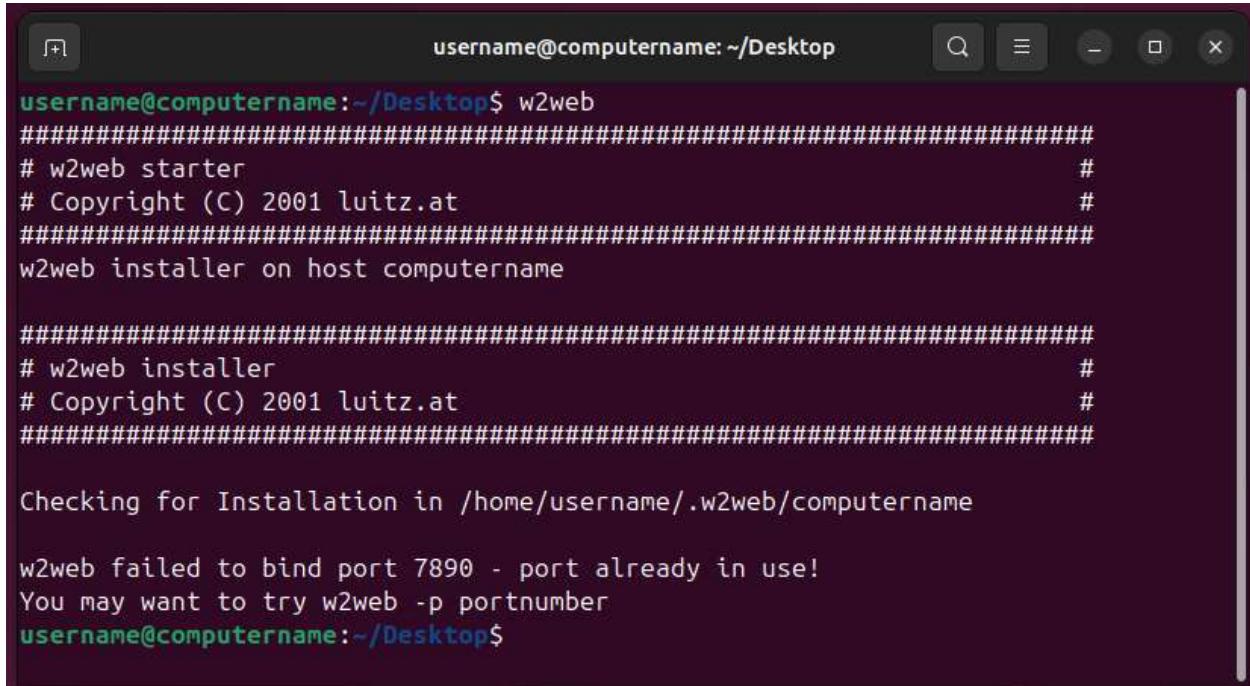
```
username@computername:~/Desktop$ w2web
#####
# w2web starter
# Copyright (C) 2001 luitz.at
#####
w2web installer on host computername

#####
# 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

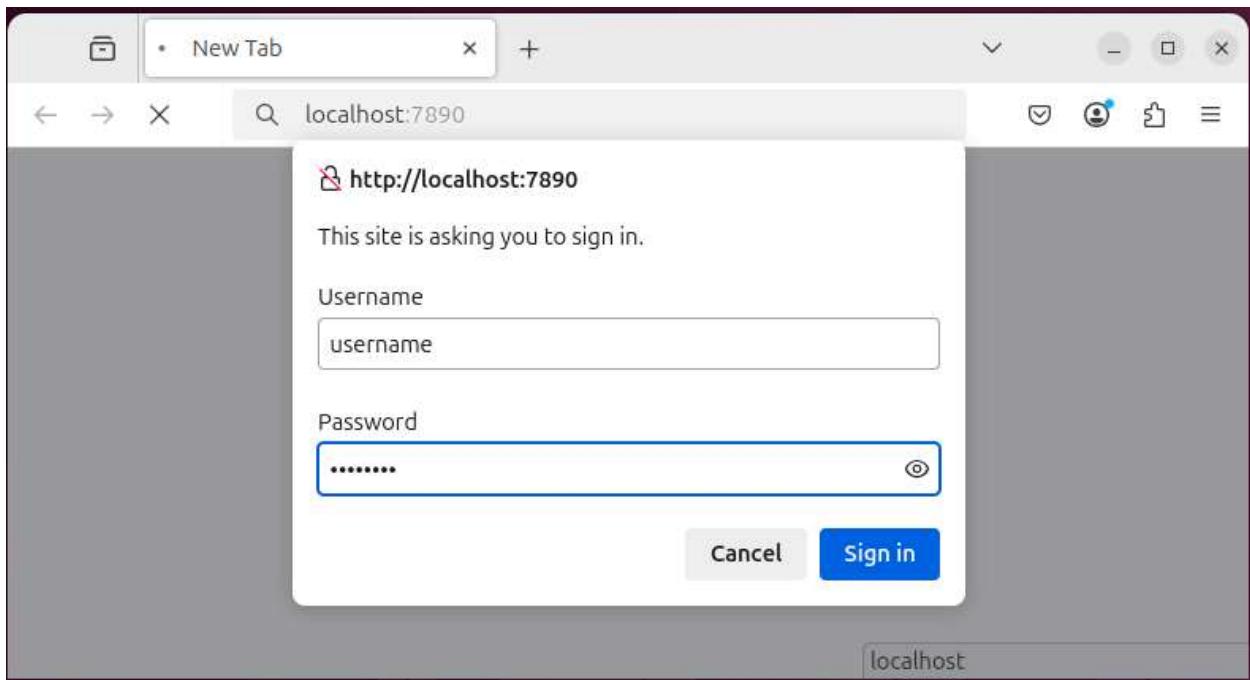
w2web failed to bind port 7890 - port already in use!
You may want to try w2web -p portnumber
username@computername:~/Desktop$
```

Open Firefox and login to w2web

3. Click on the Firefox icon to open Firefox:

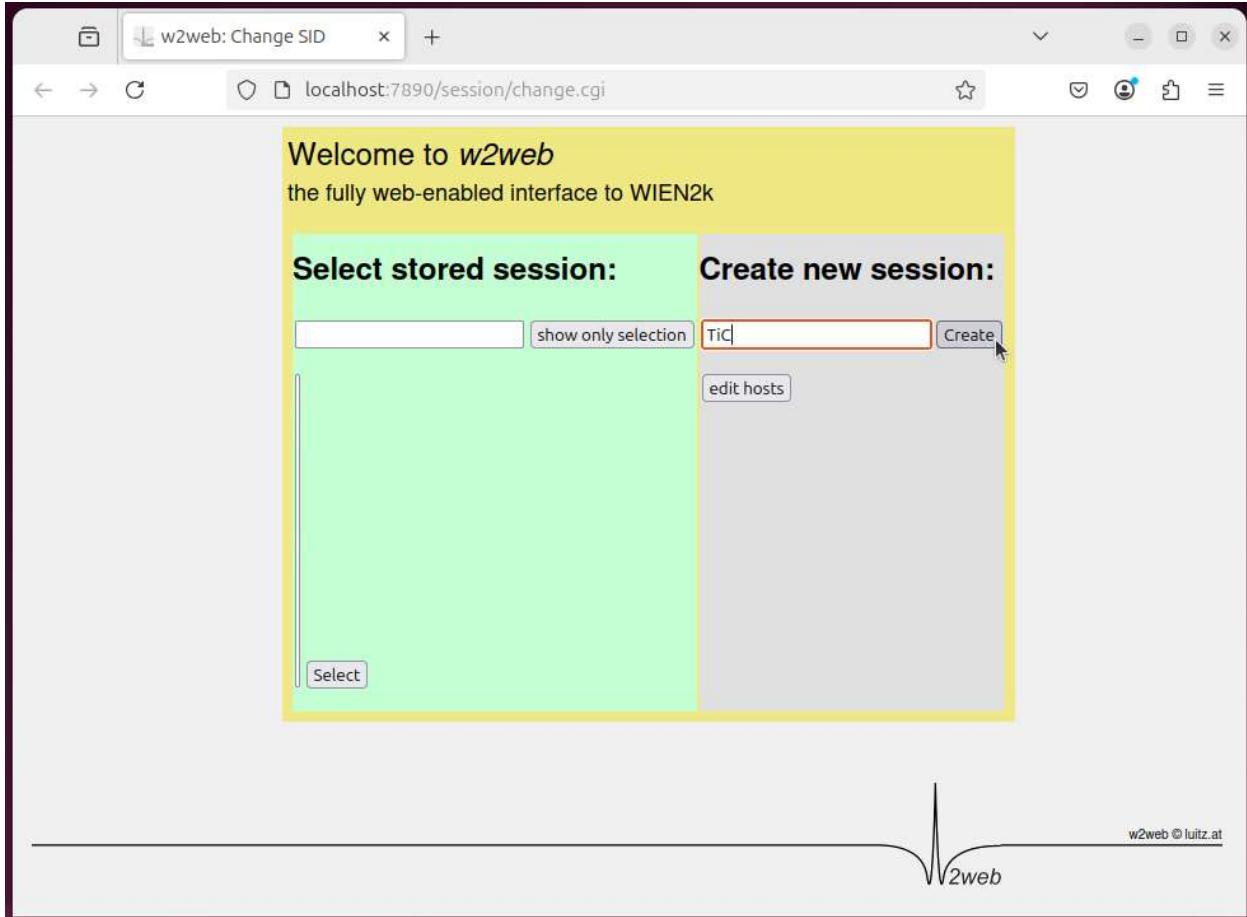


4. Enter url <http://localhost:7890>, type your w2web username and password, then click “Sign in” to login to w2web:

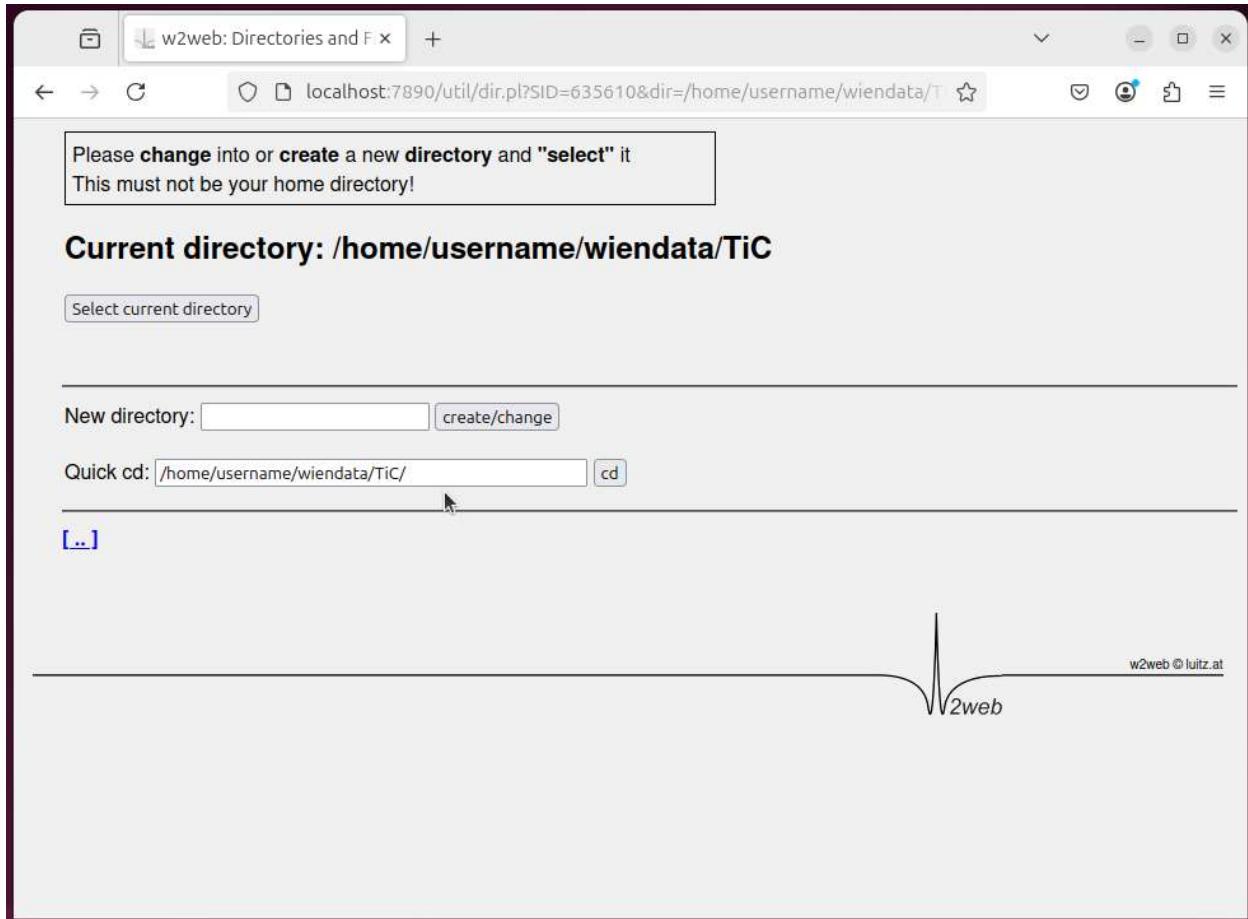


Create a new session (calculation)

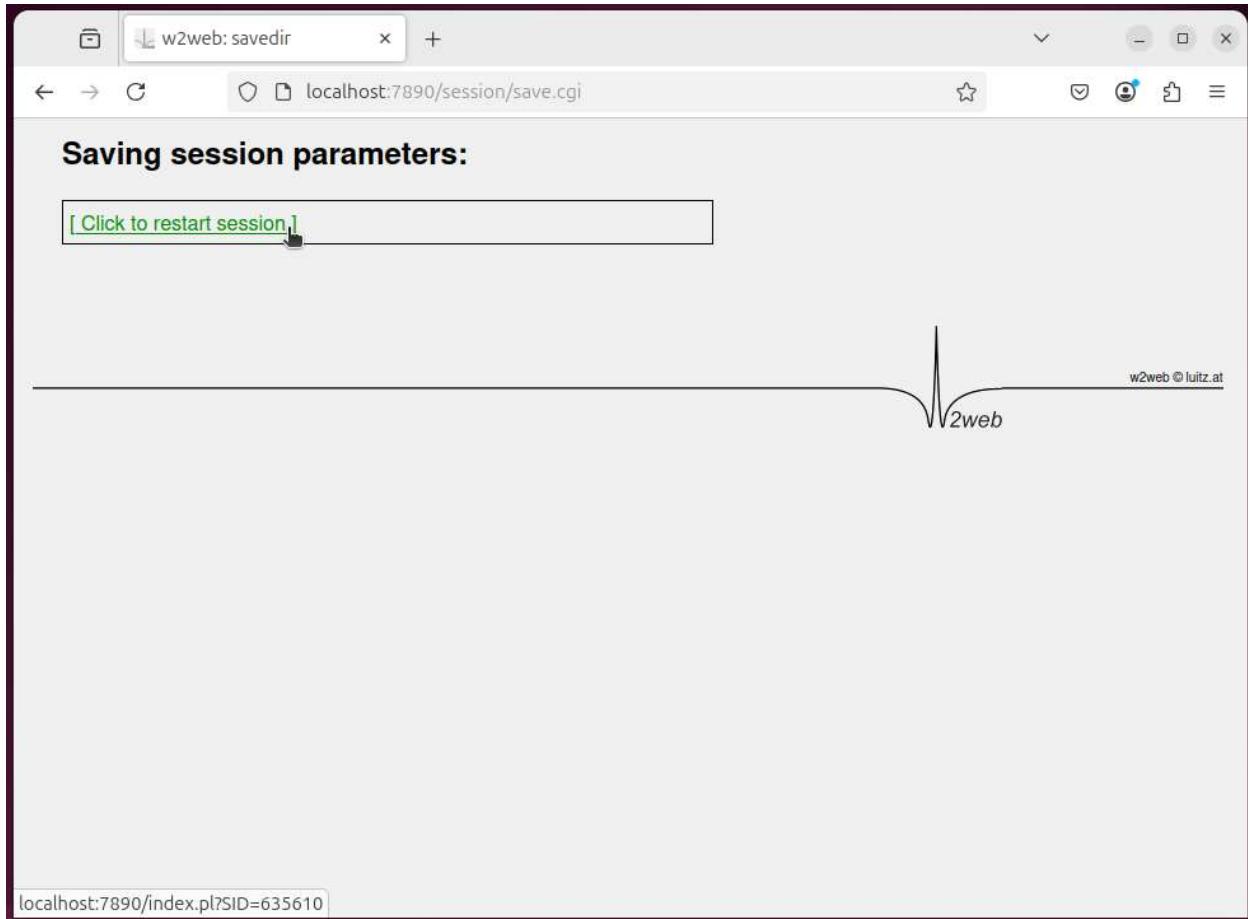
5. Enter “TiC” in the “Create new session.” box and then click the “Create” button:



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:

TiC@localhost

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

18:01:24 idle
[refresh] | [no refresh]

w2web, the fully web-enabled interface to WIEN2k

Session Name: TiC
Session ID: 199979
Directory: /home/username/wiendata/TiC
Last changed: Sun Feb 1 18:00:51 2026
Comments:
 spin polarized calculation
 AFM calculation
 complex calculation (no inversion)
 parallel calculation

Change session information

w2web © luitz.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]
Idea and realization by
[luitz.at] © 2001-2006

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 TiC@localhost web interface. The left sidebar has a yellow background with various navigation links. The main content area has a white background. It features a molecular model of TiC with atoms labeled T, I, E, N, W, and 2k. A message says "You do not have a TiC.struct file yet." Below it, a box says "You can create it using STRUCTGEN. Please specify the number of independent atoms of your initial structure!" with a "Number of atoms: 2" input field and a "Generate template" button. There are also sections for "Use cif2struct to convert a 'cif' file:" and "Use xyz2struct to convert a 'xyz' file:", both with "Upload" buttons. At the bottom, there's a note about uploading files from the local computer.

