

WIEN2k TiC Example

Ubuntu 24.04.3 LTS

WIEN2k_24.1 (Release 1/8/2024)

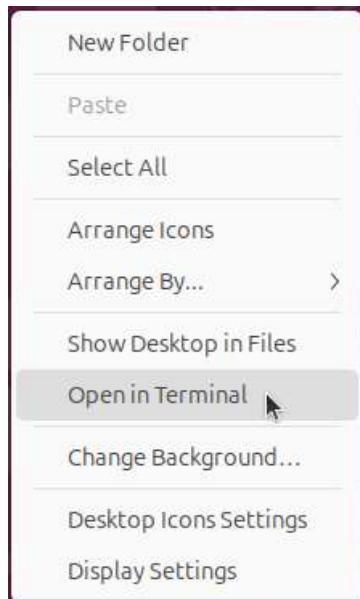
ifx version 2025.2.1

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

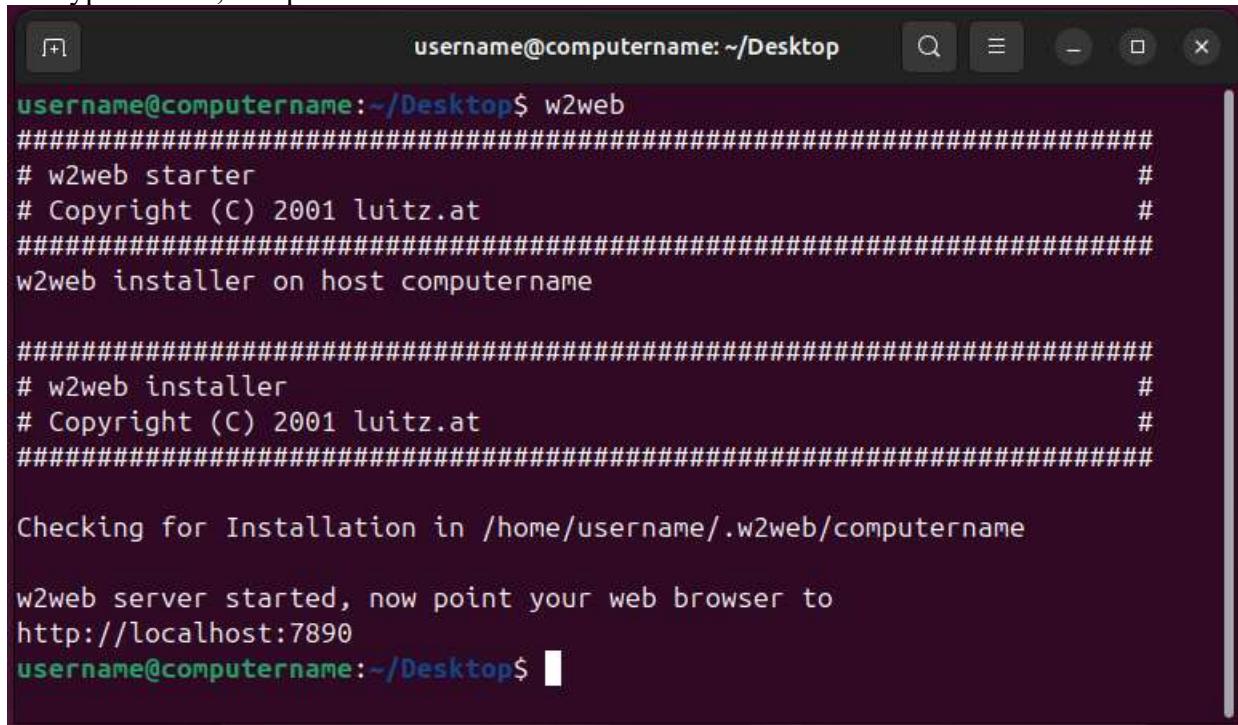
[1] <https://github.com/gsabo/WIEN2k-Patches/tree/master/24.1>

Open a terminal and start w2web

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



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



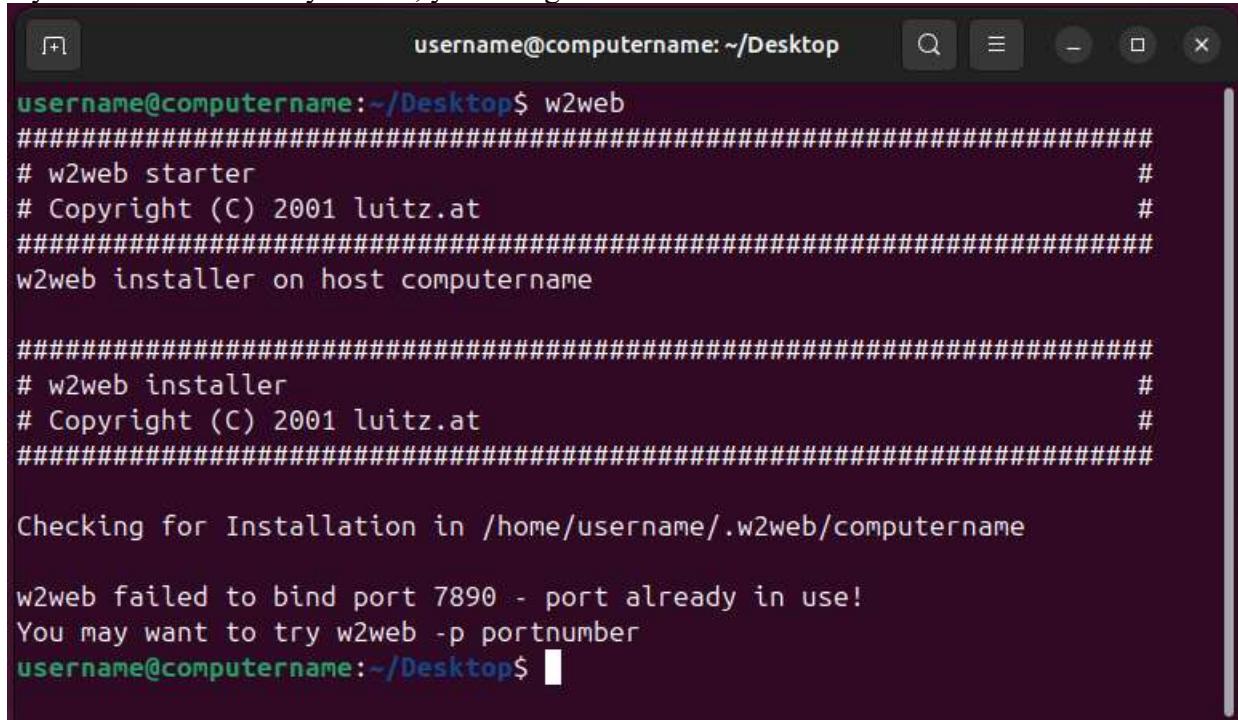
```
username@computername: ~/Desktop$ w2web
#####
# w2web starter
# Copyright (C) 2001 luitz.at
#####
w2web installer on host computername

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

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

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

If your w2web is already started, you will get:



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

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

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

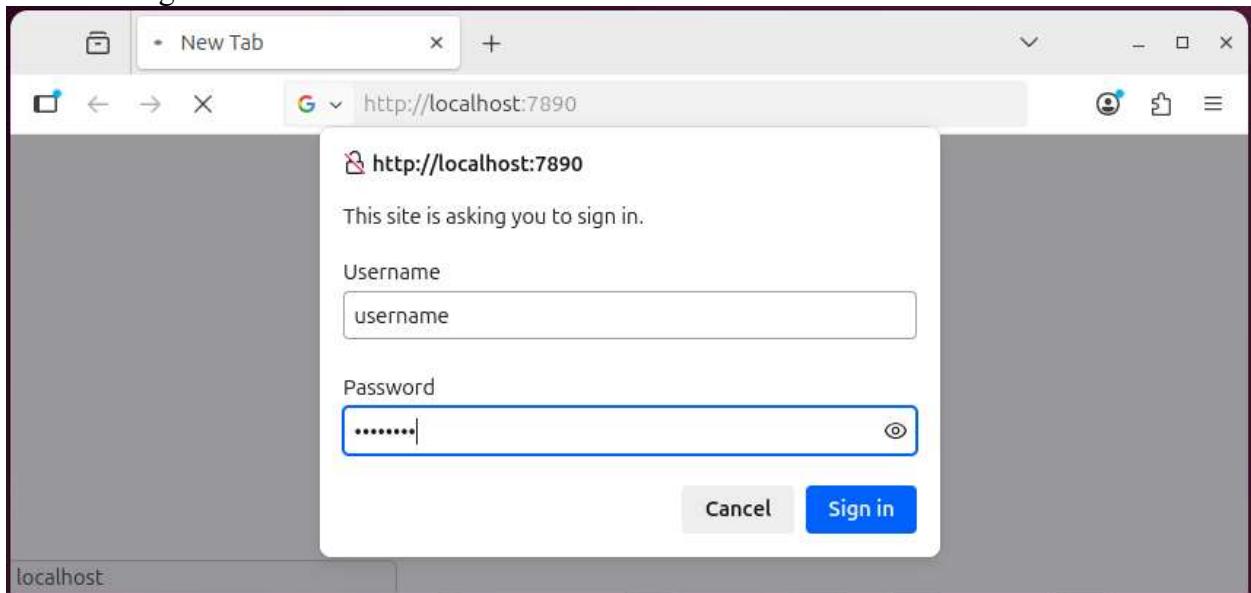
w2web failed to bind port 7890 - port already in use!
You may want to try w2web -p portnumber
username@computername:~/Desktop$
```