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 StructGen™ software interface running in a web browser (localhost:7890/index.pl?SID=635610). The session is titled "TiC".

Execution >>

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

Utils. >>

- [Tasks >>]

Files >>

- [struct file(s)]
- [input files]
- [output files]
- [SCF files]

Session Mgmt. >>

- [change session]
- [change dir]
- [change info]

Configuration

Usersguide

- [html-Version]
- [pdf-Version]

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

StructGen™

You have to click "Save Structure" for changes to take effect!

Title: TiC

Lattice:

Type: P

P
F
B
CXY
CYZ
CXZ
R
H
1_P1

[Spacegroups from Bilbao Cryst Server.]

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 Z = 0.000 RMT = 2.0000 [remove atom]
 Pos 1: x = 0.00000000 y = 0.00000000 z = 0.00000000 [remove] [split]
 [add position]

Atom 2: C Z = 0.000 RMT = 2.0000 [remove atom]
 Pos 1: x = 0.5 y = 0.5 z = 0.5 [remove] [split]
 [add position]

[add an atom]

Number of symmetry operations: generate

You have to click "Save Structure" for changes to take effect!

Save Structure

20. Click the “Save Structure” button

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

TiC@localhost

localhost:7890/index.pl?SID=635610

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

12:57:23 idle
[refresh] | [no refresh]

StructGen™

- **[set automatically RMT and continue editing] (do it at least once!)**
- [\[save file and clean up \] \(when you are done\)](#)
- [\[continue editing \]](#)
- [\[abort editing and restore original file \]](#)

w2web © luitz.at

Execution >>

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

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]

localhost:7890/util/structrmt.pl?SID=635610

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

Session: [[TiC](#)]
 /home/username/wiendata/TiC

12:57:23 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

w2web © luitz.at

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

The screenshot shows the StructGen™ software interface. On the left, there is a sidebar with various menu options like "Execution >>", "StructGen™", "view structure", etc. The main area has a yellow header bar with "Session: [TiC]" and the path "/home/username/wiendata/TiC". The title "StructGen™" is displayed prominently. A message at the top says "You have to click "Save Structure" for changes to take effect!" with a "Save Structure" button below it. The "Title" field contains "TiC". Under "Lattice", "Type: F" is selected. A dropdown menu lists space groups: P, F, B, CXY, CYZ, CXZ, R, H, and 1_P1. Below this, "Spacegroups from Bilbao Cryst Server" is mentioned. "Lattice parameters in A" are listed as $a=4.32800003862$, $b=4.32800003862$, $c=4.32800003862$, $\alpha=90.000000$, $\beta=90.000000$, and $\gamma=90.000000$. The "Inequivalent Atoms: 2" section shows two atoms: Atom 1 (Ti) with Z=22.000, RMT=2.17, and Atom 2 (C) with Z=6.000, RMT=1.77. Both atoms have "remove atom", "remove", "split", and "add position" buttons. There is also a "[add an atom]" link. A note at the bottom says "Number of symmetry operations: generate". The footer includes a copyright notice: "Idea and realization by [juitz.at] © 2001-2006".

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.php?SID=635610). The session is titled "TiC".

Lattice Parameters:

- Type: F
- Spacegroups from Bilbao Cryst Server: 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	Symbol	X	Y	Z	RMT
Atom 1	Ti	0.00000000	0.00000000	22.000	2.0000
Atom 2	C	0.50000000	0.50000000	6.000	1.9000

Number of symmetry operations: generate

View only mode -->[edit STRUCT file]

Idea and realization by [Jürgen Jauzat](#) © 2001-2006

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:

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

12:59:25 idle
[refresh] | [no refresh]

Initialize WIEN2k calculation

Fast mode (recommended):

This is in general the **recommended** way of initialization (except for antiferromagnets, supercells and slabs with unclear symmetry).

Specify the **precision level** to get an adapted input for your selected case. It will adapt RKMAX, GMAX, HDLOs and K-mesh to your problem.

Check STDOUT for errors. When errors occur, run in individual mode (at least the symmetry programs)

- select spin-polarized calculation
- Precision level (0-3; 0n-3n for non-metals, default=1)
- RMT reduction by X % (default: RMT not changed)
- VXC option (13=PBE, 5=LDA, 11=WC, 19=PBEsol) [default=13]
- energy separation between core/valence (default: -6.0 Ry)
- RKMAX (3.0 - 10.0, be careful, this may influence the cputime by ORDERS of magnitude) [[Click here for more info.](#))
- use TEMP (extrapolated to 0K) with smearing by X Ry (default: TETRA)
- use TEMPS (finite T) with smearing by X Ry (default: TETRA)
- use X k-points in full BZ (be careful, this may influence the cputime by ORDERS of magnitude; [[Click here for more info.](#))
- do not run dstart (after a first scf calculation in order to create higher precision inputs)

[CHECK BATCH VALUES](#)

Individual mode (phase 1)

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	check TiC.in1_st set RKmax (usually 5.0-9.0). [Click here for more info.)	view TiC.outputnd and cp TiC.in0_std TiC.in0	check if gmax>gmin
view outputnn	check TiC.in2_st set Fermi-method and GMAX	Perform spin-polarized calc.?	
x sgroup	Prepare input files	<input type="button" value="No"/>	
view outputsgroup			
x symmetry			

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

The screenshot shows a web browser window titled "TiC@localhost" at the URL "localhost:7890/index.pl?SID=635610". The page displays a molecular structure with atoms labeled I, E, W, N, and 2k. A message at the top right says "NN needs input". Below the structure, a text input field contains the value "2" and a button labeled "Execute!". To the left of the main content area, there is a sidebar with various navigation links under categories like "Execution >>", "StructGen™", "view structure", etc. At the bottom left, there is a note about the source: "Idea and realization by Jultz.at © 2001-2006".

31. Click the “initlapw” button:

Session: [TiC]
/home/username/wiendata/TiC
13:00:26 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)]
dfac,DSTMAX: 2.0000000000000000 20.00000000000000
iix,iiy,iiz 5 5 5 40.89369000000000
40.89369000000000 40.89369000000000

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
NN ENDS
0.002u 0.005s 0:00.00 0.0% 0+0k 0+32io 0pf+0w

```

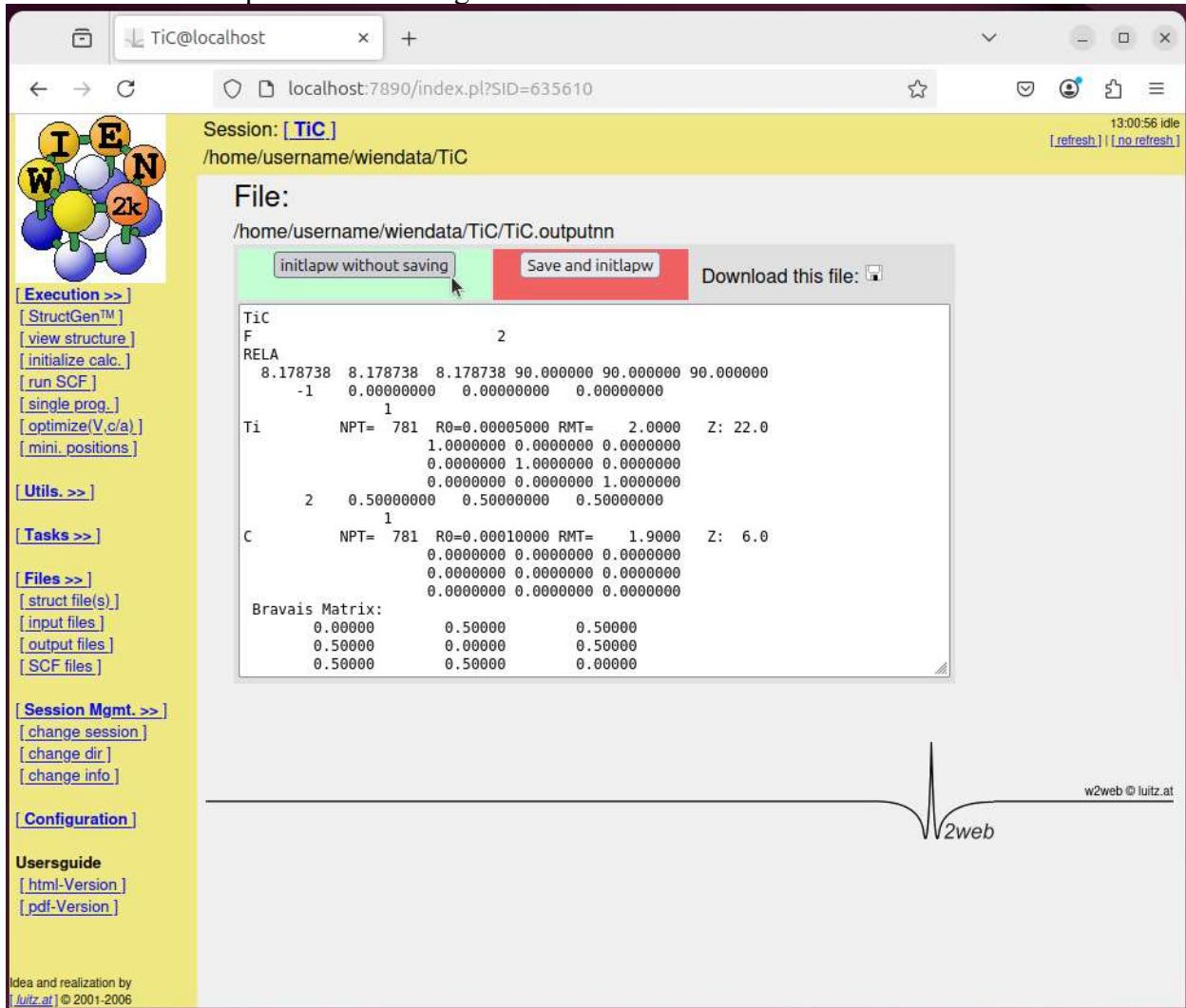
Continue with

initlapw

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w2web © luitz.at

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



The screenshot shows a web browser window titled "TiC@localhost" displaying session information for "TiC". The URL is "localhost:7890/index.pl?SID=635610". The session path is "/home/username/wiendata/TiC". On the left, there is a sidebar with various navigation links under categories like "Execution >>", "Utils. >>", "Tasks >>", "Files >>", "Session Mgmt. >>", "Configuration", and "Usersguide". A molecular model of TiC is shown at the top left. The main area contains session details and a command-line interface. The command-line interface shows the following output:

```

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

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

initlapw without saving
Save and initlapw
Download this file: □

TiC
F
RELA
 8.178738 8.178738 8.178738 90.000000 90.000000 90.000000
 -1 0.00000000 0.00000000 0.00000000
           1
Ti      NPT= 781 R0=0.00005000 RMT= 2.0000 Z: 22.0
        1.0000000 0.0000000 0.0000000
        0.0000000 1.0000000 0.0000000
        0.0000000 0.0000000 1.0000000
 2 0.50000000 0.50000000 0.50000000
           1
C       NPT= 781 R0=0.00010000 RMT= 1.9000 Z: 6.0
        0.0000000 0.0000000 0.0000000
        0.0000000 0.0000000 0.0000000
        0.0000000 0.0000000 0.0000000
Bravais Matrix:
 0.00000 0.50000 0.50000
 0.50000 0.00000 0.50000
 0.50000 0.50000 0.00000

```

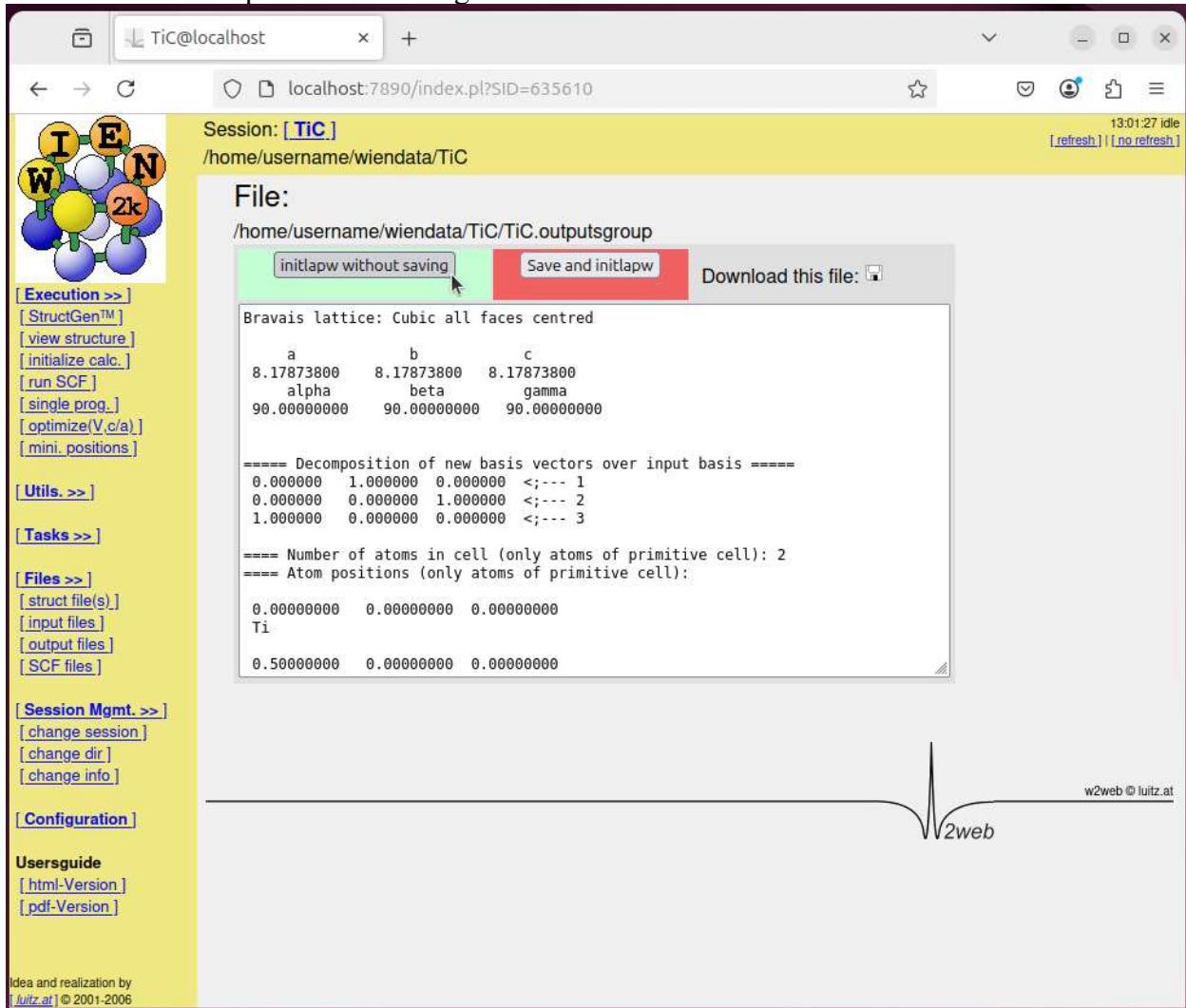
At the bottom right, there is a watermark "w2web © luitz.at" with a small logo.

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=635610". The page displays session information for "Session: [TiC]" located at "/home/username/wiendata/TiC". The commandline is "x sgroup" and the program input is empty. Resource usage is shown as 0.000u 0.001s 0:00.00 0.0% CPU, 0+0k 0+8io 0pf+0w. A "Continue with" section contains a button labeled "initlapw", which is being clicked by a mouse cursor. On the left, a sidebar lists various execution and utility options like "StructGen™", "view structure", "initialize calc.", etc. Below the sidebar are sections for "Files >>", "Session Mgmt. >>", "Configuration", and "Usersguide". At the bottom, there is a copyright notice: "Idea and realization by luitz.at © 2001-2006". The top right corner of the window shows the status "13:01:27 idle" and refresh/no refresh buttons.

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



The screenshot shows a web browser window titled "TiC@localhost" at the URL "localhost:7890/index.pl?SID=635610". The page displays session information for "Session: [TiC.]" located at "/home/username/wiendata/TiC". On the left, there's a sidebar with various navigation links under categories like "Execution >>", "Utils. >>", "Tasks >>", "Files >>", "Session Mgmt. >>", "Configuration", and "Usersguide". The main content area shows a molecular model of TiC and a text box containing the following output from a calculation:

```

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

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

initlapw without saving Save and initlapw 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
  
```

The "initlapw without saving" button is highlighted with a green background. The "Save and initlapw" button is red. A "Download this file:" link is also present. The bottom right corner of the page features a logo with the text "w2web © luitz.at" and a stylized "w2web" logo.

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

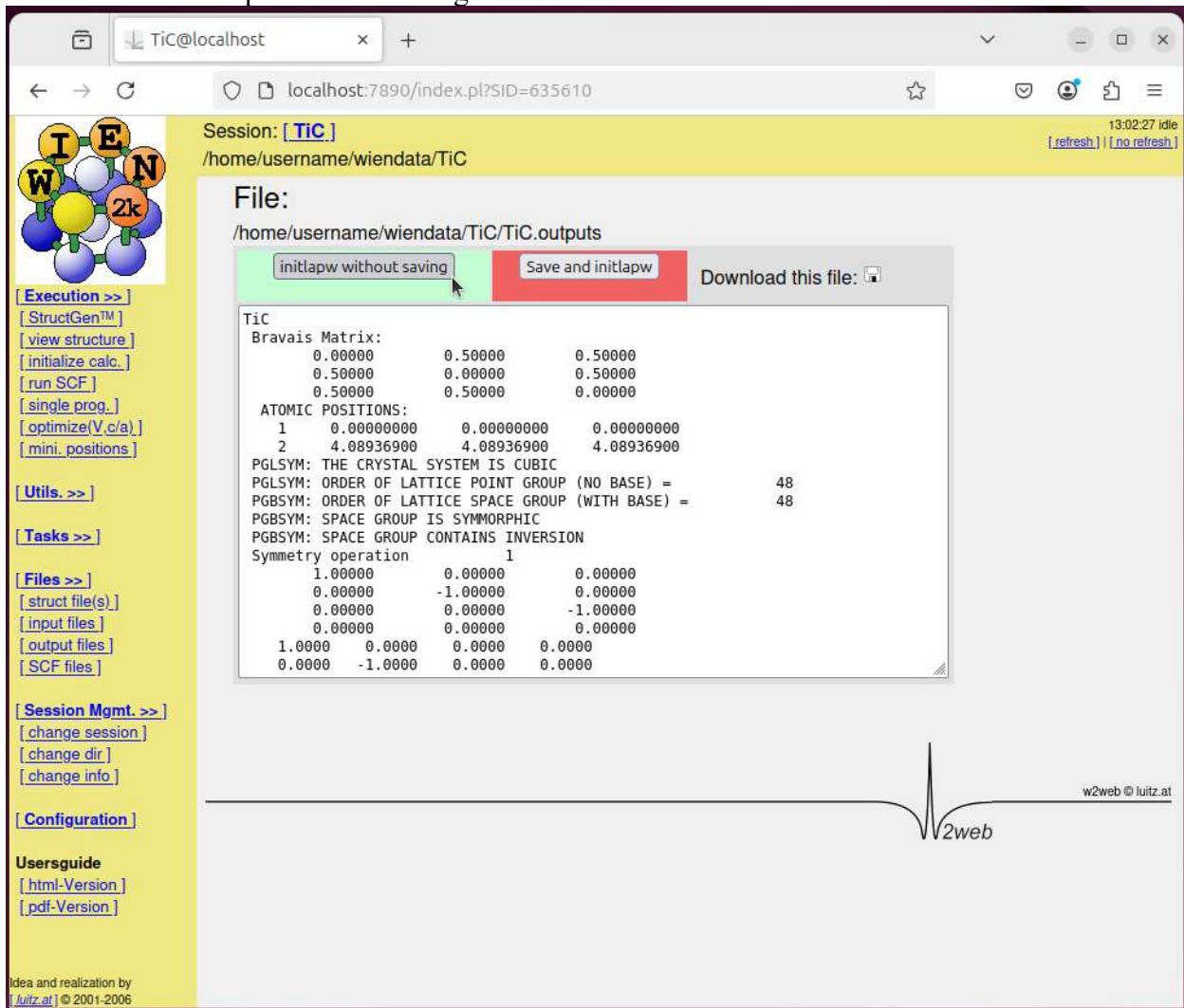
The screenshot shows the TiC@localhost web interface. On the left is a sidebar with various links like 'Execution >>', 'StructGen™', 'view structure', etc. The main area shows session details for 'TiC' at '/home/username/wiendata/TiC'. It includes several configuration options and a 'CHECK BATCH VALUES' button. Below this is a section titled 'Individual mode (phase 6)'. A prominent red box highlights a modal dialog box with the question 'Use struct-file generated by sgroup? (Usually NO, unless WARNINGS appeared above)'. Inside this dialog, a mouse cursor is clicking the 'No' button. To the right of the dialog, there are other buttons for 'x nn', 'check TiC.in1_st', 'view outputnn', 'x group', 'view outputgroup', 'x kgen', 'view klist', 'x start', and 'view outputst'. There are also checkboxes for 'RKmax', 'Fermi-method and GMAX', 'Prepare input files', and 'interactively'. At the bottom of the main area, there are links for 'x symmetry', 'copy struct_st', 'instgen_lapw', and 'view outputst'.

39. Click the “x symmetry” button

40. Click the “initlapw” button:

The screenshot shows a web browser window titled "TiC@localhost" at the URL "localhost:7890/index.pl?SID=635610". The page displays a session titled "Session: [TiC.]" with the path "/home/username/wiendata/TiC". The commandline is "x symmetry" and the program input is "". The output section shows "SPACE GROUP CONTAINS INVERSION" followed by a series of numerical values. Below this, there is a "Continue with" section containing a button labeled "initlapw", which is being clicked by a mouse cursor. To the right of the main content area, there is a small logo with the text "w2web © luitz.at" and "2web". On the left side of the page, there is a sidebar with various navigation links under categories like "Execution >>", "Tasks >>", "Files >>", "Session Mgmt. >>", "Configuration", and "Usersguide". At the bottom left, there is a note about the source: "Idea and realization by luitz.at © 2001-2006".

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



The screenshot shows a web browser window titled "TiC@localhost" at "localhost:7890/index.pl?SID=635610". The session name is "TiC" and the path is "/home/username/wiendata/TiC". The output pane displays crystallographic information:

```

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

```

The "initlapw without saving" button is highlighted in green. The "Save and initlapw" button is red. A "Download this file:" link is also present.

43. Click the “instgen_lapw” button

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

The screenshot shows a web browser window titled "TiC@localhost" with the URL "localhost:7890/index.pl?SID=635610". The page displays a molecular model of TiC with atoms labeled Ti, C, W, E, N, and 2k. On the left sidebar, there are several menu options under "Execution >>" and "Files >>". The main content area is titled "Specify options for instgen_lapw" and asks "Chose atomic configurations as:". There are three radio button options: "spin up (default)", "spin dn", and "no spin-polarization", with "no spin-polarization" selected. Below this, it says "selected below: chose u,d,n for each atom. (For AFM calculations you must define the proper magnetic order here !!!)". It shows "atom 1: Ti" with a spin value of "u" and "atom 2: C" also with a spin value of "u". A large "Execute!" button is at the bottom of this section. In the top right corner of the main area, there is a message "instgen_lapw needs input" and a timestamp "13:02:57 idle". The bottom right corner features a logo with the text "w2web @ luitz.at" and "2web".

45. Click the “initlapw” button:

TiC@localhost

localhost:7890/index.pl?SID=635610

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

13:02:57 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

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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]

Idea and realization by
[luitz.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:

The screenshot shows a web browser window titled "TiC@localhost" at the URL "localhost:7890/index.pl?SID=635610". The session is identified as "TiC." and the working directory is "/home/username/wiendata/TiC". A message at the top right says "LSTART needs input". On the left, there's a sidebar with various menu items under "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", and "Usersguide" (html-Version, pdf-Version). Below the sidebar, it says "Idea and realization by [luitz.at](#) © 2001-2006". The main content area has a molecular model of TiC with atoms labeled T, I, E, W, N, and 2k. It displays a dropdown menu for "Select Exchange Correlation Potential" set to "PBE-GGA (Perdew-Burke-Ernzerhof 96)". Below that, it asks for "ENERGY to separate core and valence states" with a field containing "-6.0" and a note "(recommended: -6.0 Ry)". It also says "(check how much core charge leaks out of MT-sphere)". At the bottom is a large "Execute!" button. In the bottom right corner of the main area, there's a small logo with the text "w2web" and "2web" above it.

48. Click the “initlapw” button:

TiC@localhost localhost:7890/index.pl?SID=635610 13:03:27 idle
[\[refresh.\]](#) | [\[no refresh.\]](#)

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

Commandline: x lstart
 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
 0.054u 0.002s 0:00.05 100.0% 0+0k 0+968io 0pf+0w

Continue with [initlapw](#)

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

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

The figure shows a screenshot of a web browser window titled "TiC@localhost". The URL is "localhost:7890/index.pl?SID=635610". The session name is "[TiC]". The main content area displays a molecular model of Titanium Carbide (TiC) with atoms labeled W, E, N, and Ti. Below the model, there is a sidebar with various execution and utility options like "StructGen™", "view structure", "initialize calc.", etc. The central part of the screen shows the output of a calculation. The output starts with "Ti" and "RHFS", followed by iteration information: "NUMBER OF ITERATIONS 350", "PRECISION OF ENERGIES 5.00E-07", "WAVEFUNCTION 1.00E-06", and "POTENTIAL 1.00E-06". It then details an integration step: "INTEGRATION WITH 971 POINTS STARTING AT 0.0011/22 AND INCREMENT 0.0136". Finally, it lists orbital occupation and trial energies:

ORBITAL	OCCUPATION	TRIAL ENERGIES
15	1.000	-1.210000E+02
15	1.000	-1.210000E+02

At the bottom right, there is a watermark for "w2web" with the URL "w2web @ luitz.at".

51. Click the “check TiC.in1_st” button
52. Change “emax” in the file from 1.5 to 2.0
53. Click the “Save and initlapw” button:

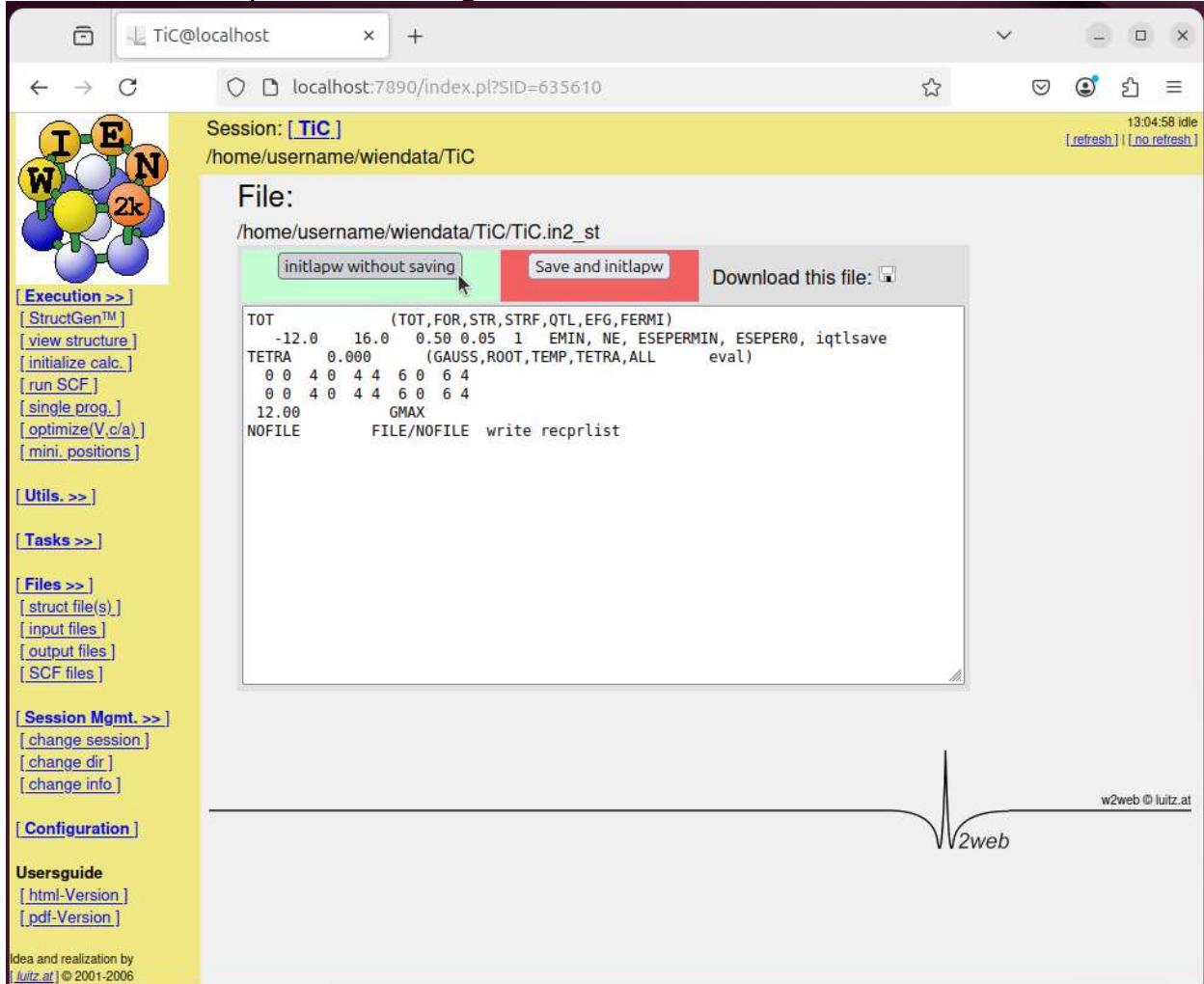
The screenshot shows a web-based graphical user interface for a quantum chemistry program. On the left, there's a sidebar with various menu items like 'Execution >>', 'Files >>', 'Session Mgmt. >>', 'Configuration', and 'Usersguide'. The main area features a molecular model of TiC and a code editor displaying a configuration file. The code editor has a red box around the 'Save and initlapw' button. The status bar at the top right shows '13:04:58 idle [refresh] [no refresh]'.

```

Session: [TiC]
/home/username/wiendata/TiC
File:
/home/username/wiendata/TiC/TiC.in1_st
initlapw without saving Save and initlapw Download this file: □
WFFIL EF= 0.50000 (WFFIL, WFPRI, ENFIL, SUPWE)
7.00 10 4 ELPS xg BL 64 (R-MT*K-MAX,MAX L IN WE,V,NMT,LIB)
0.30 5 0 (GLOBAL E-PARAMETER WITH n OTHER CHOICES, global APW/LAPW)
0 0.30 0.0000 CONT 1
0 -4.30 0.0001 STOP 1
1 0.30 0.0000 CONT 1
1 -2.54 0.0010 CONT 1
2 0.30 0.0010 CONT 1
0.30 3 0 (GLOBAL E-PARAMETER WITH n OTHER CHOICES, global APW/LAPW)
0 0.30 0.0000 CONT 1
0 -0.71 0.0010 CONT 1
1 0.30 0.0000 CONT 1
K-VECTORS FROM UNIT:4 -9.0 2.0 37 emin / de (emax=Ef+de) / nband

```

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



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

File:
 /home/username/wiendata/TiC/TiC.in2_st

initlapw without saving Save and initlapw Download this file:

```

TOT          (TOT,FOR,STR,STRF,QTL,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 recplist
  
```

w2web © luitz.at

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

The screenshot shows a web browser window titled "TiC@localhost" at the URL "localhost:7890/index.pl?SID=635610". The main content area displays session configuration options for a TiC session. On the left, a sidebar contains links for "Execution >>", "StructGen™", "view structure", "initialize calc.", "run SCF", "single prog.", "optimize(V,c/a)", "mini_positions", "Utils. >>", "Tasks >>", "Files >>", "Session Mgmt. >>", "Configuration", and "Usersguide". The "Configuration" section includes links for "html-Version" and "pdf-Version". At the bottom of the sidebar, it says "Idea and realization by [J. Luitz](#) © 2001-2006".

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

Session configuration options:

- RMT reduction by X % (default: RMT not changed)
- VXC option (13=PBE, 5=LDA, 11=WC, 19=PBESol) [default=13]
- energy separation between core/valence (default: -6.0 Ry)
- RKMAX (3.0 - 10.0, be careful, this may influence the cputime by ORDERS of magnitude) [\[Click here for more info.\]](#)
- use TEMP (extrapolated to 0K) with smearing by X Ry (default: TETRA)
- use TEMPS (finite T) with smearing by X Ry (default: TETRA)
- use X k-points in full BZ (be careful, this may influence the cputime by ORDERS of magnitude; [\[Click here for more info.\]](#))
- do not run dstart (after a first scf calculation in order to create higher precision inputs)

Your input seems to be ok and you can start the initialization

RUN BATCH INITIALISATION

Individual mode (phase 16)

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.

Buttons and status messages:

- x nn
- check TiC.in1_st set RKmax (usually 5.0-9.0). [\[Click here for more info.\]](#)
- view outputnn
- check if gmax>gmin
- x group
- view outputgroup
- check TiC.in2_st set Fermi-method and GMAX
- x symmetry
- copy struct_st and view outputs
- in0, in1, in2, inc and inm files generated
- instgen_lapw TiC.inst exists, run instgen_lapw only for non-default spin-configuration
- x lstart
- x kgen
- view klist
- view outputst
- x start interactively

57. Click the “x kgen” button

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

The screenshot shows a web browser window titled "TiC@localhost" with the URL "localhost:7890/index.pl?SID=635610". The page displays a session configuration for "TiC" with the path "/home/username/wiendata/TiC". On the left, there is a sidebar with various execution and utility buttons. The main area contains fields for "Number of k-points" (set to 1000), "Shift k-mesh (if applicable)" (set to Yes), and an "Execute!" button. A note below the input fields states: "(For experts: if Number of k-points is set to zero, you must specify 3 divisions of the reciprocal lattice vectors yourself, otherwise leave these fields blank!)" There are three empty input fields below the note. The bottom right corner features a logo with the text "w2web © luitz.at" and "2web".

59. Click the “initlapw” button:

The screenshot shows a web-based graphical user interface for a computational chemistry program named TiC. On the left, there is a sidebar with various buttons categorized under sections like 'Execution >>', 'Utils. >>', 'Tasks >>', 'Files >>', 'Session Mgmt. >>', 'Configuration', and 'Usersguide'. A large molecular structure diagram is displayed at the top left. The main area contains session information, command-line input, and output logs. A prominent button labeled 'initlapw' is highlighted with a mouse cursor. The bottom right corner features a logo for 'w2web'.

Session: [TiC]
 /home/username/wiendata/TiC
 Commandline: x kgen
 Program input is: " 1000 1 "
 NUMBER OF K-POINTS IN WHOLE CELL: (0 for 3 divisions of K, -1 for delta-K)
 length of reciprocal lattice vectors (bohr^-1): 1.331 1.331 1.331
 47 k-points generated, ndiv= 10 10 10
 delta-K (bohr^-1): 0.1331 0.1331 0.1331
 KGEN ENDS
 0.004u 0.006s 0:00.01 0.0% 0+0k 0+200io 0pf+0w

Continue with

initlapw

w2web © luitz.at
 w2web

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60. Click the “view klist” button

61. Click the “initlapw without saving” button:

The screenshot shows a web browser window titled "TiC@localhost" displaying a session for "TiC". The URL is "localhost:7890/index.pl?SID=635610". The page content includes a molecular model of TiC, a sidebar with various menu options, and a central area for viewing and manipulating klists. A modal dialog box is open, showing a table of data with the following rows:

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

The "initlapw without saving" button is highlighted with a green background and white text. Other buttons in the row include "Save and initlapw" and "Download this file: .

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

The screenshot shows a web browser window titled "TiC@localhost" at the URL "localhost:7890/index.pl?SID=635610". The page displays session information for "Session: [TiC.]" located at "/home/username/wiendata/TiC". The commandline is "x dstart" and the program input is empty. A detailed execution log follows:

C	T	F	DSTART ENDS	0.785u 0.006s 0:00.79 98.7%	0+0k 0+368io 0pf+0w
Continue with					
<input type="button" value="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 "Idea and realization by [luitz.at](#) © 2001-2006". On the right, there is a watermark for "w2web © luitz.at" with a stylized heart logo.

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:

```

kmt(min)*kmax =    7.00000
      9         9         9         7         7         7
      9         9         9
gmin =    7.36842
gmax =   12.00000

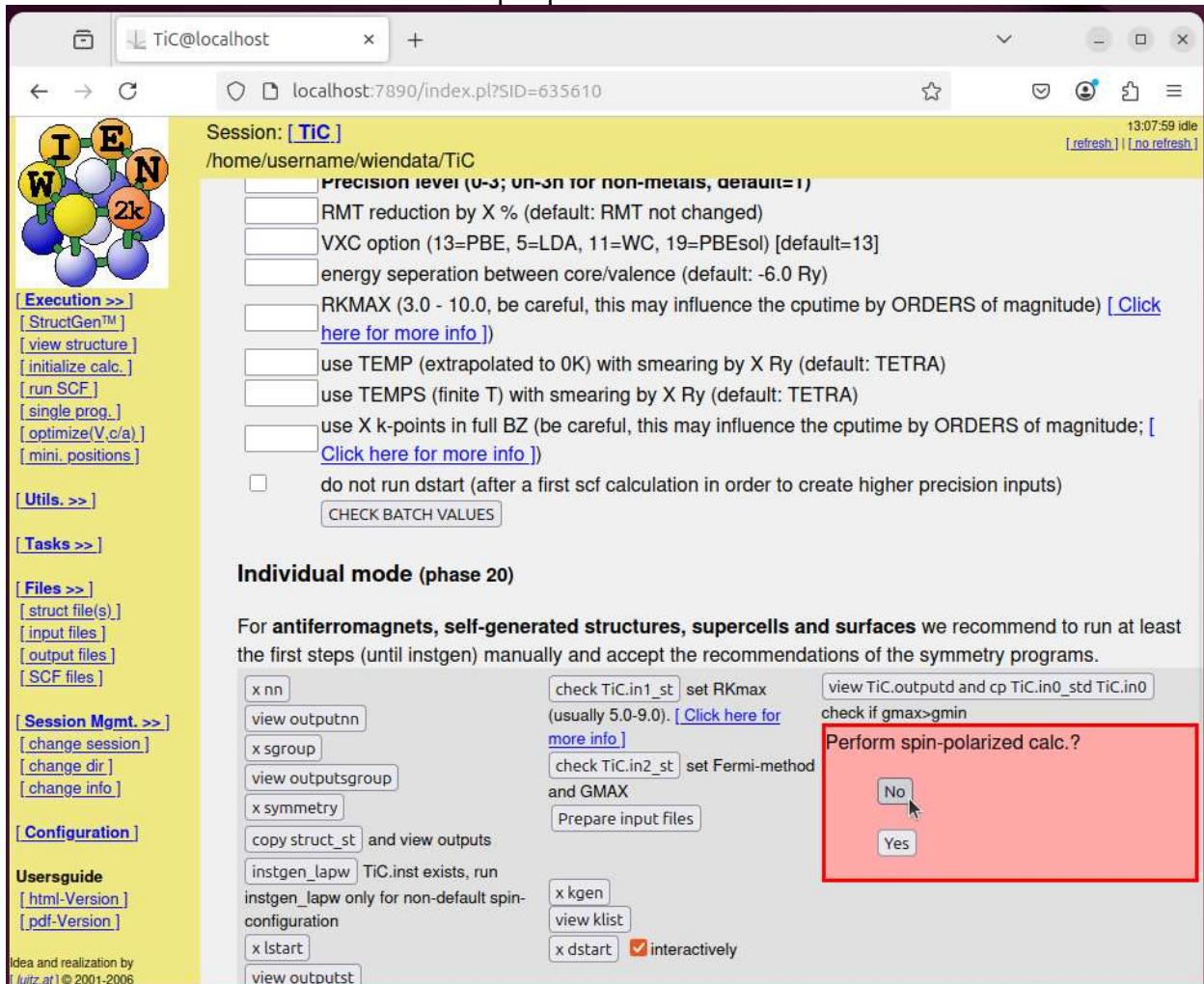
cutoff distance for superposition:   16.205
unitcell range:   4   4   4

ATOM =    1 ATOMNAME =Ti
LMAX =  5 LM =  0 0 4 0 4 4 6 0 6 4
Charge decomposition: ZZ MT tail MT+tail
          22.00000 19.39153 2.60847 22.00000
Calculated number of neighbours, nneg = 251
:INT001: CHARGE SPHERE 1 = 19.823810

ATOM =    2 ATOMNAME =C
  
```

w2web © luitz.at
 w2web

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



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

TiC@localhost x +

localhost:7890/index.pl?SID=635610

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

13:08:29 idle
[\[refresh\]](#) | [\[no refresh\]](#)

use T EMPIR (extrapolated to 0K) with smearing by X Ry (default: TETRA)
 use TEMPS (finite T) with smearing by X Ry (default: TETRA)
 use X k-points in full BZ (be careful, this may influence the cputime by ORDERS of magnitude; [[Click here for more info.](#)])
 do not run dstart (after a first scf calculation in order to create higher precision inputs)
[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	check TiC.in1_st set RKmax (usually 5.0-9.0). [Click here for more info.]	view TiC.outputn and cp TiC.in0_std TiC.in0
view outputnn		check if gmax>gmin
x sgroup	check TiC.in2_st set Fermi-method and GMAX	Prepare input files
view outputsgroup		
x symmetry		
copy struct_st and view outputs	x kgen	
instgen_lapw TiC.inst exists, run	view klist	
instgen_lapw only for non-default spin-configuration	x start	<input checked="" type="checkbox"/> interactively
x start	view outputst	

Initialization done

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

localhost:7890/exec/scf.pl?SID=635610

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:

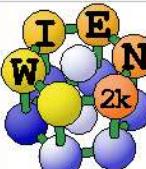
70. As shown, this calculation converges after 12 cycles:

TiC@localhost

localhost:7890/index.pl?SID=635610

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

13:10:00 idle
[\[refresh.\]](#) | [\[no refresh.\]](#)



Execution >>

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

Utils. >>

Tasks >>

Files >>

- [\[struct file\(s\)\]](#)
- [\[input files\]](#)
- [\[output files\]](#)
- [\[SCF files\]](#)

Session Mgmt. >>

- [\[change session\]](#)
- [\[change dir\]](#)
- [\[change info\]](#)

Configuration

Usersguide

- [\[html-Version\]](#)
- [\[pdf-Version\]](#)

Idea and realization by
[Jürgen Lutz](#) © 2001-2006

```

LAPW0 END
LAPW1 END
LAPW2 END
CORE END
MIXER END
ec cc fc and str_conv 1 0 1 1
in cycle 9      ETEST: .0002736650000000    CTEST: .0396237    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
  
```

Plot electron density

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

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

13:10:30 idle

Electron density plots

You must have a valid TiC.vector file (from an scf calculation).
 If you don't have it, you must run "x lapw1" with an appropriate input.

Select E-range for lapw2 for a density without semicore or within an E-window.
 For proper values check energy-parameters and eigenvalues or band-ranges in the corresponding scf-files

Calculate climval with Emin and Emax so

For difference densities only !

default valence states: put P for all your states

Calculate atomic valence densities

Calculate atomic valence densities as defined above

(or create TiC.in5 / execute lapw5 below)

Edit input-file and select the appropriate option for lapw5 below

-val Calculate density with: -diff -val/-tot -pot/-coulomb/-exchange(2)/-halfr2v/-tau -sub/-add/-none

Plot Density or download [\[TiC.rho.\]](#) for plotting with your own plotting program

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

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

TiC@localhost x +

localhost:7890/index.pl?SID=635610

Session: [TiC]
/home/username/wiendata/TiC
13:10:30 idle
[refresh] [no refresh]

Commandline: x lapw2 -emin -1.0
Program input is: " "

LAPW2 END
0.131u 0.137s 0:00.26 100.0% 0+0k 0+520io 0pf+0w

Continue with

continue with electron density

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2web

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]

Configuration

Usersguide
[html-Version]
[pdf-Version]

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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

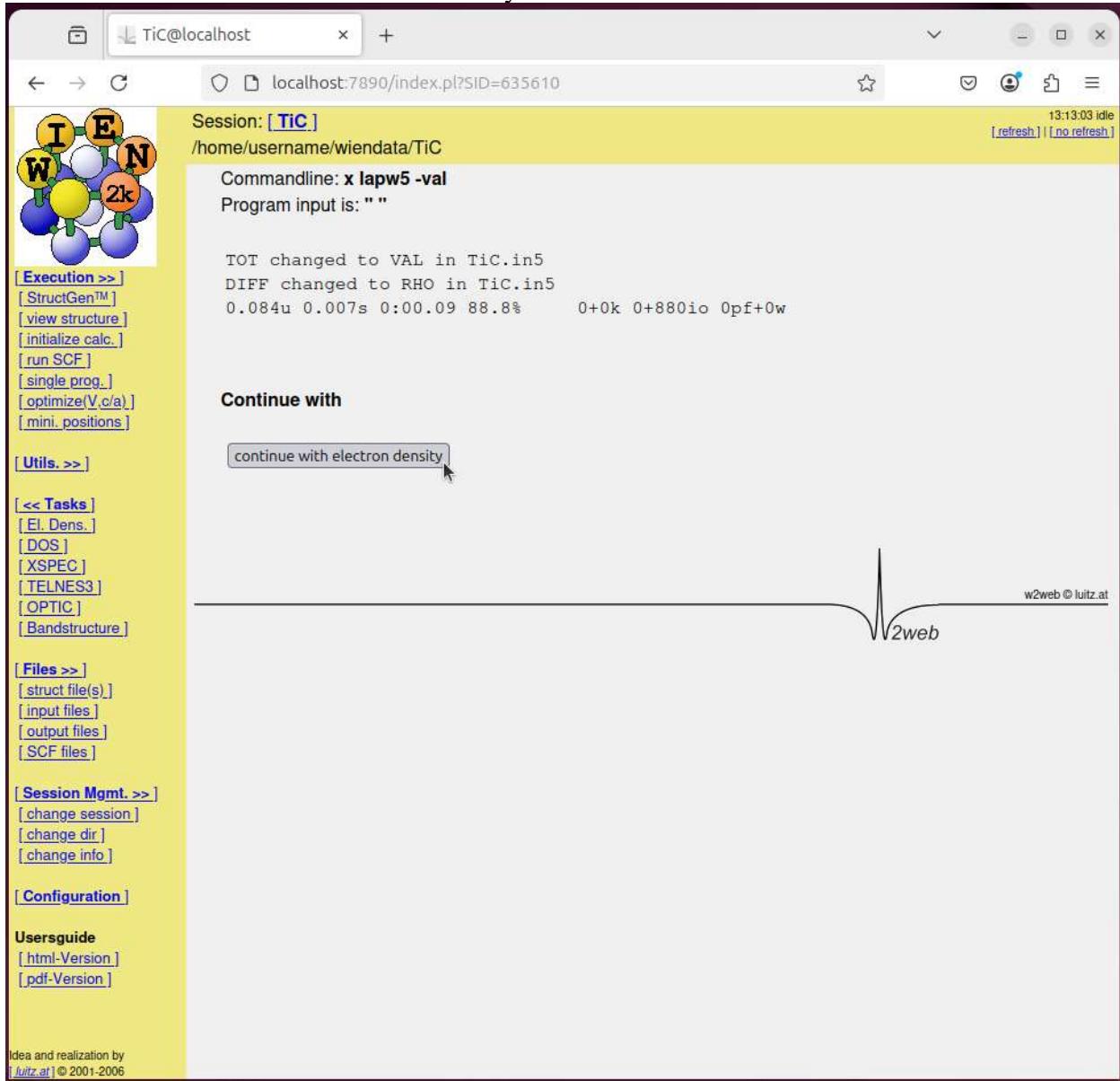
ADD was removed

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

The screenshot shows the WIEN2k web interface. On the left, there's a sidebar with various buttons for execution, tasks, files, session management, and configuration. The main area shows a session titled "Session: [TiC]" with the path "/home/username/wiendata/TiC". A text input field contains the command "continue with electron density without saving". To its right is a red-bordered button labeled "Save and continue with electron density", which is the target of a mouse cursor. Below the text input, there's a code editor window displaying an input file with several lines of text. At the bottom right of the screen, there's a small logo for "w2web" and the URL "w2web@luitz.at".

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”

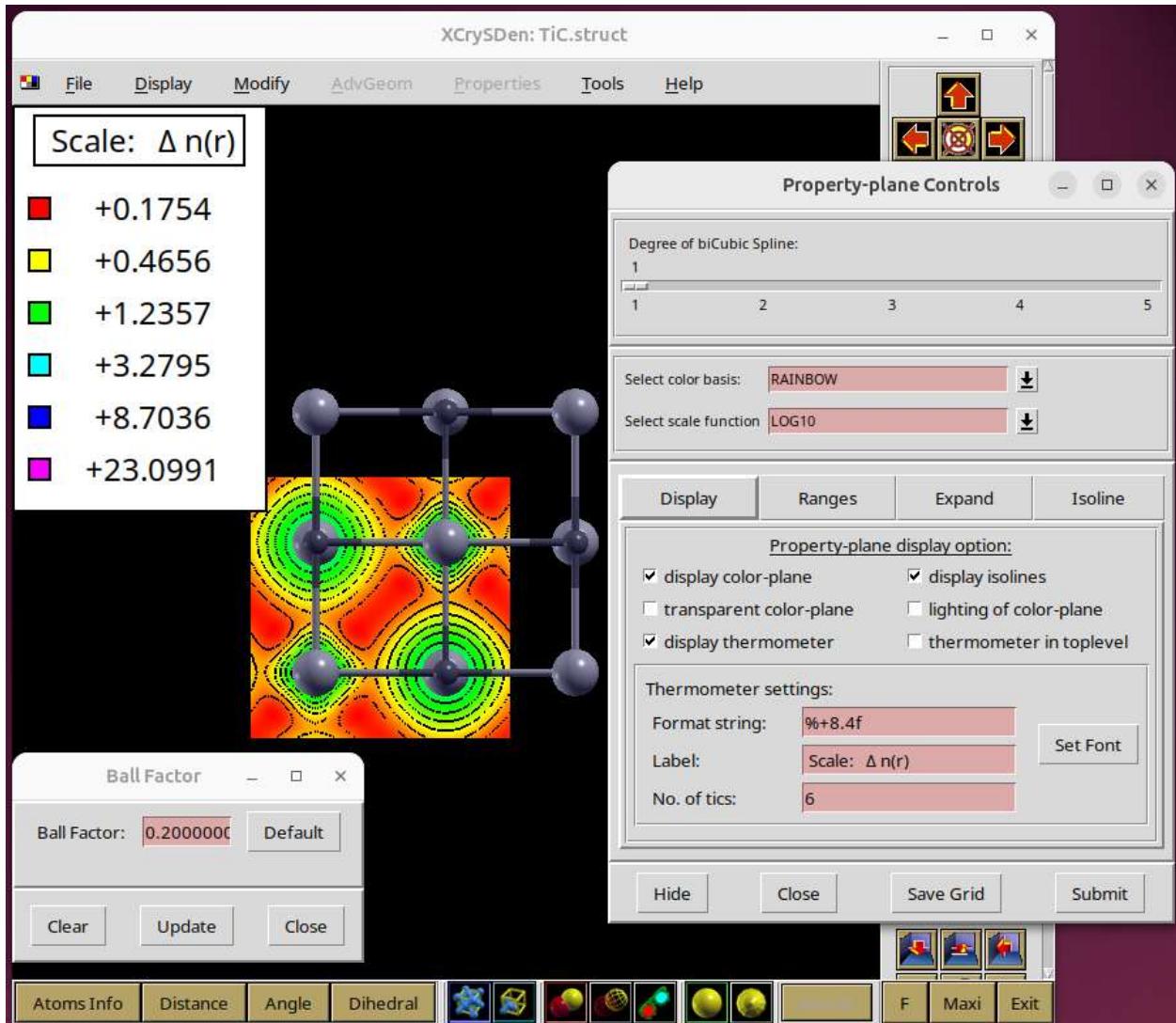
83. Click the “Submit” button

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]):



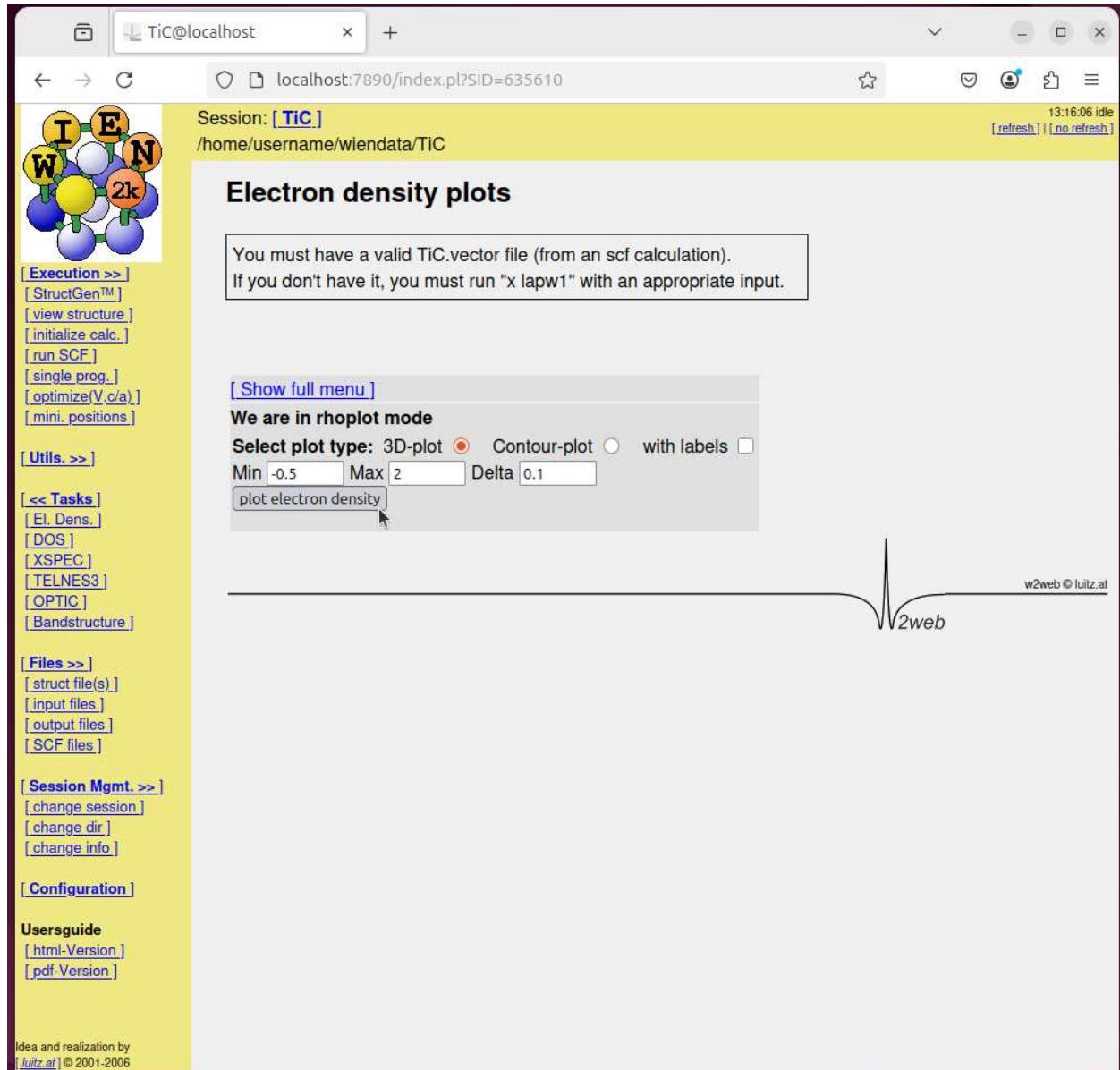
[2] http://www.wien2k.at/reg_user/textbooks/usersguide.pdf

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

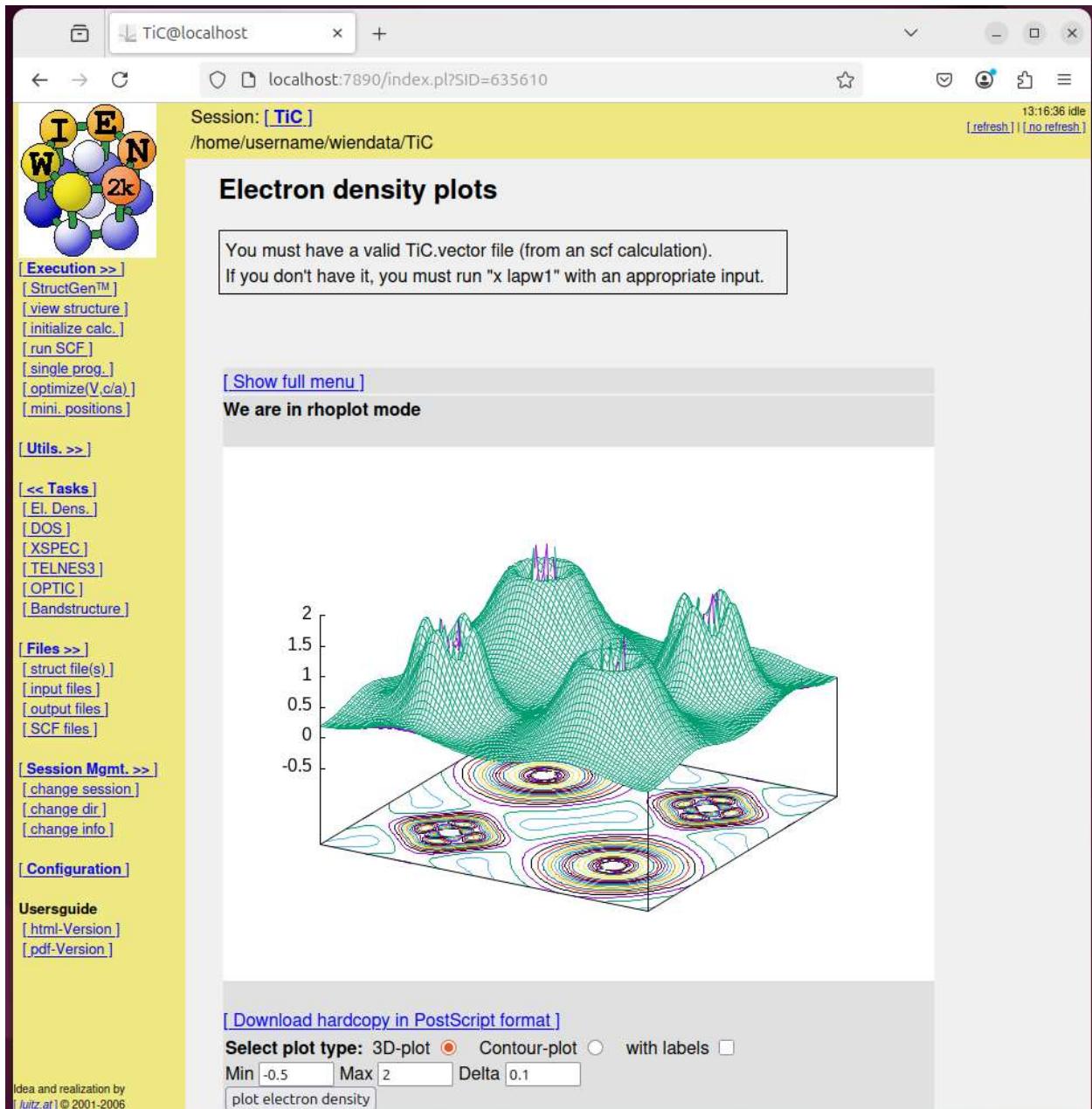
89. In the left menu, click “El. Dens.” under “Tasks”

90. Click the “rhoplot” button

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



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



Plot density of states (DOS)

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

94. Click on “x lapw2 -qtl”:

Density of states

Optional steps:

- `edit TiC.in1` Edit TiC.in1 and specify a larger E-max (bottom of file)
- `x kgen` Prepare a denser k-mesh
- `x lapw1` Create eigenvalues at denser k-mesh or higher E-max interactively

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

- `edit TiC.inq` Edit input-file for QTL
- `x qtl` Calculate partial charges with QTL program so interactively

Necessary steps:

- `x lapw2 -qtl` Calculate partial charges so interactively

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

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

`x tetra` Calculate partial DOS interactively

`view TiC.outputt` Check output of TETRA

OPTIONAL: Calculate renormalized DOS

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

`dosplot` Plot DOS using renormalized DOS or download DOS-data for plotting with your plotting program:

`save_lapw -dos` with name:

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

95. Click on “continue with DOS”:

TiC@localhost

localhost:7890/index.pl?SID=635610

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

13:17:07 idle
[refresh] | [no refresh]

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

LAPW2 END
0.041u 0.031s 0:00.07 100.0% 0+0k 0+480io 0pf+0w

Continue with

continue with DOS

w2web © luitz.at

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]

Configuration

Usersguide [html-Version.] [pdf-Version]

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

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
```