Open Firefox and login to w2web

3. Click on the Firefox icon to open Firefox:

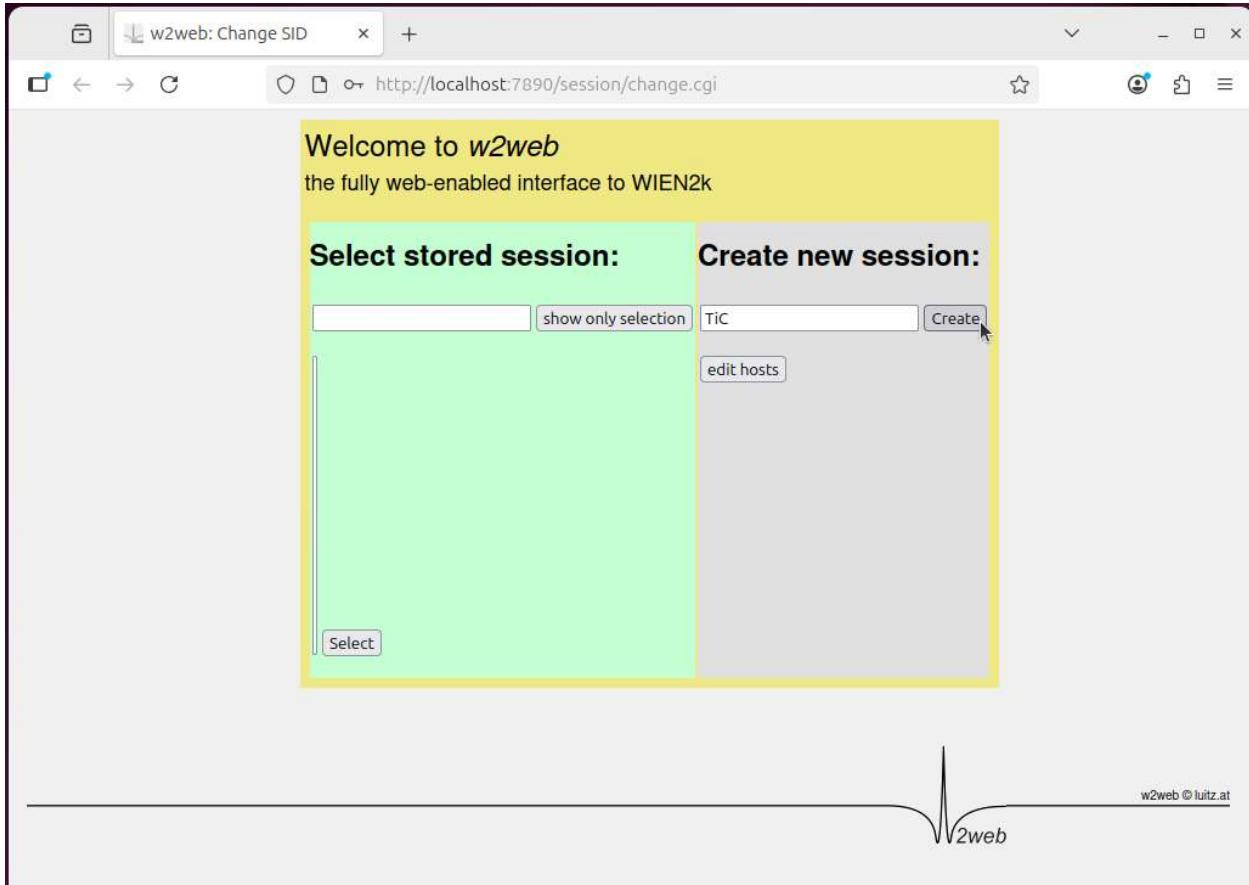


4. Enter url `http://localhost:7890`, type your w2web username and password, then click "Sign in" to login to w2web:

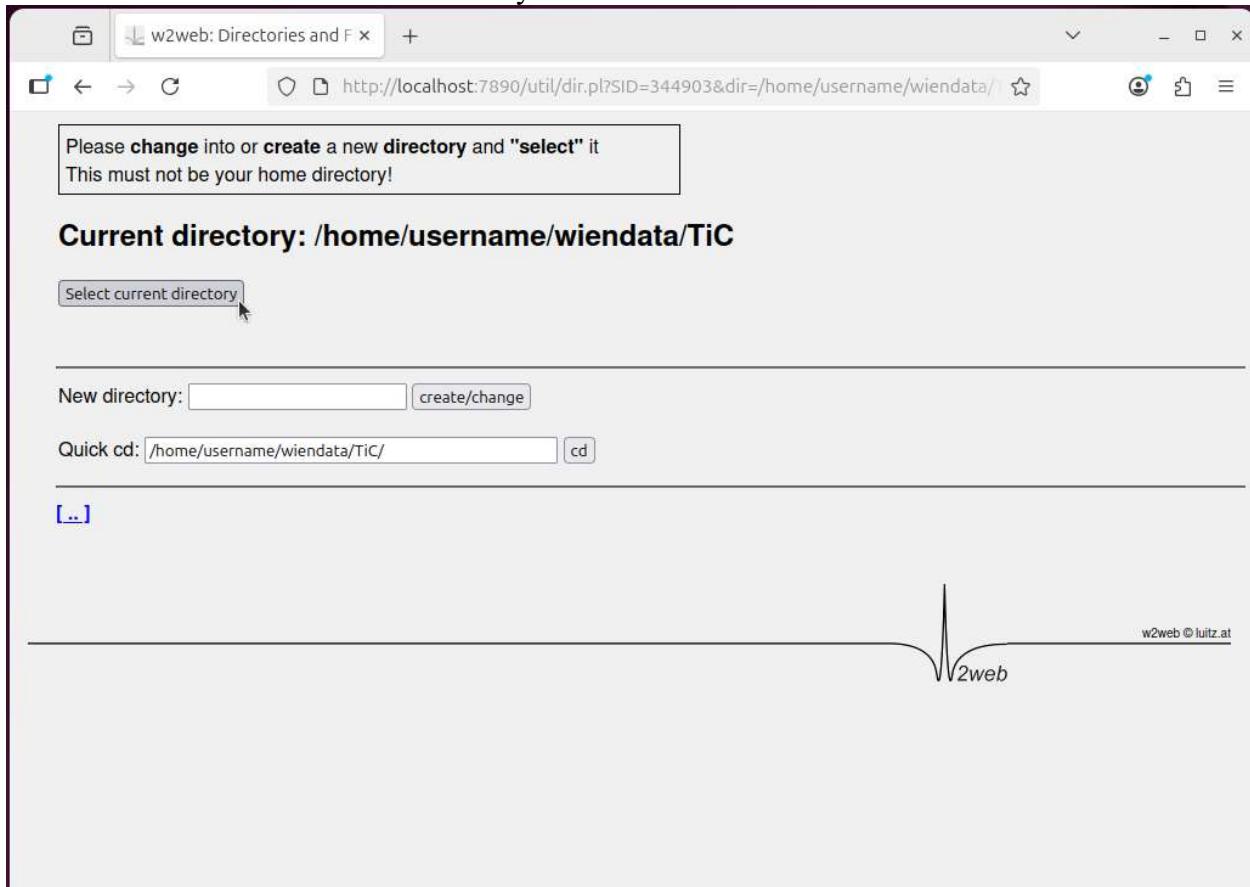


Create a new session (calculation)

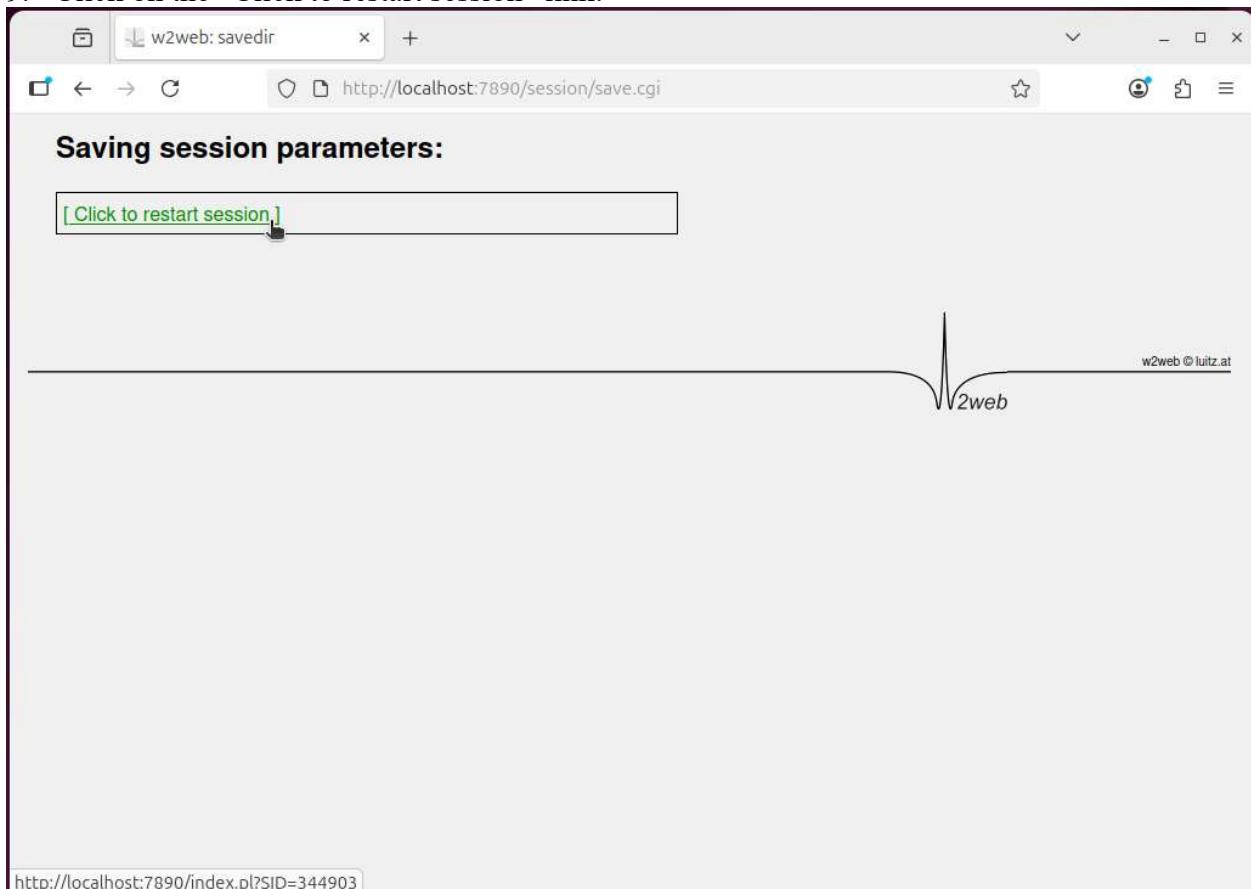
5. Enter “TiC” in the “Create new session:” box and then click the “Create” button:



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



9. Click on the “Click to restart session” link:



10. The following window should appear:

The screenshot shows a web browser window titled "TiC@localhost" displaying the "w2web, the fully web-enabled interface to WIEN2k". The URL is "http://localhost:7890/index.pl?SID=344903". The session information is as follows:

- Session Name:** TiC
- Session ID:** 344903
- Directory:** /home/username/wiendata/TiC
- Last changed:** Sun Aug 31 16:52:24 2025

Comments:

- spin polarized calculation
- AFM calculation
- complex calculation (no inversion)
- parallel calculation

[Change session information](#)

w2web © luitz.at

Navigation menu (left sidebar):

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

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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:

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

16:53:02 idle
[refresh] || [no refresh]

StructGen™

You do not have a TiC.struct file yet.

You can create it using STRUCTGEN. Please specify the number of independent atoms of your initial structure!

Number of atoms: 2

Alternatively:

Use cif2struct to convert a "cif" file: to convert a "txt" file:
(e.g. from the Inorganic crystal structure database) (for input definition see UG: cif2struct)

Use selected CIF/TXT file

Use xyz2struct to convert a "xyz" file: .

Here you can a "cif" or "xyz" file from your 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 (TiC@localhost) at http://localhost:7890/index.pl?SID=344903. The session is named "TiC".

Left Sidebar (Yellow Area):

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

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Main Content Area:

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

16:54:02 idle
[refresh] || [no refresh]

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
α= 90.000000 β= 90.000000 γ= 90.000000

Inequivalent Atoms: 2

Atom 1: Ti Z= 0.000 RMT= 2.0000 [remove atom]
Pos 1: x= 0.00000000 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

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

16:54:33 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)
- [\[continue editing \]](#)
- [\[abort editing and restore original file \]](#)

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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]

http://localhost:7890/util/structrmt.pl?SID=344903

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

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

16:54:33 idle
[refresh] || [no refresh]

Automatic determination of RMTs

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

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

Reduce RMTs by % using new or old scheme

do it

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

do it

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2web

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

The screenshot shows the StructGen™ software interface running in a web browser (TiC@localhost) at http://localhost:7890/index.pl?SID=344903. The session is titled "TiC".

Left Sidebar (Yellow Background):

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

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Main Content Area:

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

Title: TiC

Lattice: Type: F

- P
- F
- B
- CXY
- CYZ
- CXZ
- R
- H
- 1_P1

Spacegroups from Bilbao Cryst Server:

Lattice parameters in A:

a = 4.32800003862	b = 4.32800003862	c = 4.32800003862
$\alpha = 90.000000$	$\beta = 90.000000$	$\gamma = 90.000000$

Inequivalent Atoms: 2

Atom 1: Ti Z = 22.000 RMT = 2.17 [remove atom]
 Pos 1: x = 0.00000000 y = 0.00000000 z = 0.00000000 [remove] [split]
 [add position]

Atom 2: C Z = 6.000 RMT = 1.77 [remove atom]
 Pos 1: x = 0.50000000 y = 0.50000000 z = 0.50000000 [remove] [split]
 [add position]

[add an atom]

Number of symmetry operations: generate

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 the StructGen™ software interface running in a web browser (TiC@localhost). The main window displays a 3D ball-and-stick model of a crystal structure with atoms labeled Ti, C, N, E, and W. A legend indicates the color coding for these elements. On the left, a sidebar contains a navigation menu with sections like Execution, Utilities, Tasks, Files, Session Management, Configuration, and User Guide, along with links for HTML and PDF versions.

Session Information:

- Session: TiC
- Path: /home/username/wiendata/TiC
- Date: 16:56:04 idle
- Links: [refresh] | [no refresh]
- StructView /home/username/wiendata/TiC

StructGen™ Interface:

Title: TiC

Lattice: F

Type: F

Spacegroups from Bilbao Cryst Server:

- P
- F
- B
- CXY
- CYZ
- CXZ
- R
- H
- 1_P1

Lattice parameters in A:

a = 4.32800003862	b = 4.32800003862	c = 4.32800003862
$\alpha = 90.000000$	$\beta = 90.000000$	$\gamma = 90.000000$

Inequivalent Atoms: 2

Atom 1: Ti Z = 22.000 RMT = 2.0000
Pos 1: x = 0.00000000 y = 0.00000000 z = 0.00000000

Atom 2: C Z = 6.000 RMT = 1.9000
Pos 1: x = 0.50000000 y = 0.50000000 z = 0.50000000