The screenshot shows a web-based graphical user interface for the TiC software. The title bar says "TiC@localhost". The URL in the address bar is "localhost:7890/index.pl?SID=635610". The session name is "Session: [TiC]" and the path is "/home/username/wiendata/TiC". The time "13:20:08 idle" is shown in the top right.

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

Buttons: "continue with DOS without saving" (green), "Save and continue with DOS" (red, highlighted), "Download this file:

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, max_nr_of_summands
2 5              # this sums dos-cases 2+5 from the input above
```

Left sidebar (yellow background):

- [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]
- [Configuration]
- Usersguide
 - [html-Version]
 - [pdf-Version]

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

w2web © iulz.at

2web

98. Click "Save and continue with DOS"

99. Click “x tetra”

100. Click “continue with DOS”:

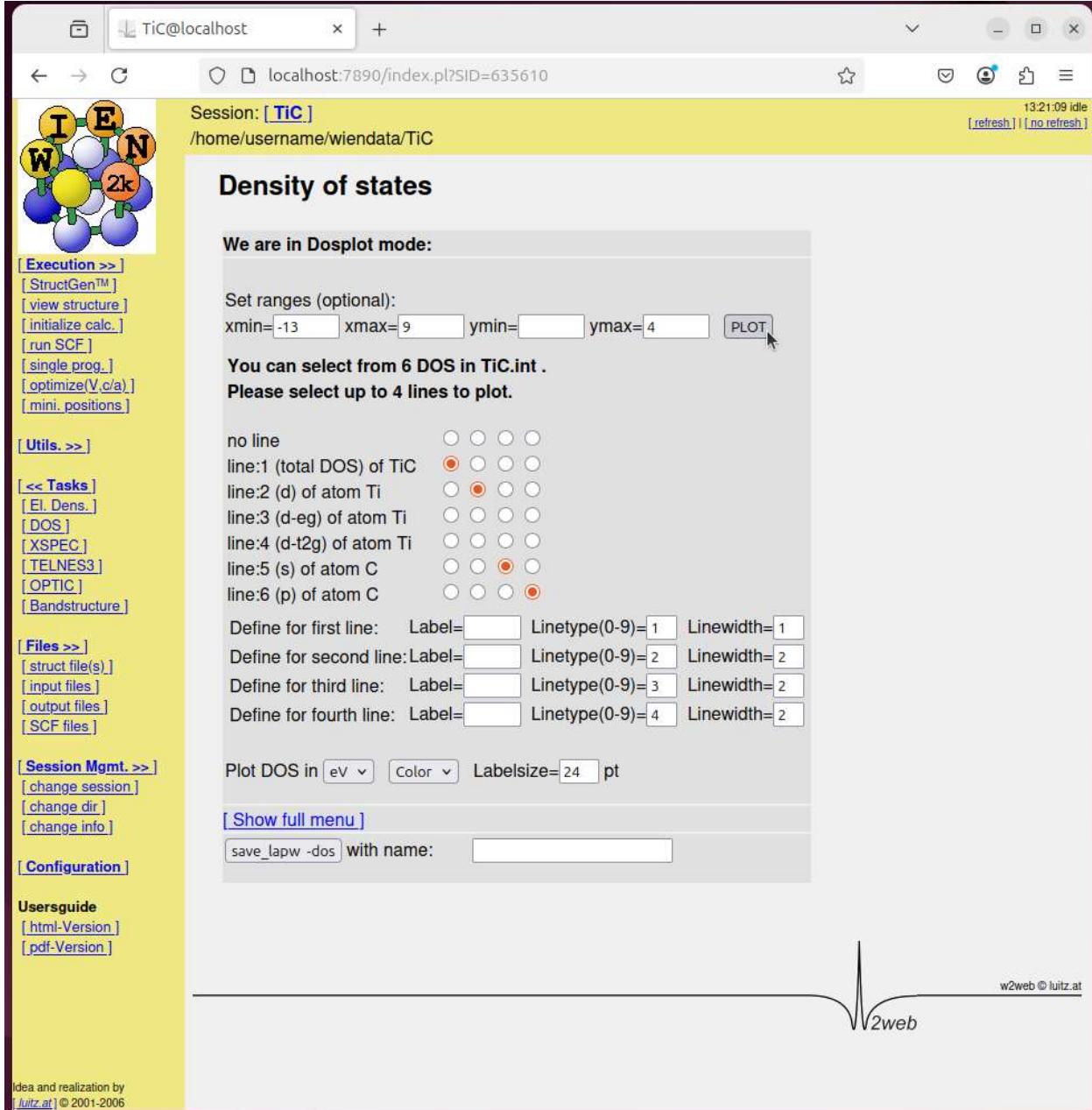
The screenshot shows a web-based graphical user interface for a computational chemistry application. The title bar reads "TiC@localhost". The address bar shows the URL "localhost:7890/index.pl?SID=635610". The main content area displays a DOS (Density of States) plot for tetrahedra around the K point. The plot features a single prominent peak at the center. Above the plot, the session information is shown as "Session: [TiC]" and the commandline entered is "Commandline: x tetra". The program input is listed as "Program input is: '". Below the plot, there is a section titled "Continue with" containing a button labeled "continue with DOS". On the left side of the interface, there is a vertical sidebar with several sections and their sub-options:

- 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]
- Configuration**
- Usersguide**: [html-Version.], [pdf-Version.]

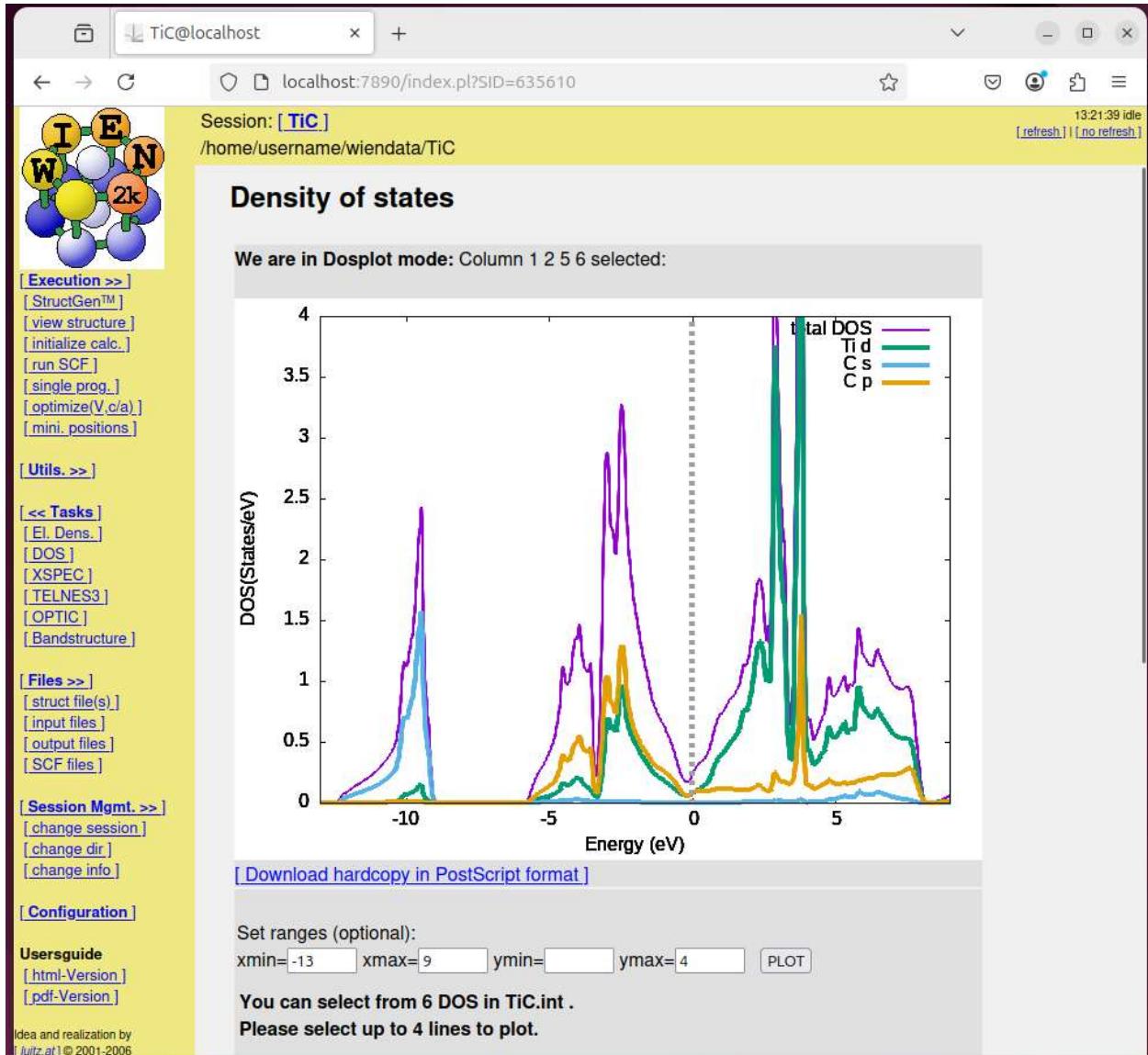
At the bottom of the sidebar, it says "Idea and realization by [luitz.at] © 2001-2006". The right side of the interface has a watermark "w2web @ luitz.at" and "2web".

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”:

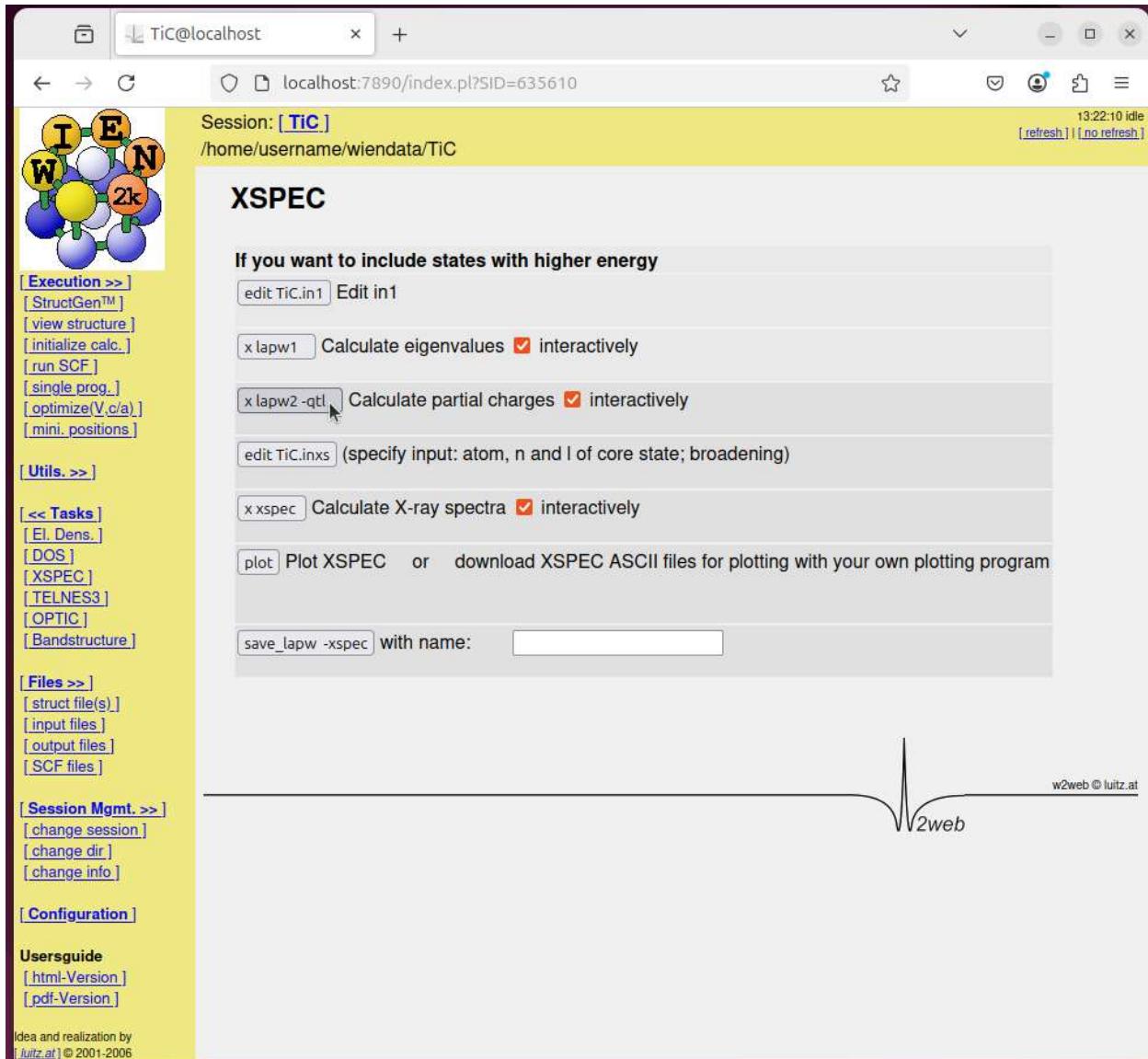


103. The resulting plot is (this is similar to Figure 3.10 in the usersguide):

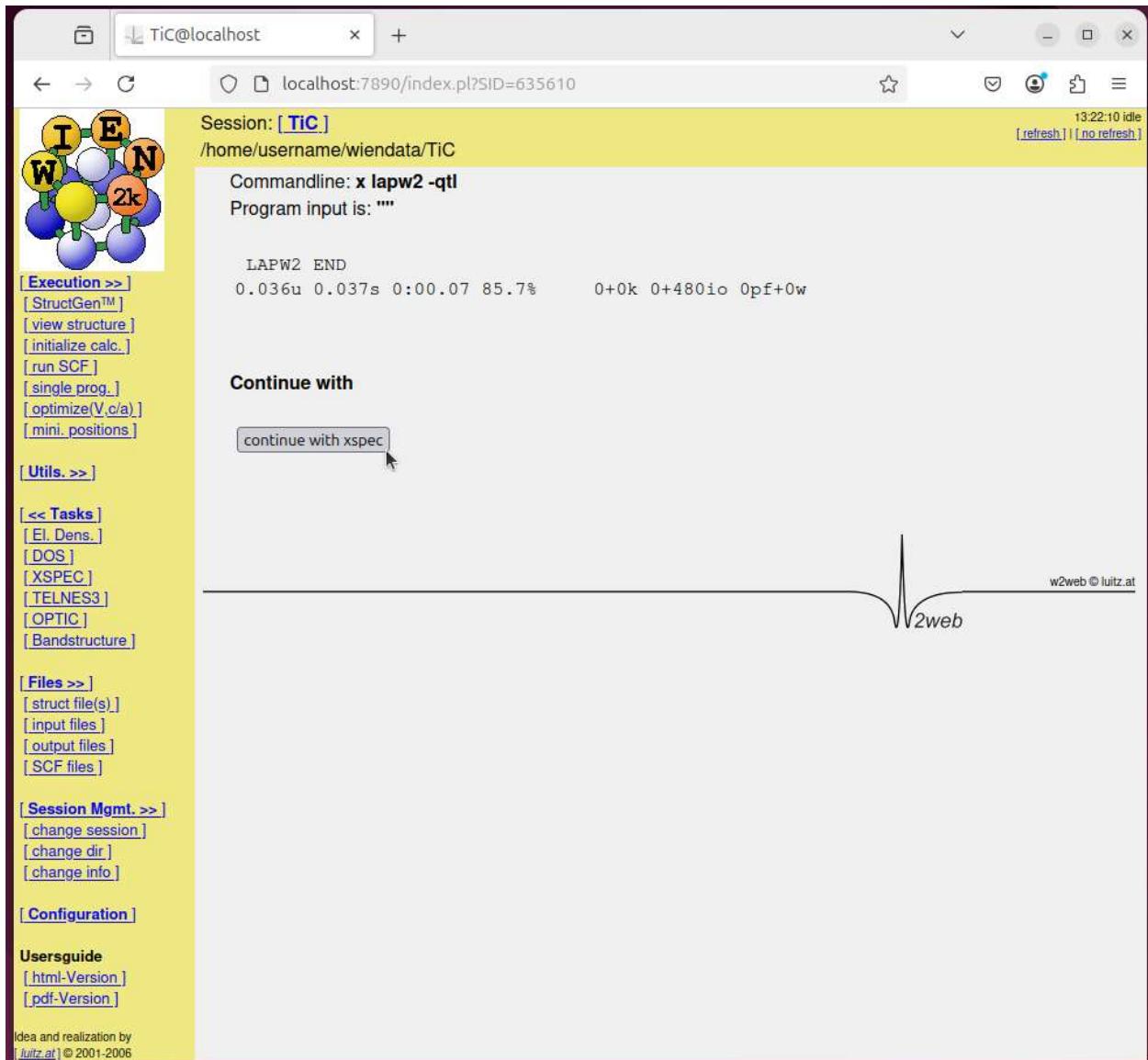


Plot x-ray spectra

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

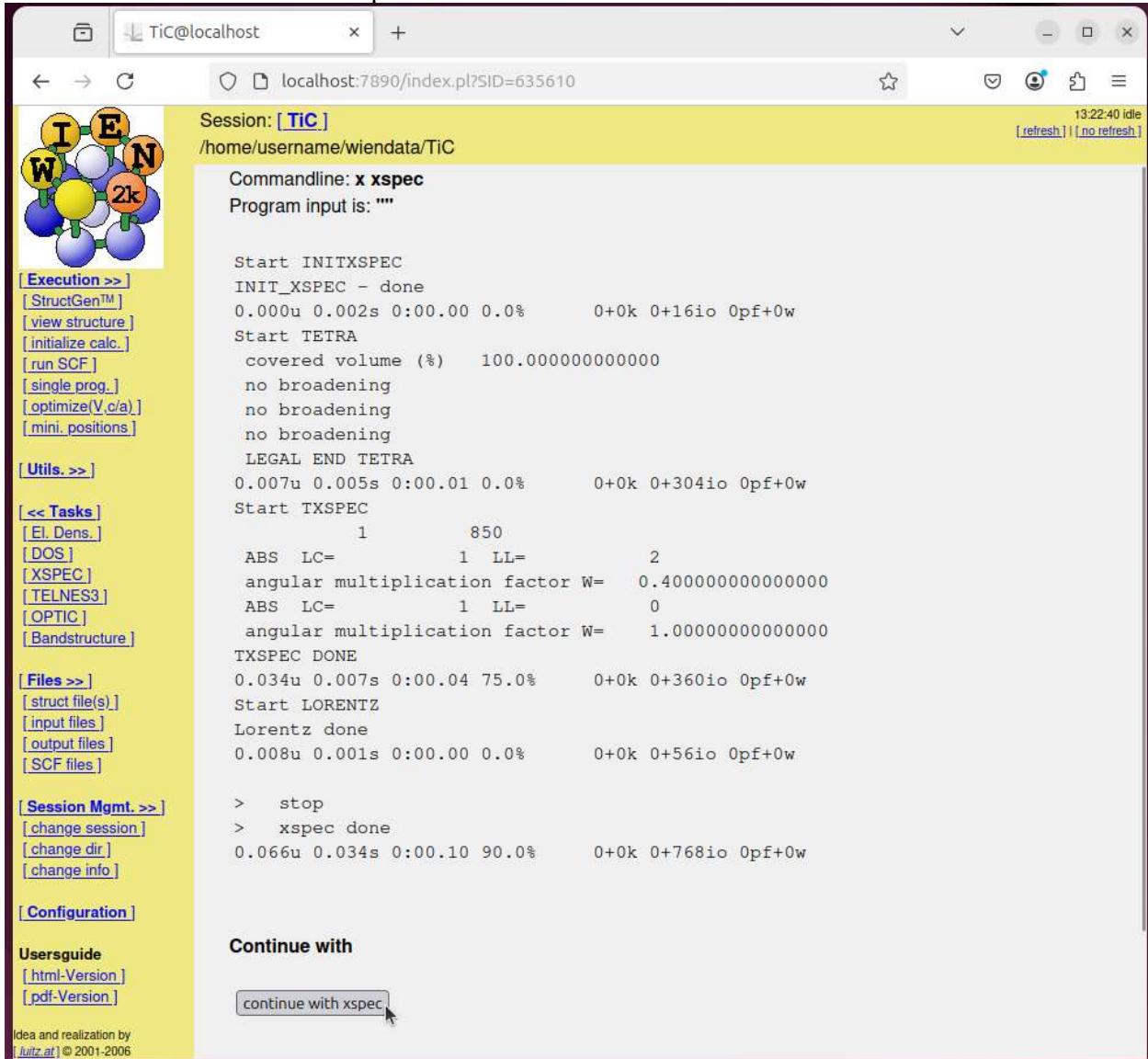


106. Click “continue with xspec”:



107. Click "x xspec"

108. Click “continue with xspec”:

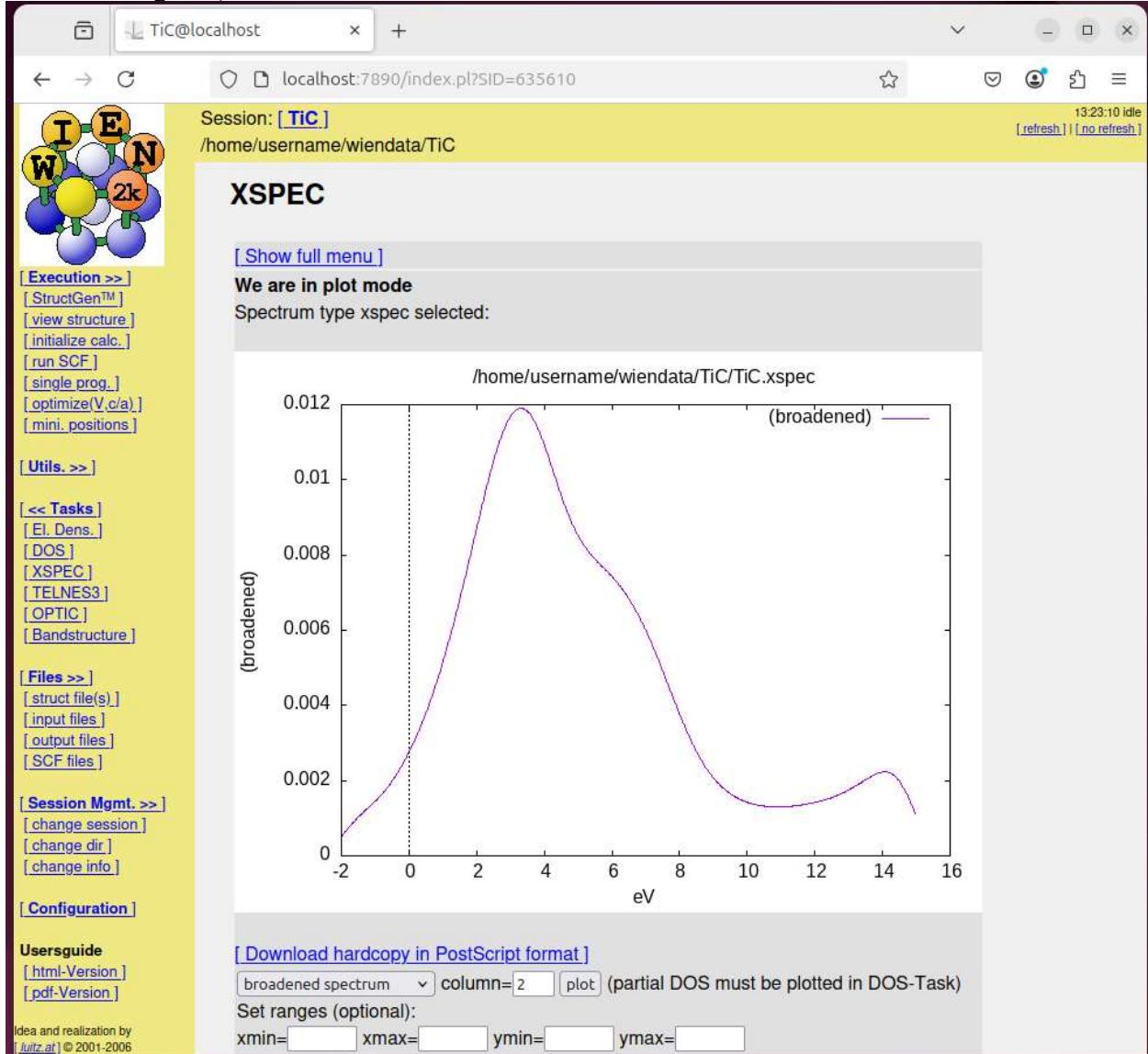


109. Click “plot”

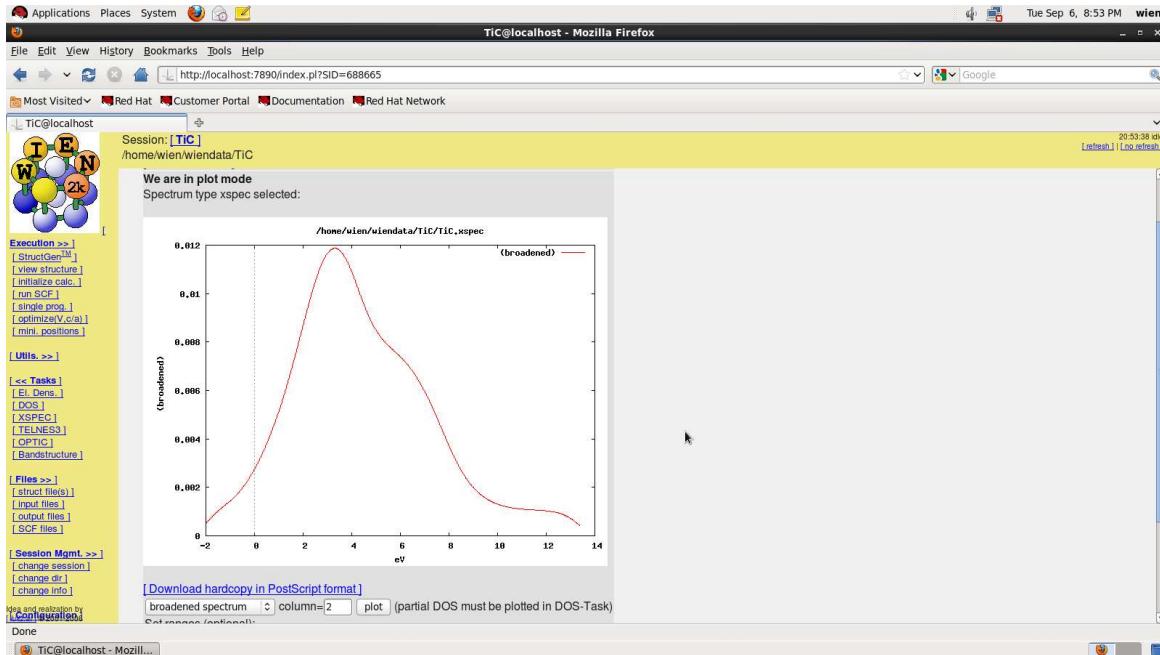
110. Click “plot”:

The screenshot shows a web browser window for 'TiC@localhost' at port 7890. The session is named 'TIC' and the path is '/home/username/wiendata/TiC'. The main content area is titled 'XSPEC' and displays the 'plot' mode configuration. It includes a 'broadened spectrum' dropdown set to 'column=' with a highlighted 'plot' button, and optional range inputs for 'xmin', 'xmax', 'ymin', and 'ymax'. Below these are fields for 'save_lapw -xspec' and 'with name:' followed by an empty input field. A watermark 'w2web @ luitz.at' is visible in the bottom right. On the left, a sidebar lists various tasks and utilities, such as 'Execution >>', 'StructGen™', 'XSPEC', 'OPTIC', and 'Configuration'. At the bottom, there's a note about the idea and realization by 'luitz.at'.

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

Fcc [\[Brillouinzones from Bilbao Cryst Server.\]](#)

or **(save klist as TiC.klist_band)**

Calculate Eigenvalues interactively

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

Calculate irreducible representations so interactively

for band character plots only!

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

Insert correct EF

Calculate bandstructure so interactively

Plot bandstructure or download Xmgrace files for plotting with xmgrace

with name:

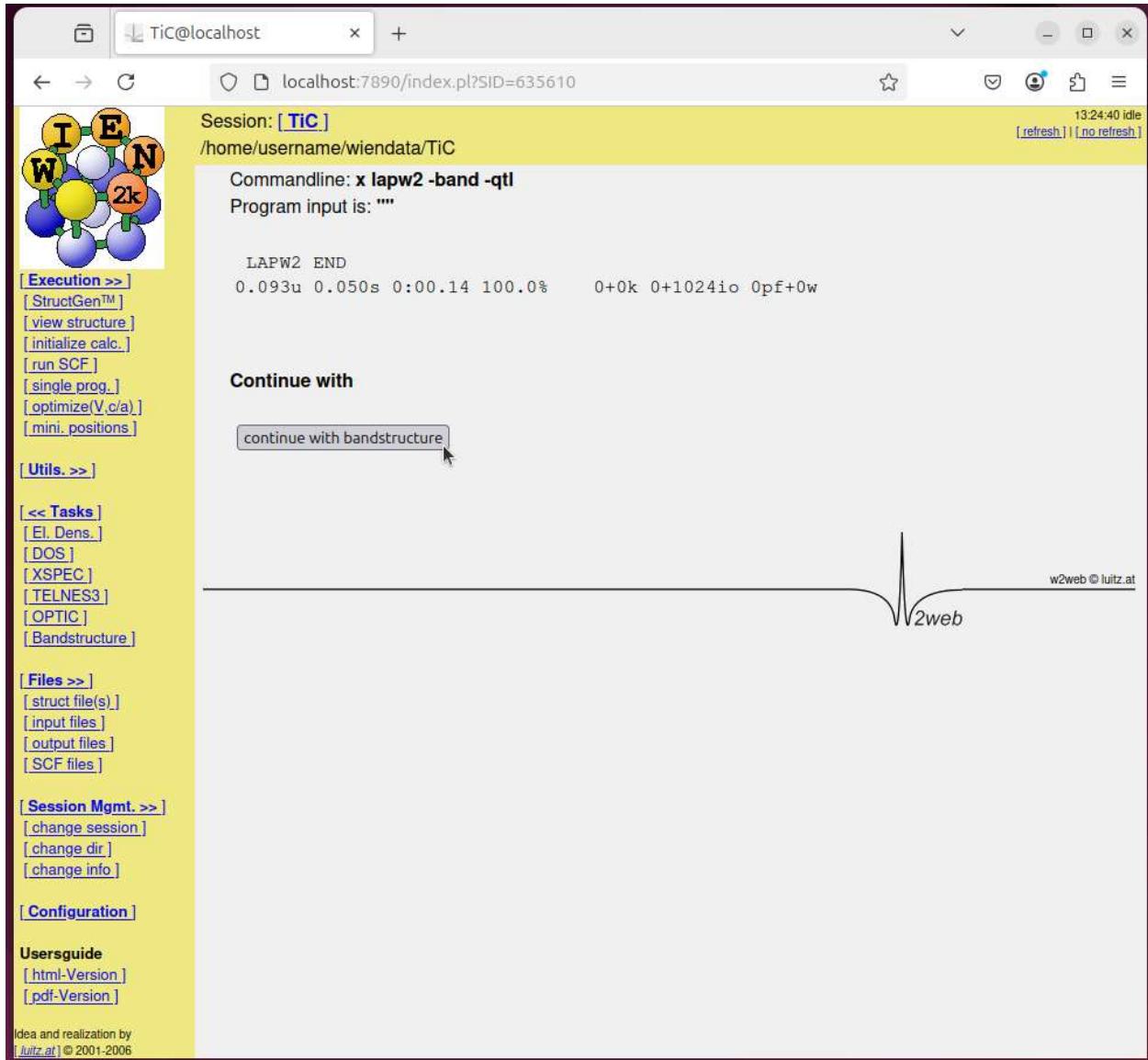
w2web © luitz.at

114. Click on “x lapw1 -band”

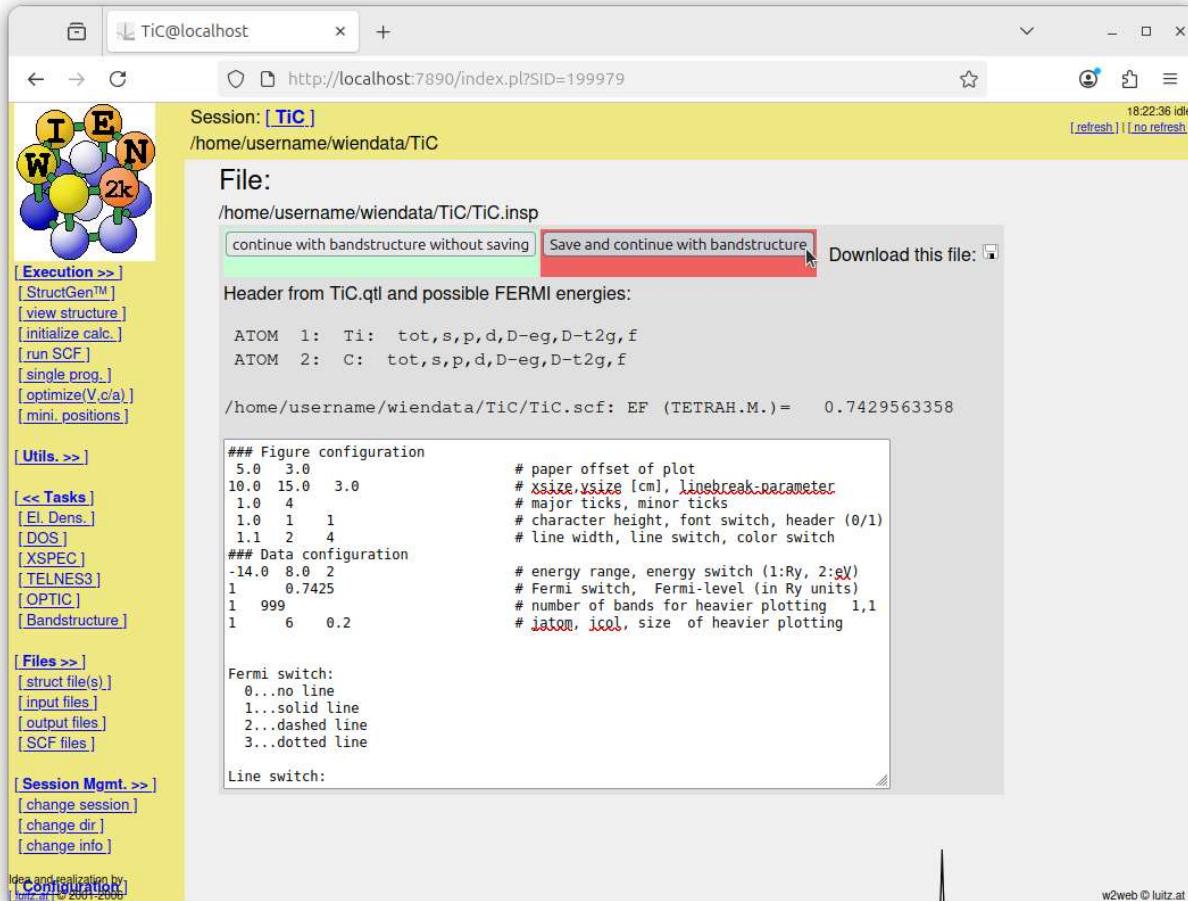
115. Click “continue with bandstructure”:

The screenshot shows a web browser window for 'TiC@localhost' at 'localhost:7890/index.pl?SID=635610'. The page displays a session titled 'Session: [TiC]' with the path '/home/username/wiendata/TiC'. The commandline is listed as 'Commandline: x lapw1 -band' and 'Program input is: ""'. Below this, the output of the LAPW1 calculation is shown: 'LAPW1 END' followed by performance metrics: '0.816u 0.290s 0:01.11 99.0%' and resource usage: '0+0k 0+5976io 0pf+0w'. A section titled 'Continue with' contains a button labeled 'continue with bandstructure', which has a mouse cursor hovering over it. To the right of the button is a small plot of a band structure with a sharp peak. The left sidebar of the interface contains various navigation links such as 'Execution >>', 'StructGen™', 'View structure', etc., and sections like 'Tasks', 'Files >>', 'Session Mgmt. >>', 'Configuration', and 'Usersguide'.

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 0.7429563358 shown on the screen):



The screenshot shows the WiEN2k software interface. The title bar says "TiC@localhost". The address bar shows "http://localhost:7890/index.pl?SID=199979". The left sidebar has a "Session: [TiC]" section with "Header from TiC.qtl and possible FERMI energies:" and a list of ATOM entries. Below this is a code editor window containing the TiC.insp file. The file includes configuration sections for figure and data plotting, Fermi switch settings, and line switches. A red box highlights the "Save and continue with bandstructure" button in the toolbar above the code editor.