Number of symmetry operations: generate

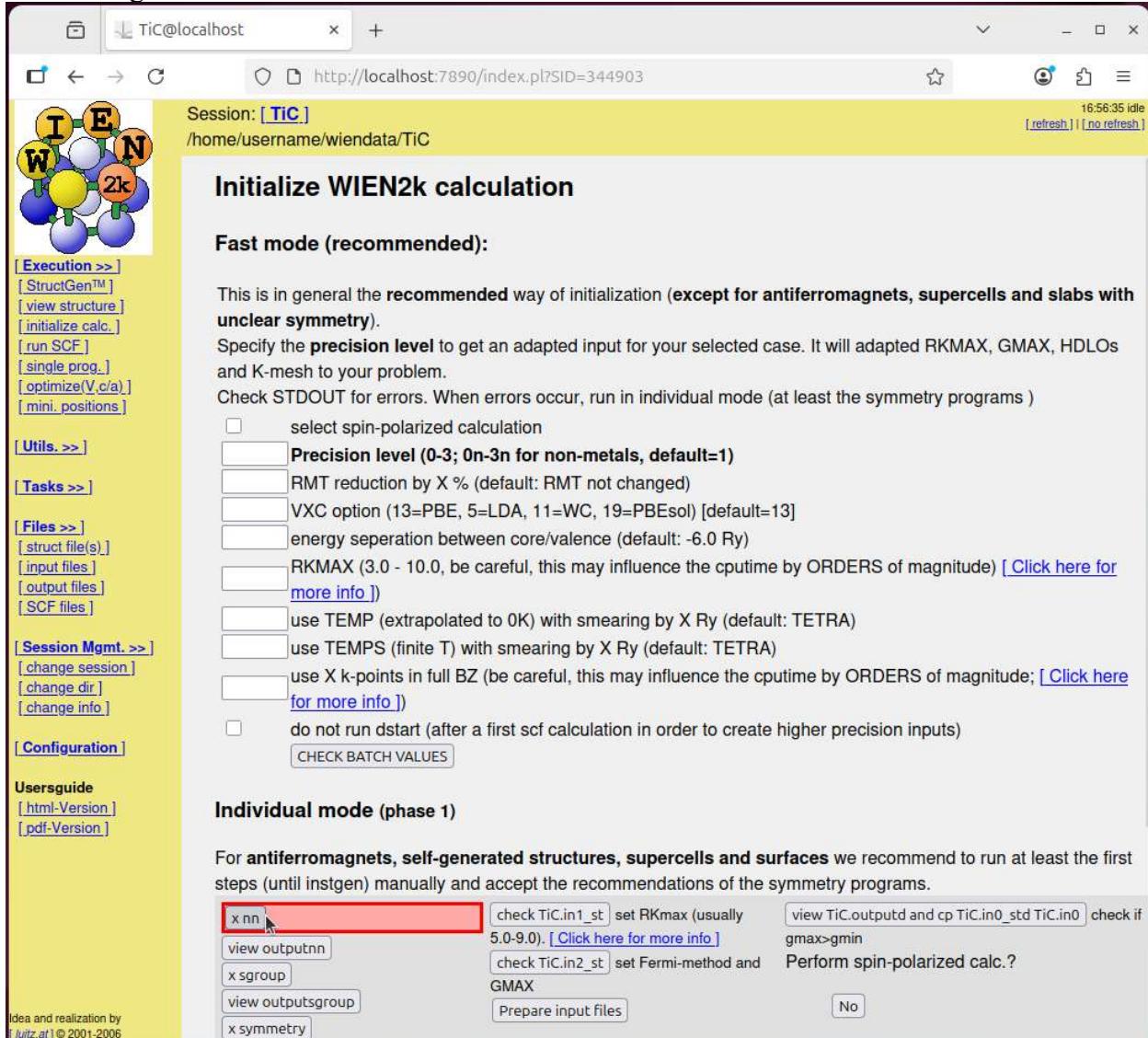
View only mode --> [edit STRUCT file.]

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Initialize the calculation

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



The screenshot shows the WIEN2k web interface for initializing a calculation. The main title is "Initialize WIEN2k calculation". Under "Fast mode (recommended)", there are several configuration options with checkboxes. One option, "select spin-polarized calculation", has a checked checkbox. Below this is a section titled "Precision level (0-3; 0n-3n for non-metals, default=1)". Other options include "RMT reduction by X % (default: RMT not changed)", "VXC option (13=PBE, 5=LDA, 11=WC, 19=PBEsol) [default=13]", "energy separation between core/valence (default: -6.0 Ry)", "RKMAX (3.0 - 10.0, be careful, this may influence the cputime by ORDERS of magnitude) [Click here for more info]", "use TEMP (extrapolated to 0K) with smearing by X Ry (default: TETRA)", "use TEMPS (finite T) with smearing by X Ry (default: TETRA)", "use X k-points in full BZ (be careful, this may influence the cputime by ORDERS of magnitude; [Click here for more info])", and "do not run dstart (after a first scf calculation in order to create higher precision inputs)". A "CHECK BATCH VALUES" button is located at the bottom of this section. Below this is a section titled "Individual mode (phase 1)". It contains a note: "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." At the bottom, there is a row of buttons: "x nn", "view outputnn", "x sgroup", "view outputsgroup", "x symmetry", "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", "view TiC.outputnd and cp TiC.in0_std TiC.in0", "check if gmax>gmin", and "Perform spin-polarized calc.?". The "x nn" button is highlighted with a red box.

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

The screenshot shows a web browser window titled "TiC@localhost" with the URL "http://localhost:7890/index.pl?SID=344903". The page displays a molecular structure of TiC (Tin Carbide) with atoms labeled T, C, N, E, W, and 2k. A sidebar on the left contains various menu options such as "Execution >>", "StructGen™", "view structure", "initialize calc.", etc. The main content area has a yellow header bar with the session information "Session: [TiC]" and the path "/home/username/wiendata/TiC". Below this, a message says "please specify nn-bondlength factor: (usually=2)" with a text input field containing "2" and a button labeled "Execute!". In the top right corner, there is a timestamp "16:56:35 idle" and refresh/no-refresh buttons. The bottom right corner features a logo with the text "w2web © luitz.at" and "2web". At the bottom left, there is a copyright notice: "Idea and realization by [luitz.at] © 2001-2006".

31. Click the “initlapw” button:

TiC@localhost http://localhost:7890/index.pl?SID=344903

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

16:56:35 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 20.000000000000000
iix,iiy,iiz 5 5 5 40.893690000000000
        40.893690000000000

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
0.003u 0.003s 0:00.00 0.0%    0+0k 0+32io 0pf+0w

```

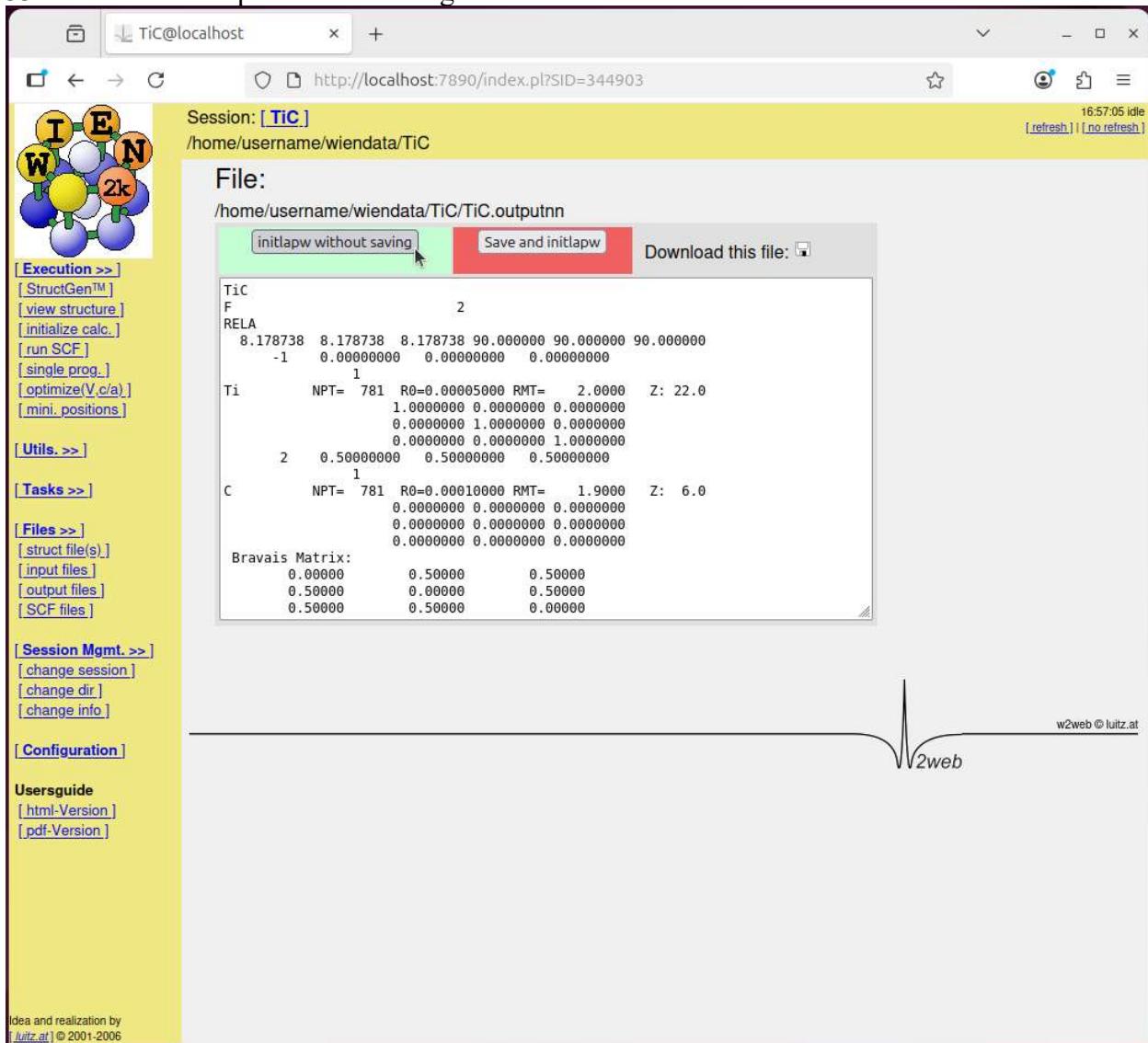
Continue with



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



The screenshot shows a web browser window for 'TiC@localhost' at 'http://localhost:7890/index.pl?SID=344903'. The session is named 'TiC' and the path is '/home/username/wiendata/TiC'. The main content area displays a molecular structure diagram with atoms labeled I, E, N, W, and 2k. Below the diagram is a 'File:' section containing the path '/home/username/wiendata/TiC/TiC.outputnn'. A modal dialog box is overlaid on the page, containing three buttons: 'initlapw without saving' (highlighted in green), 'Save and initlapw' (in red), and 'Download this file:'. The 'initlapw without saving' button is currently active. The text in the modal box shows the content of the 'TiC.outputnn' file, which includes atomic coordinates and a Bravais Matrix.