```

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.) = 0.7429563358

### 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, jcol, size of heavier plotting

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

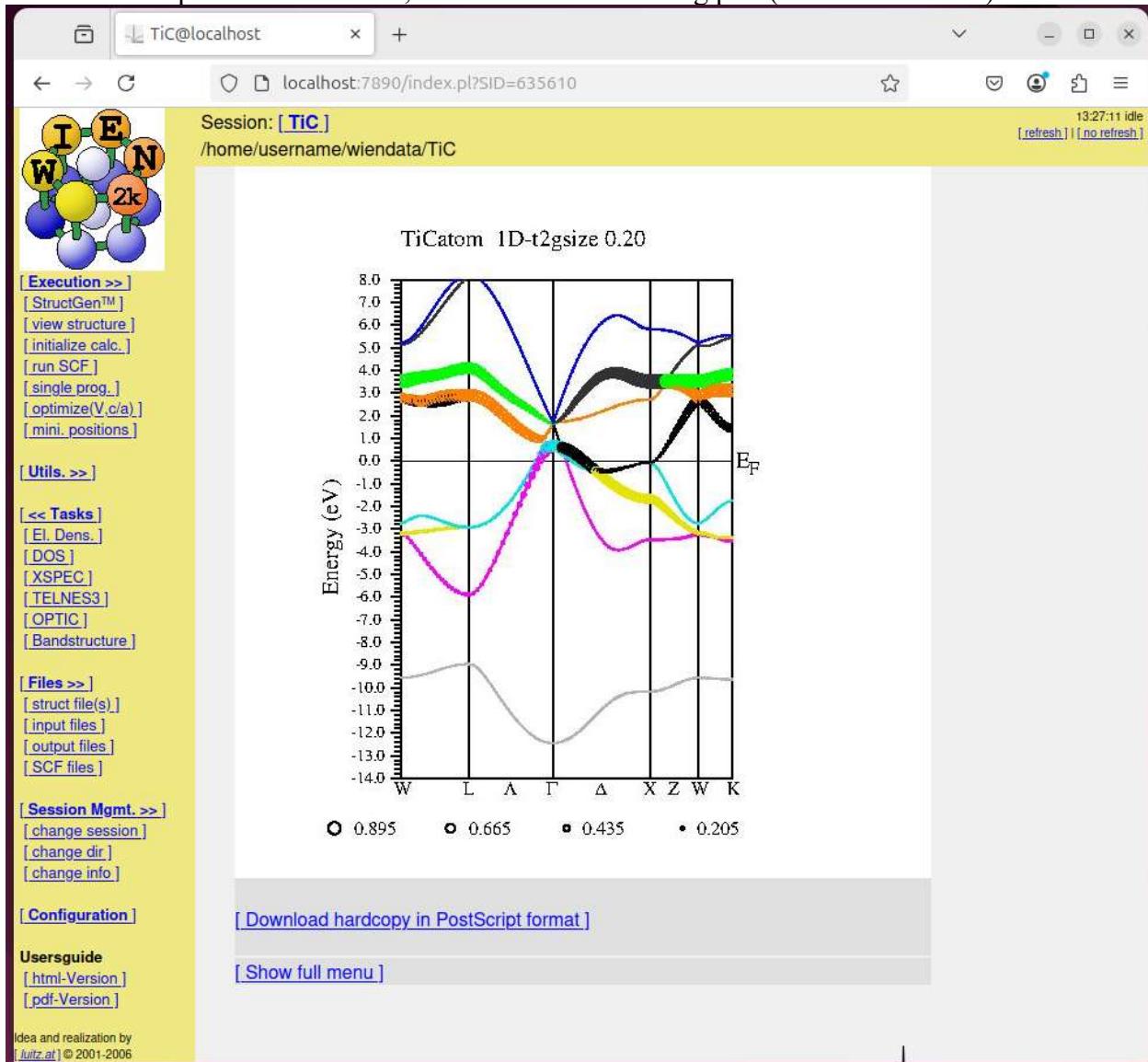
Line switch:

```

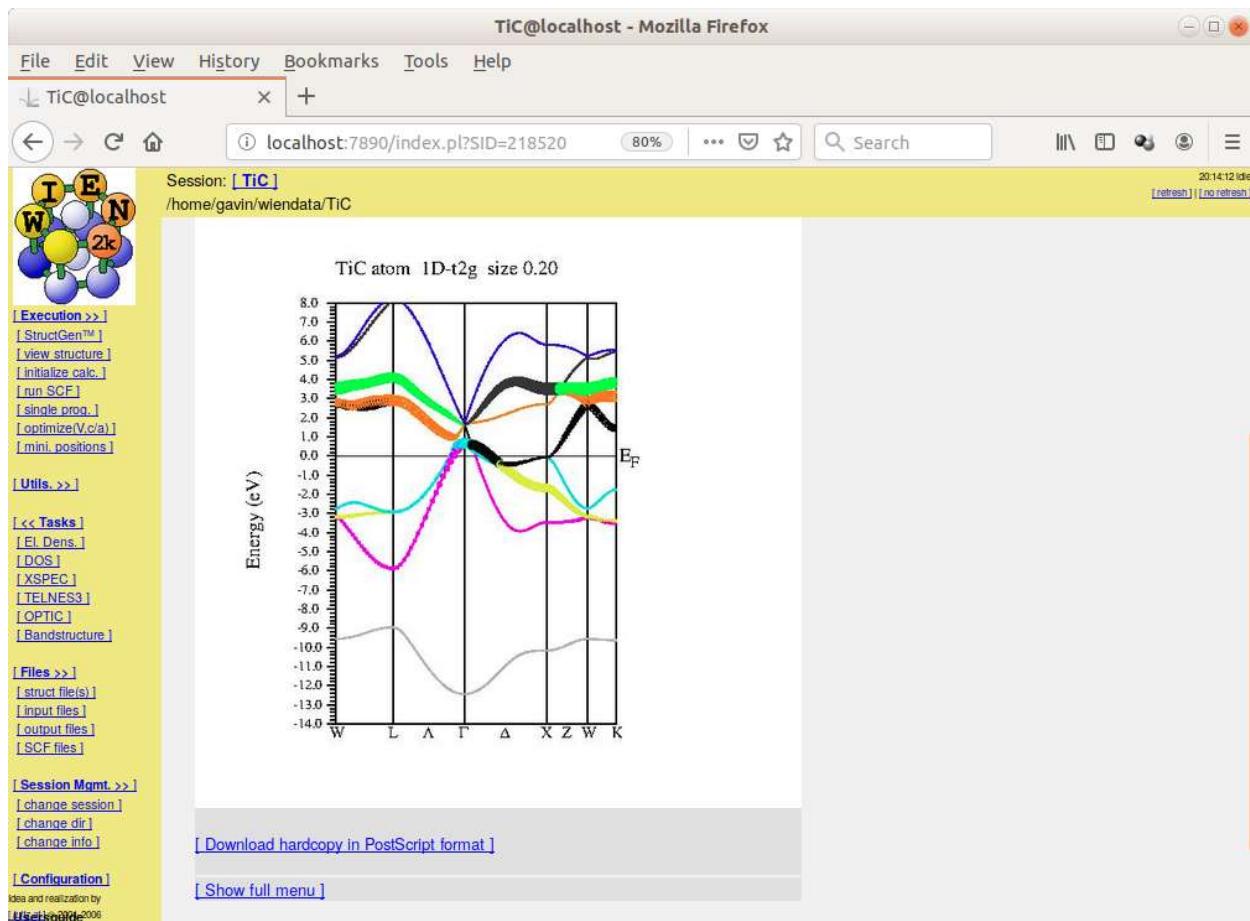
119. Click “Save and continue with bandstructure”
120. Click “x spaghetti”
121. Click “continue with bandstructure”:

The screenshot shows a web browser window for the Wien2k software. The URL is `localhost:7890/index.pl?SID=635610`. The session name is `TiC`. The commandline is `x spaghetti` and the program input is `""`. The output window displays a band structure plot with several bands crossing the Fermi level. A legend on the left identifies atoms: Ti (orange), C (grey), N (blue), O (red), and W (yellow). Below the plot, there are several execution buttons: `Execution >>`, `StructGen™`, `view structure`, `Initialize calc.`, `run SCF`, `single prog.`, `optimize(V_c/a)`, and `mini_positions`. Under `Utils. >>`, there are links for `<< Tasks`, `El. Dens.`, `DOS`, `XSPEC`, `TELNES3`, `OPTIC`, and `Bandstructure`. The `Continue with` section contains a button labeled `continue with bandstructure`. The bottom right corner of the window has a watermark: `w2web © luitz.at`.

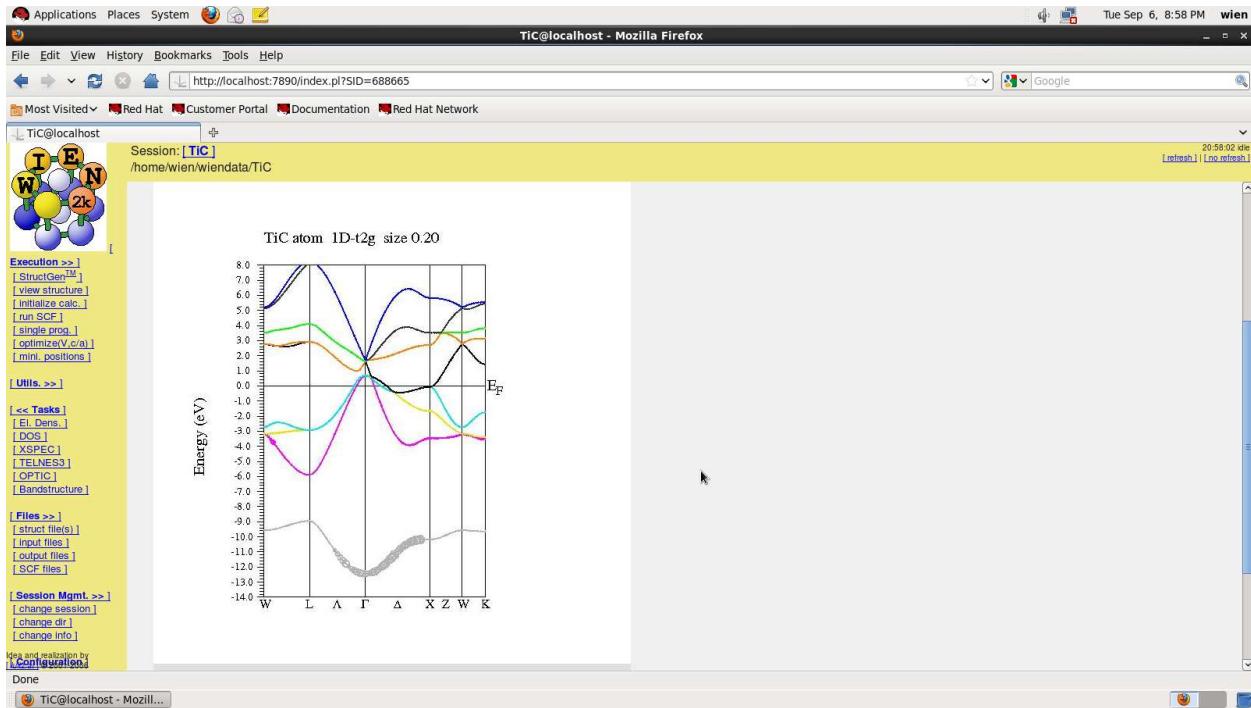
122. Click “plot bandstructure”, the creates the following plot (version 24.1-23.2):



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”:

The screenshot shows the Wiendata software interface. On the left, there's a vertical sidebar with a molecular model of TiC and several menu items under 'Execution >>', 'Utils. >>', 'Tasks >>', 'Files >>', 'Session Mgmt. >>', 'Configuration', and 'Usersguide'. The main area displays a dialog titled 'Optimize volume, c/a-ratio, ...'. Inside the dialog, there are several input fields and buttons: a radio button for 'x optimize' (which is selected), a checkbox for 'Generate structure files from TiC.struct', a link 'edit optimize.job', a button 'run optimize.job', a dropdown 'Type of execution: background', and a button 'plot' which is highlighted. At the bottom right of the dialog, there's a small logo with the text 'w2web'. The top status bar shows the session name 'TiC@localhost' and the URL 'localhost:7890/index.pl?SID=635610'. The top right corner shows the time '13:28:42 idle' and refresh options.

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!”:

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

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

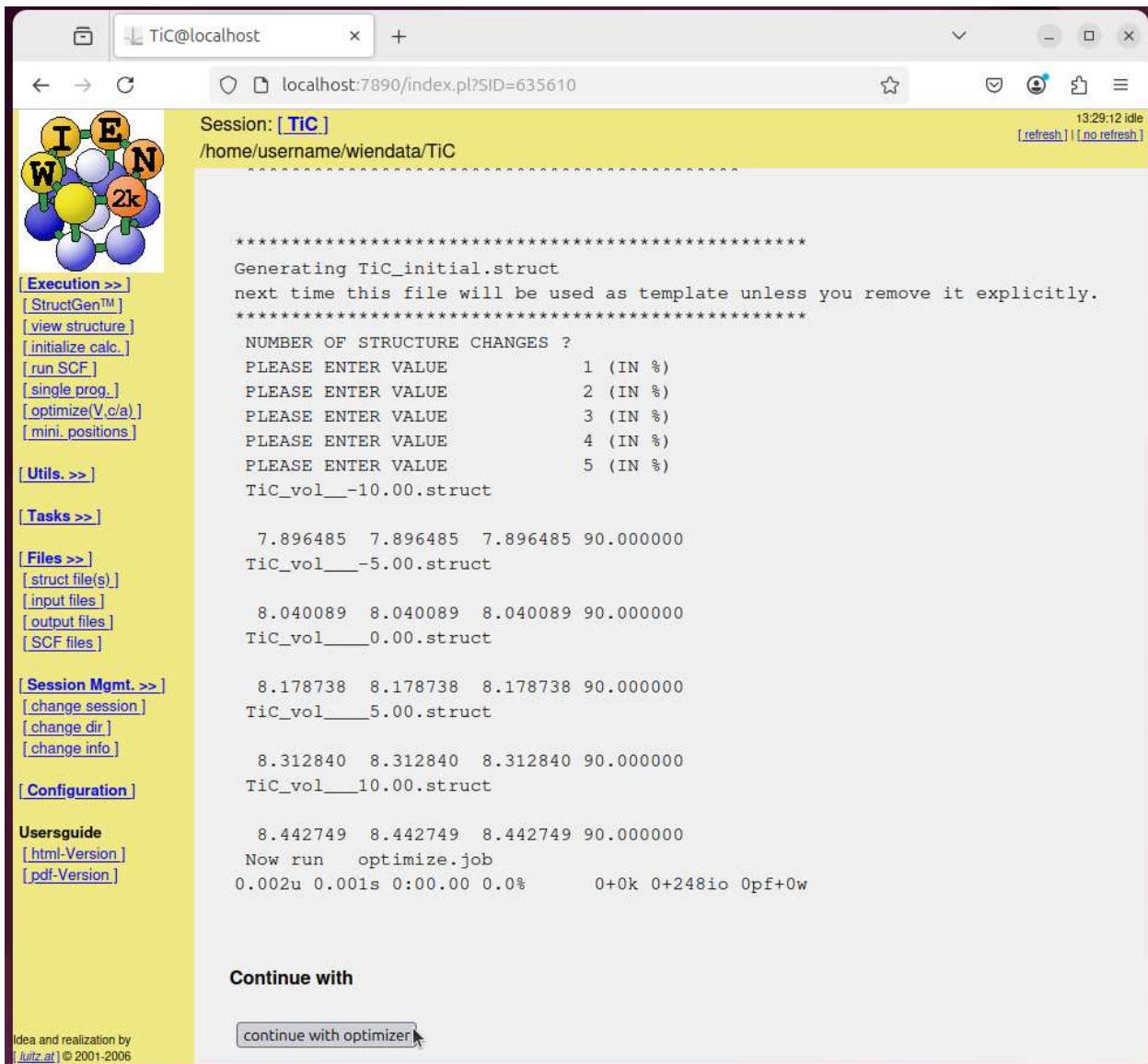
For option 7: specify number of structures: 15, 81 (3x3x3x3), 256 (4x4x4x4)

Execute!

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127. Click “continue with optimizer”:



The screenshot shows a web browser window for `TiC@localhost` at `localhost:7890/index.pl?SID=635610`. The session is titled `TiC.` The main content area displays a molecular structure diagram with atoms labeled T, E, N, W, and 2k. Below the structure are several lines of text representing input parameters for an optimization job. At the bottom of the page, there is a button labeled "Continue with" followed by a button labeled "continue with optimizer".

```

Session: [ TiC. ]
/home/username/wiendata/TiC
13:29:12 idle
[ refresh ] [ no refresh ]

*****
Generating TiC_initial.struct
next time this file will be used as template unless you remove it explicitly.
*****
NUMBER OF STRUCTURE CHANGES ?
PLEASE ENTER VALUE      1 (IN %)
PLEASE ENTER VALUE      2 (IN %)
PLEASE ENTER VALUE      3 (IN %)
PLEASE ENTER VALUE      4 (IN %)
PLEASE ENTER VALUE      5 (IN %)
TiC_vol__-10.00.struct

7.896485 7.896485 7.896485 90.000000
TiC_vol__-5.00.struct

8.040089 8.040089 8.040089 90.000000
TiC_vol__0.00.struct

8.178738 8.178738 8.178738 90.000000
TiC_vol__5.00.struct

8.312840 8.312840 8.312840 90.000000
TiC_vol__10.00.struct

8.442749 8.442749 8.442749 90.000000
Now run optimize.job
0.002u 0.001s 0:00.00 0.0%      0+0k 0+248io 0pf+0w

Continue with
continue with optimizer

```

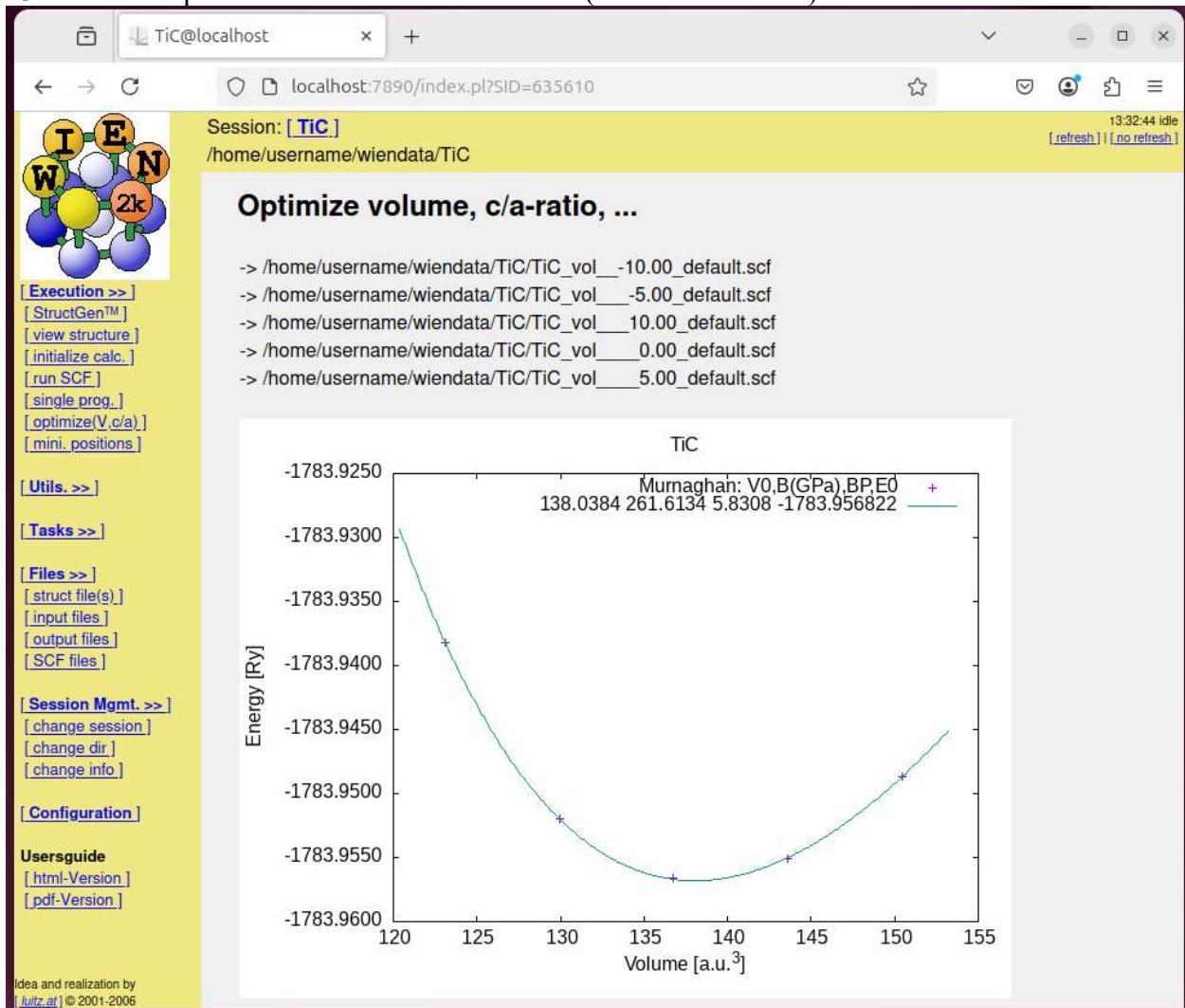
Idea and realization by
[[Juiz.at](#)] © 2001-2006

128. Click “run optimize.job”

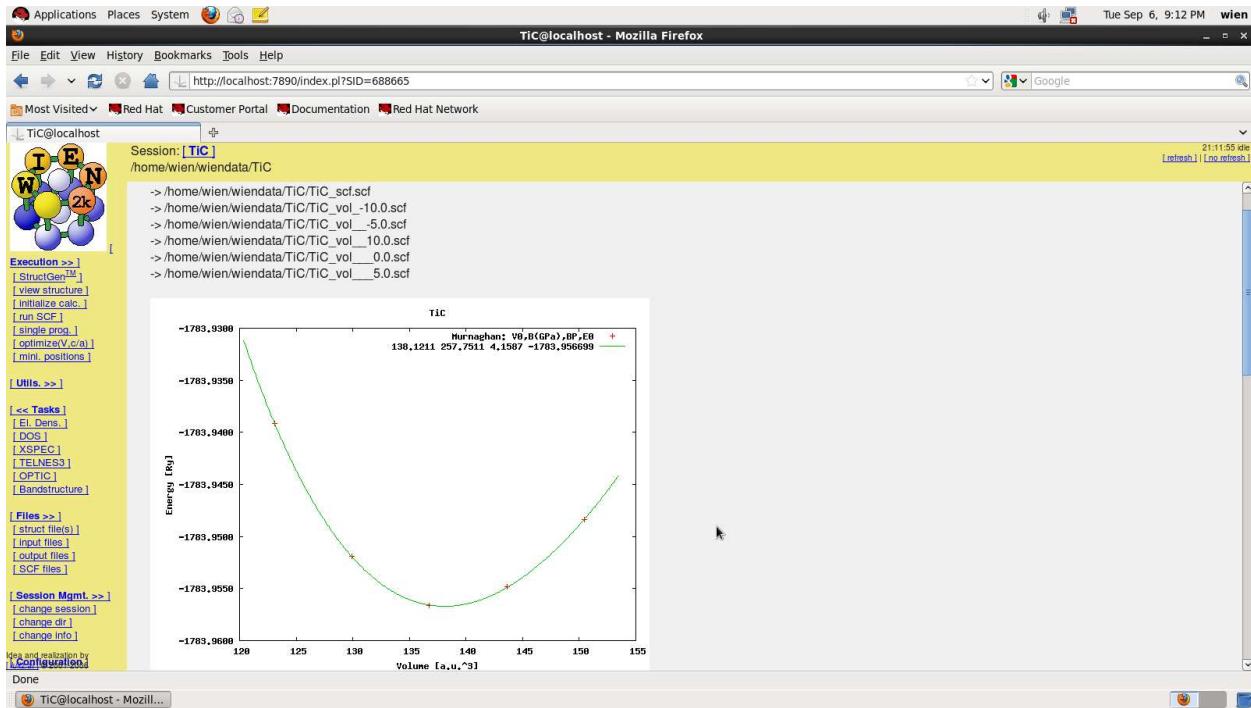
129. Click “continue with optimizer”:

The screenshot shows a web browser window with the URL `localhost:7890/index.pl?SID=635610`. The page title is "Session: [TiC]". The session path is `/home/username/wiendata/TiC`. The command line is listed as "Commandline: ./optimize.job" and the program input is """. A note says "[View STDOUT] to monitor the progress of this command". Below this, there is a button labeled "Continue with" and a sub-button labeled "continue with optimizer" which is being clicked by a mouse cursor. On the left side, there is a sidebar with various menu items under categories like "Execution >>", "Tasks >>", "Files >>", "Session Mgmt. >>", "Configuration", and "Usersguide". At the bottom of the sidebar, it says "Idea and realization by [luitz.at] © 2001-2006". The top right corner of the page shows the time "13:30:42 idle" and links for "[refresh.]" and "[no refresh.]". The bottom right corner has a logo with the text "w2web @ luitz.at" and "w2web".

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.