```

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

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
      1.00000000 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:
  0.00000  0.50000  0.50000
  0.50000  0.00000  0.50000
  0.50000  0.50000  0.00000

```

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34. Click the “x sgroup” button

35. Click the “initlapw” button:

The screenshot shows a web browser window for 'TiC@localhost' at 'http://localhost:7890/index.pl?SID=344903'. The page displays a molecular structure with atoms labeled I, E, N, W, and 2k. The session information is as follows:

- Session: [TiC](#)
- Program input is: ""
- Resource usage: 0.000u 0.000s 0:00.00 0.0% CPU, 0+0k 0+8io 0pf+0w

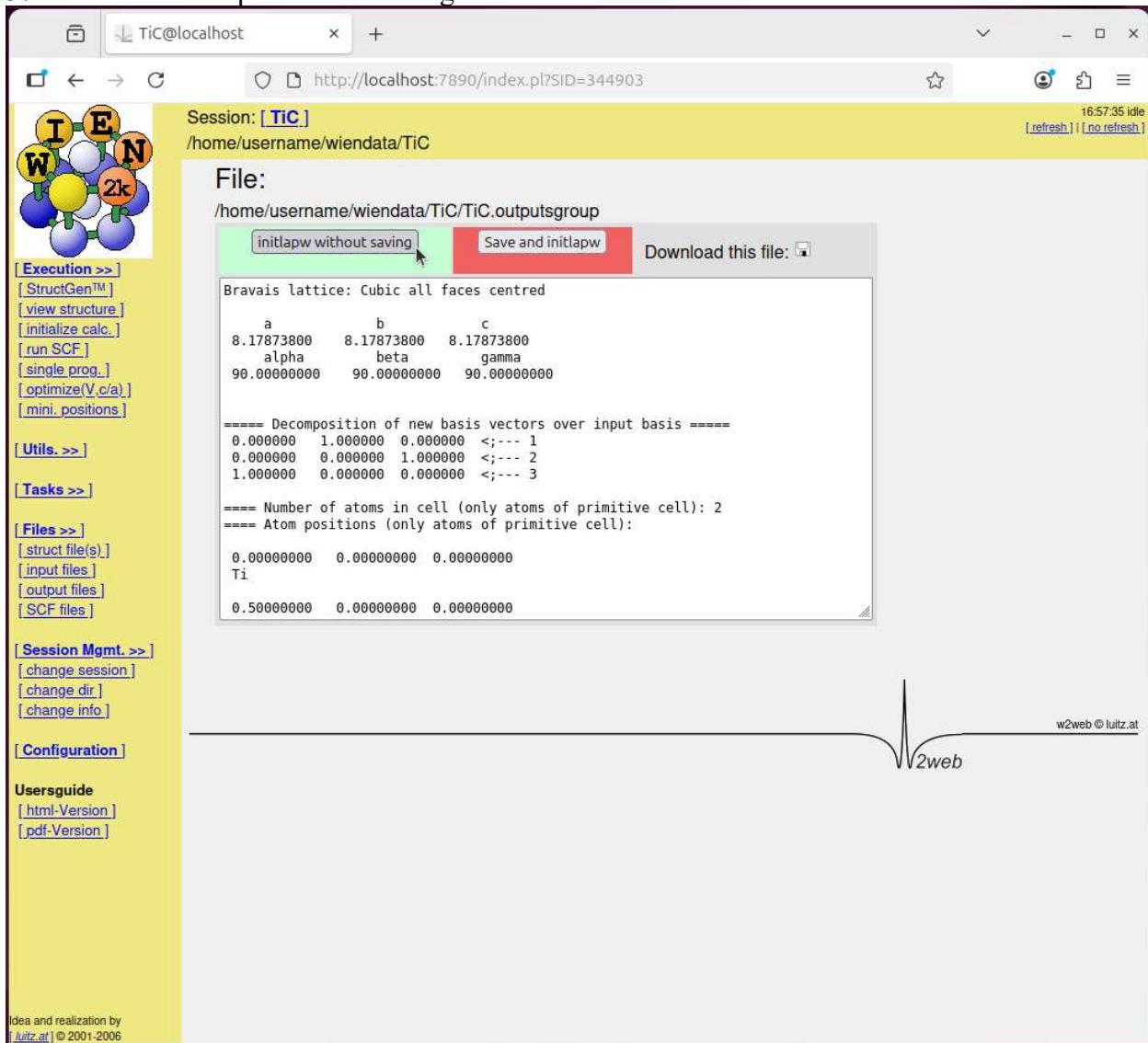
Below this, there is a 'Continue with' section containing a button labeled 'initlapw' which is being clicked by a mouse cursor. To the right of the button is a logo for 'w2web' featuring a stylized heart-like shape.

The left sidebar contains a navigation menu with the following sections and 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](#).

At the bottom left, it says 'Idea and realization by [luitz.at](#) © 2001-2006'.

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



The screenshot shows a web browser window titled "TiC@localhost" displaying session information for "TiC". The URL is "http://localhost:7890/index.pl?SID=344903". 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., and Configuration. The main content area shows session details and output files. A modal dialog box is open, showing the command "initlapw without saving" highlighted in green, indicating it was just clicked. Below the command, there are other buttons: "Save and initlapw" (red) and "Download this file: ". The output text in the modal includes structural parameters (Bravais lattice: Cubic all faces centred, lattice constants a, b, c, alpha, beta, gamma), decomposition of basis vectors, atom positions, and atomic species (Ti). The footer of the page includes copyright information: "Idea and realization by lutz.at © 2001-2006" and a logo "w2web © lutz.at" with a stylized heart symbol.

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

The screenshot shows a web browser window for 'TiC@localhost' at 'http://localhost:7890/index.pl?SID=344903'. The session is 'TiC'.

Session: [TiC]

/home/username/wiendata/TiC

16:57:35 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]

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

16:57:35 idle
[refresh] || [no refresh]

RMI reduction by X % (default: HMI 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 6)

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
sgroup found: 225 (F m -3 m)

check TiC.in1_st set RKmax
(usually 5.0-9.0). [\[Click here for more info\]](#)
view TiC.output and cp TiC.in0_std TiC.in0
check if gmax>gmin
Perform spin-polarized calc.?

check TiC.in2_st set Fermi-method and GMAX
and GMAX
Prepare input files
No
Yes

Use struct-file generated by sgroup?
(Usually NO, unless WARNINGS appeared above)

Yes
No

x kgen
view klist
x dstart interactively

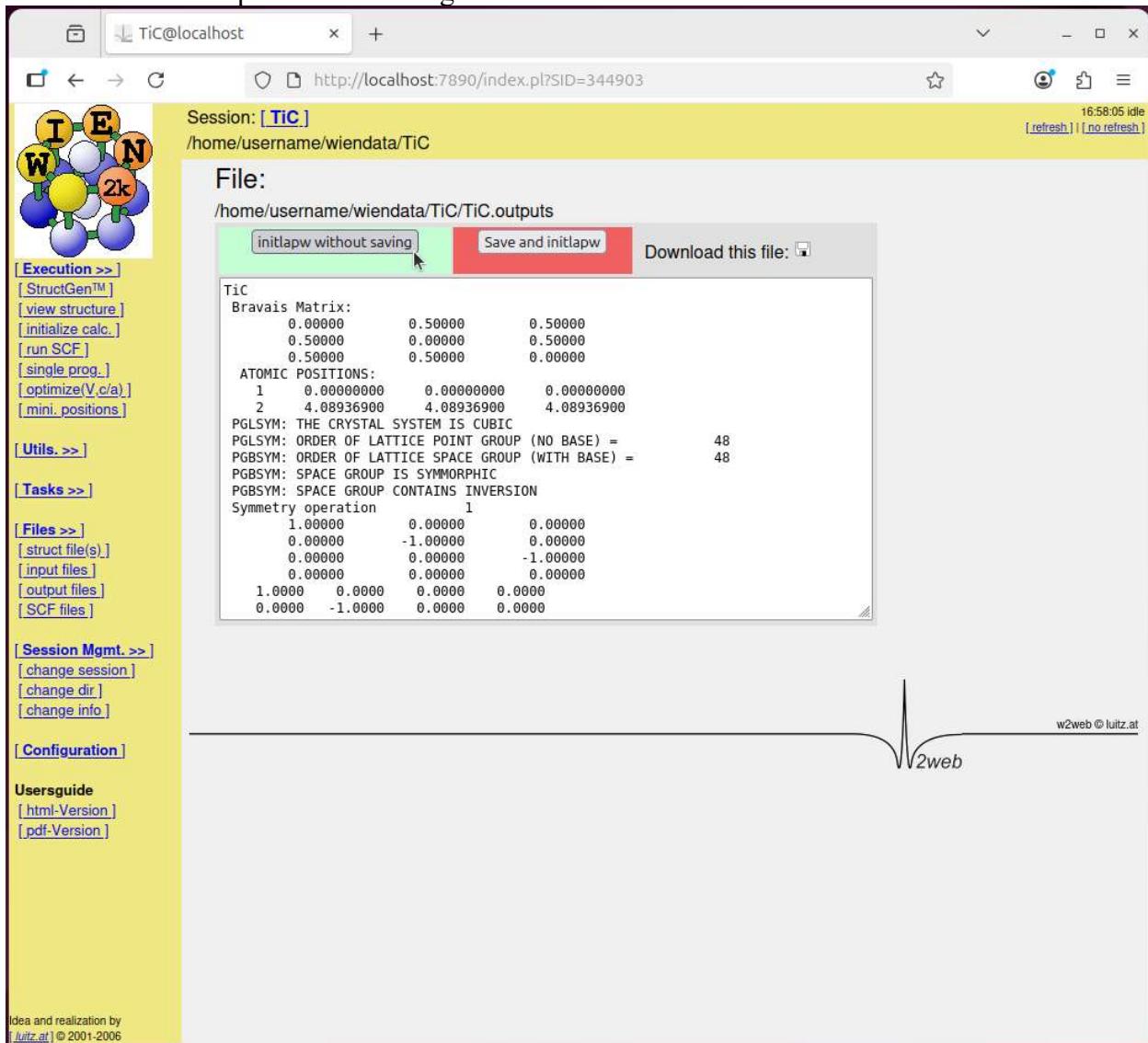
x symmetry
copy struct_st and view outputs
instgen_lapw TiC.inst needs to be generated by instgen_lapw
view outputst

39. Click the “x symmetry” button

40. Click the “initlapw” button:

The screenshot shows a web browser window for 'TiC@localhost' at 'http://localhost:7890/index.pl?SID=344903'. The page displays a molecular structure with atoms labeled I, E, N, W, and 2k. On the left, a sidebar contains navigation links for 'Execution', 'StructGen™', 'view structure', 'initialize calc.', 'run SCF', 'single prog.', 'optimize(V,c/a)', 'mini. positions', 'Utils. >>', 'Tasks >>', 'Files >>', 'Session Mgmt. >>', and 'Configuration'. The main content area shows the commandline: 'x symmetry' and 'Program input is: ""'. It also displays output: 'SPACE GROUP CONTAINS INVERSION 0.005u 0.001s 0:00.00 0.0% 0+0k 0+64io 0pf+0w'. Below this is a 'Continue with' section with a button labeled 'initlapw' which has a mouse cursor hovering over it. The bottom right corner of the page features a logo with the text 'w2web © luitz.at'.

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



The screenshot shows a web browser window for the TiC@localhost application. The URL is <http://localhost:7890/index.pl?SID=344903>. The session name is **TiC**.

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

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

Buttons at the top of the output area:
 (highlighted)

Output content:

```

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

```

Left sidebar menu:

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

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43. Click the “instgen_lapw” button

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

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

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

Execute!

16:58:05 idle
[refresh](#) ||| [no refresh](#)

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45. Click the “initlapw” button:

The screenshot shows a web browser window titled "TiC@localhost" with the URL "http://localhost:7890/index.pl?SID=344903". The session is labeled "TiC" and the commandline is "instgen_lapw -s -nm". The program input is "u u". A message indicates "2 Atoms found: with labels Ti C generate atomic configuration for atom 1 : Ti generate atomic configuration for atom 2 : C". Below this, there is a "Continue with" section containing a button labeled "initlapw". The left sidebar contains various navigation links such as "Execution >>", "StructGen™", "view structure", "initialize calc.", etc. The bottom left corner of the sidebar notes "Idea and realization by [luitz.at](#) © 2001-2006". The bottom right corner of the main area has a logo for "w2web" with the text "w2web © luitz.at".

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 "http://localhost:7890/index.pl?SID=344903". The session is identified as "Session: [TiC] /home/username/wiendata/TiC". A message in the top right corner says "LSTART needs input". On the left, there's a sidebar with various links like "Execution >>", "StructGen™", "view structure", etc. The main content area has a heading "Select Exchange Correlation Potential:" with a dropdown menu set to "PBE-GGA (Perdew-Burke-Ernzerhof 96)". Below it, there's a section for "ENERGY to separate core and valence states" with a note about charge localization and a text input field containing "-6.0" with a tooltip "(recommended: -6.0 Ry)". An "Execute!" button is visible. The bottom right of the page features a logo with the text "w2web © luitz.at" and "2web". At the bottom left, there's a note: "Idea and realization by luitz.at © 2001-2006".

48. Click the “initlapw” button:

TiC@localhost http://localhost:7890/index.pl?SID=344903 16:59:05 idle [refresh] || [no refresh]

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

Commandline: **x Istart**
 Program input is: "13 -6.0 "

```

SELECT XC POT:
recommended: PBE      [(13) GGA of Perdew-Burke-Ernzerhof 96]
              LDA      [( 5)]
              WC       [(11) GGA of Wu-Cohen 2006]
              PBESOL [(19) GGA of Perdew et al. 2008]
SELECT ENERGY to separate core and valence states:
recommended: -6.0 Ry (check how much core charge leaks out of MT-sphere)
ALTERNATIVELY: specify charge localization
(between 0.97 and 1.0) to select core state
  
```

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

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

LSTART ENDS
 0.055u 0.002s 0:00.05 100.0% 0+0k 0+968io 0pf+0w

Continue with

initlapw

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

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

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

initlapw without saving Save and initlapw Download this file: [\[\]](#)

ORBITAL	OCCUPATION	TRIAL ENERGIES
1S	1.000	-1.2100000E+02
1S	1.000	-1.2100000E+02

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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:

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

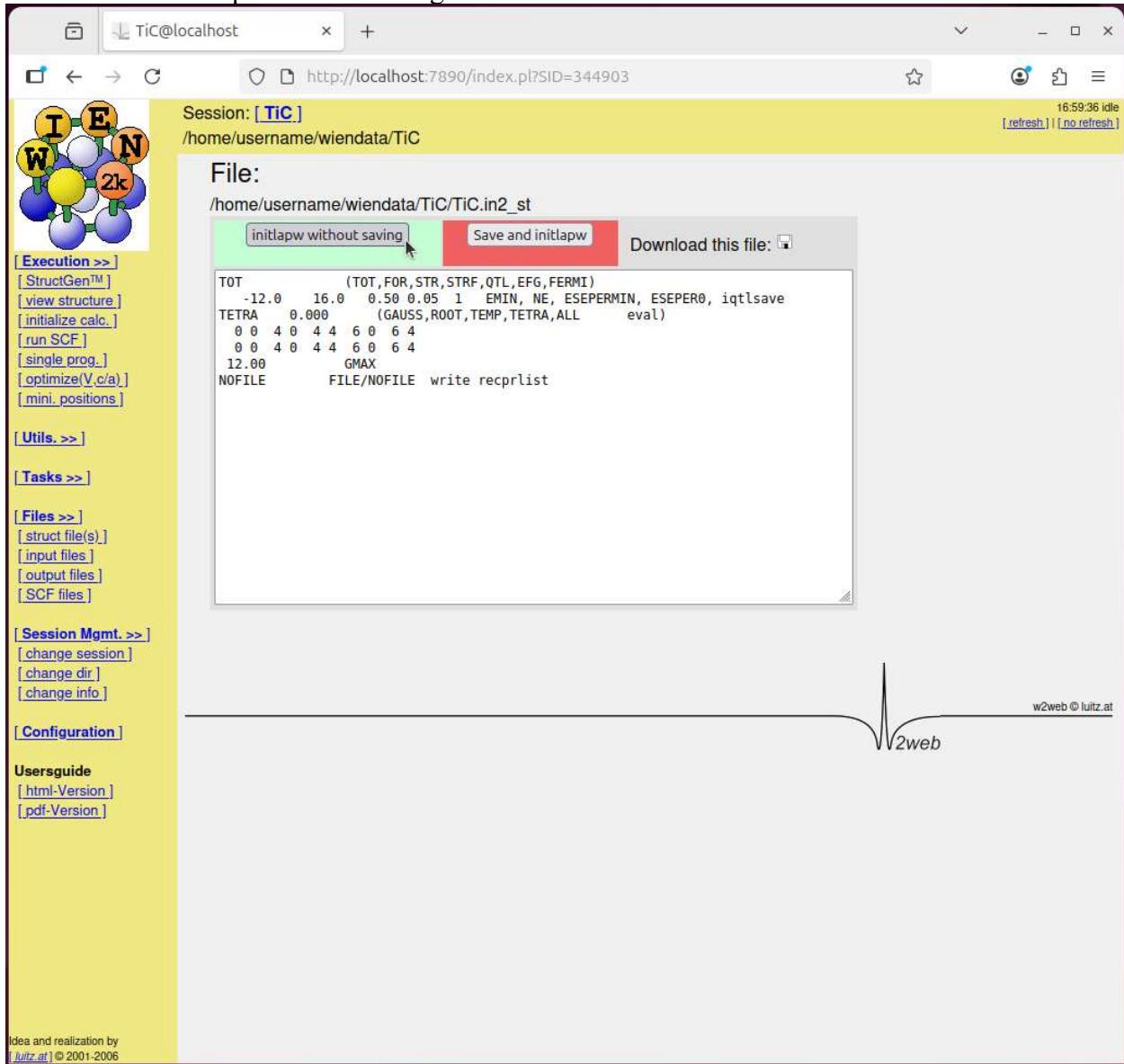
File:
/home/username/wiendata/TiC/TiC.in1_st

WEFIL EEL= 0.50000 (WEFIL, WEPRI, ENEL, SUPWE)
7.00 10 4 ELPA RKG 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

initlapw without saving Save and initlapw Download this file:

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



The screenshot shows a web browser window titled "TiC@localhost" with the URL "http://localhost:7890/index.pl?SID=344903". The page displays a session named "TiC" with the path "/home/username/wiendata/TiC". On the left, there is a sidebar with various menu items such as "Execution >>", "StructGen™", "view structure", etc. The main content area shows a molecular model of a TiC cluster and a text input field containing an input file. The input file content is as follows:

```

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

```

Below the input field, there are three buttons: "initlapw without saving" (highlighted in green), "Save and initlapw" (highlighted in red), and "Download this file: ". The status bar at the top right shows "16:59:36 idle" and "[refresh] || [no refresh]". The bottom right corner features a logo with the text "w2web © luitz.at" and "2web".

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 "http://localhost:7890/index.pl?SID=344903". The page displays a session configuration for a calculation named "TiC". On the left, there is a sidebar with various navigation links such as "Execution >>", "StructGen™", "view structure", etc. The main content area contains several input parameters:

- 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):**

A red message at the bottom states: "Your input seems to be ok and you can start the initialization". Below this is a "RUN BATCH INITIALISATION" button.

On the right side, under "Individual mode (phase 16)", there are several buttons and checkboxes:

- x nn
- x sgroup
- x symmetry
- copy struct_st and view outputs
- instgen_lapw
- 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
- in0, in1, in2, inc and inm files generated
- x kgen
- view klist
- x dstart
- checkbox for interactively

Checkboxes for "No" and "Yes" are present next to some of the buttons.

At the bottom left, there is a note: "Idea and realization by [J. Lutz](#) © 2001-2006".

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 for 'TiC@localhost' at 'http://localhost:7890/index.pl?SID=344903'. The session is named 'TiC' and is located at '/home/username/wiendata/TiC'. On the left, there's a sidebar with a molecular model icon and several menu items: Execution >>, StructGen™, view structure, initialize calc., run SCF, single prog., optimize(V,c/a), mini. positions, Utils. >>, Tasks >>, Files >>, Session Mgmt. >>, Configuration, and Usersguide (html-Version, pdf-Version). The main area has a yellow header bar with 'Session: [TiC]' and 'Number of k-points: 1000'. Below it, there's a note about specifying divisions for reciprocal lattice vectors if the number of k-points is zero. There are three empty input fields and a 'Shift k-mesh (if applicable)' dropdown set to 'Yes'. A 'Execute!' button is highlighted with a cursor. In the bottom right corner, there's a small logo with 'w2web' and 'luitz.at'. At the bottom left, it says 'Idea and realization by [luitz.at] © 2001-2006'.

59. Click the “initlapw” button:

The screenshot shows a web browser window titled "TiC@localhost" with the URL "http://localhost:7890/index.pl?SID=344903". The page displays a session for "TiC" at "/home/username/wiendata/TiC". The commandline is "x kgen" and the program input is "1000 1". The output shows K-points generation details: 47 k-points generated, ndiv= 10 10 10, and KGEN ENDS. A "Continue with" section contains a button labeled "initlapw" which is being clicked by a mouse cursor. The interface includes a sidebar with links for execution, utilities, tasks, files, session management, and configuration, along with a usersguide. A footer note credits "luitz.at" for the idea and realization.

60. Click the “view klist” button

61. Click the “initlapw without saving” button:

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

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

1	0	0	0	10	1.0	-7.0	1.5	1000 k, dj
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			

Execution >>

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

Utils. >>

Tasks >>

Files >>

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

Session Mgmt. >>

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

Configuration

Usersguide

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

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17:00:36 idle
[\[refresh \]](#) || [\[no refresh \]](#)

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

The screenshot shows a web browser window for the TiC application at <http://localhost:7890/index.pl?SID=344903>. The session name is **TiC**. The commandline is **x dstart** and the program input is **""**. The output shows a calculation summary:

C	T	F
DSTART ENDS		
0.801u	0.005s	0:00.80 100.0%
0+0k	0+368io	0pf+0w

Below the output, there is a section titled **Continue with** containing a button labeled **initlapw**, which is currently being clicked. To the right of the button is a logo consisting of a stylized heart rate line above the text **w2web**.

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

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

Output:

C	T	F
DSTART ENDS		
0.801u	0.005s	0:00.80 100.0%
0+0k	0+368io	0pf+0w

Continue with

initlapw

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Execution >>

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

Utils. >>

Tasks >>

Files >>

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

Session Mgmt. >>

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

Configuration

Usersguide

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

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64. Click the “view TiC.outputd and cp TiC.in0_std TiC.in0” button

65. Notice that the condition gmax > gmin is met and click the “initlapw without saving” button:

The screenshot shows a web browser window titled "TiC@localhost" with the URL "http://localhost:7890/index.pl?SID=344903". The session name is "TiC" and the path is "/home/username/wiendata/TiC". On the left, there's a sidebar with various menu items like "Execution >>", "StructGen™", "view structure", etc. The main area displays a molecular model of TiC with atoms labeled E, N, W, and 2k. Below the model, a "File:" section shows the path "/home/username/wiendata/TiC/TiC.outputd". A red box highlights the "initlapw without saving" button. The output text in the box includes:

```

root(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
:NT0001: CHARGE SPHERE 1 = 19.823810

```

At the bottom right, there's a watermark "w2web © lutz.at" with a small logo.

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

The screenshot shows the TiC@localhost web interface for session 'TiC'. The main content area displays initialization parameters and a configuration section. In the bottom right, a modal dialog box titled 'Perform spin-polarized calc.? ' contains two buttons: 'No' (highlighted with a red border) and 'Yes'. The background shows various input fields and checkboxes related to calculation parameters like 'Precision level', 'RMT reduction', and 'RKMAX'.

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

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 20)

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.

<input type="button" value="x nn"/> <input type="button" value="view outputnn"/>	<input #"="" type="button" value="check TiC.in1_st set RKmax (usually 5.0-9.0). [Click here for more info]"/>	<input type="button" value="view TiC.outputd and cp TiC.in0_std TiC.in0 check if gmax>gmin"/>
<input type="button" value="x sgroup"/> <input type="button" value="view outputsgroup"/>	<input type="button" value="check TiC.in2_st set Fermi-method and GMAX"/> <input type="button" value="Prepare input files"/>	
<input type="button" value="x symmetry"/> <input type="button" value="copy struct_st and view outputs"/>		
<input type="button" value="instgen_lapw"/> TiC.inst exists, run instgen_lapw only for non-default spin-configuration <input type="button" value="x lstart"/> <input type="button" value="view outputst"/>	<input type="button" value="x kgen"/> <input type="button" value="view klist"/> <input type="button" value="x dstart"/> <input checked="" type="checkbox"/> interactively	

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

The screenshot shows a web browser window for 'TiC@localhost' at the URL <http://localhost:7890/index.pl?SID=344903>. The page displays session configuration options for a TiC calculation. On the left, a sidebar lists various session management and configuration links. The main content area includes a molecular model of TiC, session information ('Session: [TiC]'), and a list of configuration parameters. A section titled 'Individual mode (phase 21)' provides instructions for antiferromagnets and self-generated structures. At the bottom, a large green button labeled '[Continue with run SCF]' is highlighted with a mouse cursor.

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

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 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.outputd and cp TiC.in0_std TiC.in0
view outputnn	if gmax>gmin	check
x sgroup	check TiC.in2_st set Fermi-method and GMAX	Prepare input files
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 kgen	
x lstart	view klist	
view outputst	x start <input checked="" type="checkbox"/> 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:

Session: [TiC] /home/username/wien2k/TiC

17:02:07 idle [[refresh](#)] [[no refresh](#)]

SCF Cycle

Options: (help)

- parallel
- optimize positions (MSR1a)
- iterative diag
- iter. after full-diag
- iter.diag (no Hinv)
- vec2pratt with iter.diag
- spinorbit
- spin polarized
- constrain moment to 0
- AFM calc.
- dm
- orbital pot (DFT+U)
- eece (hybrid-DFT for correlated e)
- DFT-D3 (dispersion corrections)
- nl-vdW (dispersion corrections)
- hf (full hybrid-DFT, expensive!)
- diaghf (diagonal-only full hybrid-DFT)
- non-scf full hybrid-DFT)
- newklist (full hybrid-DFT with new k-list)
- redklist (full hybrid-DFT with red. k-list)

Expert options:

no HNS 6
 in1new 2
 q-limit 0.05
 It-number 40
 FSM 0

Scratch Directory:

Convergence criteria:

Energy: 0.0001 Ry
 Force: 1 mRy/au
 Charge: 0.0001 e

Type of execution: interactively

E-mail notification to

only save parameters

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

```

Session: [TiC]
/home/username/wiendata/TiC
17:03:05 idle
[refresh] || [no refresh]

ec cc fc and str_conv 1 0 1 1
in cycle 8      ETEST: .0004534800000000    CTEST: .1361611    STRTEST: 0
  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: .0396235    STRTEST: 0
  LAPW0 END
  LAPW1 END
  LAPW2 END
  CORE END
  MIXER END
ec cc fc and str_conv 1 0 1 1
in cycle 10     ETEST: .0002063550000000    CTEST: .0132326    STRTEST: 0
  LAPW0 END
  LAPW1 END
  LAPW2 END
  CORE END
  MIXER END
ec cc fc and str_conv 1 0 1 1
in cycle 11     ETEST: .0000190850000000    CTEST: .0016612    STRTEST: 0
  LAPW0 END
  LAPW1 END
  LAPW2 END
  CORE END
  MIXER END
ec cc fc and str_conv 1 0 1 1
in cycle 12     ETEST: .0000148250000000    CTEST: .0005343    STRTEST: 0
  LAPW0 END
  LAPW1 END
  LAPW2 END
  CORE END
  MIXER END
ec cc fc and str_conv 1 1 1 1
> stop

```

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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/wiendata/TiC

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 clmval 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

Calculate density with: -diff -val/-tot -pot/-coulomb/-exchange(2)/-halfrho2v/-tau -sub/-add/-none

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

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w2web © luitz.at

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

The screenshot shows a web browser window titled "TiC@localhost" with the URL "http://localhost:7890/index.pl?SID=344903". The session is identified as "TiC" and the commandline is "x lapw2 -emin -1.0". The program input is empty. The output shows a LAPW2 END message with statistics: 0.153u 0.132s 0:00.28 100.0% 0+0k 0+520io 0pf+0w.

A sidebar on the left contains a molecular structure icon and a list of execution options:

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

Below this is a section for "Utils. >>" which includes:

- [<< Tasks]
- [El. Dens.]
- [DOS]
- [XSPEC]
- [TELNES3]
- [OPTIC]
- [Bandstructure.]

Under "Files >>" are links for struct file(s), input files, output files, and SCF files. There are also sections for "Session Mgmt. >>" (change session, change dir, change info) and "Configuration".

The main area has a "Continue with" button, with "continue with electron density" highlighted by a mouse cursor. A watermark "2web" is visible at the bottom right of the page.

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

```

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

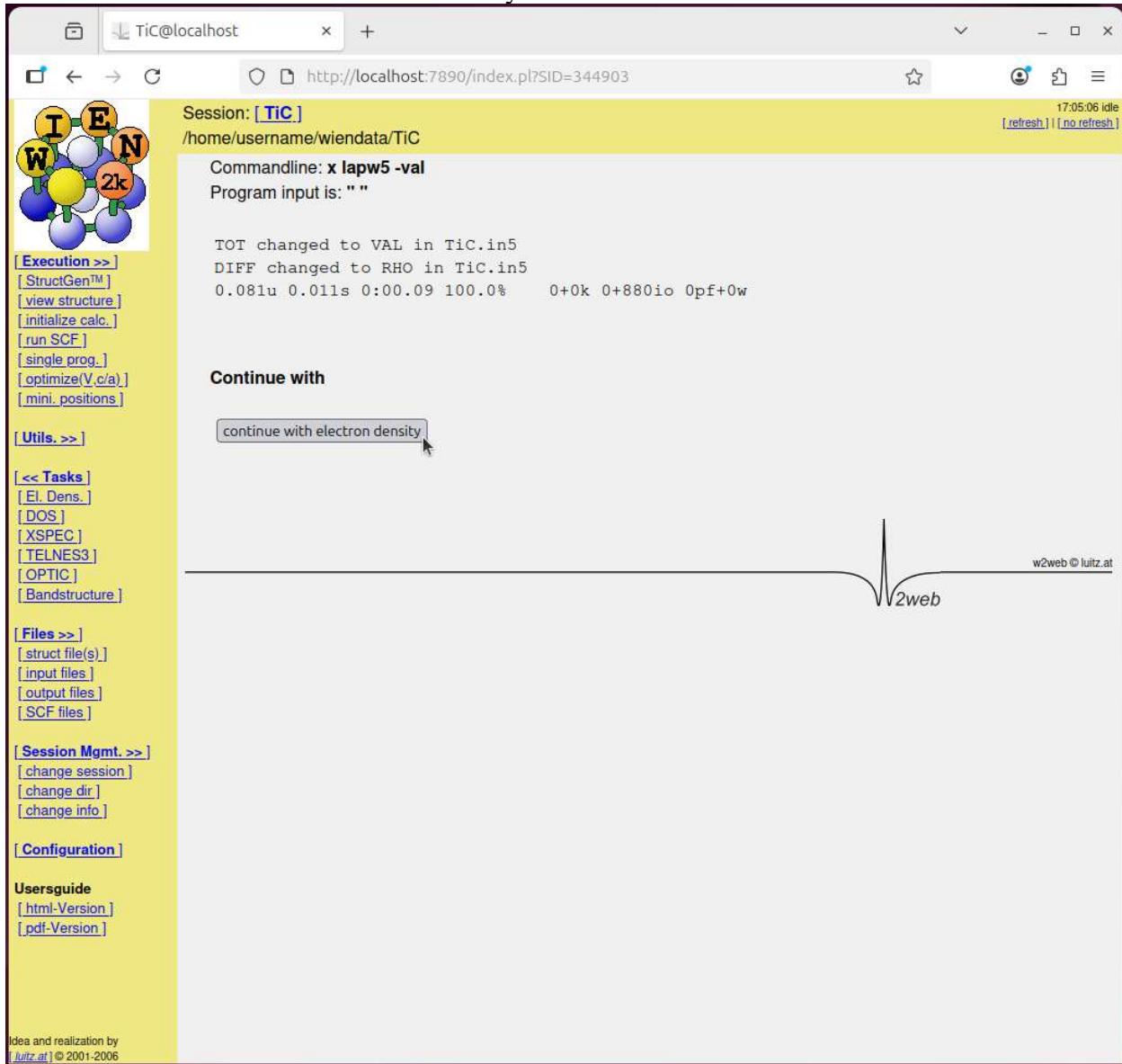
File:
/home/username/wiendata/TiC/TiC.in5

continue with electron density without saving Save and continue with electron density Download this file: □

-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
3 2 3            # number of shells
100 100          # number of points in x and y dir, (ratio close to lenght ratio
RHO              # RHO|DIFF|OVER; ADD|SUB or blank
ANG VAL NODEBUG # ANG|ATU; VAL|TOT; DEBUG|NODEBUG
ORBITQ          # optional: ORBITQ|NONORBITQ plotting directions

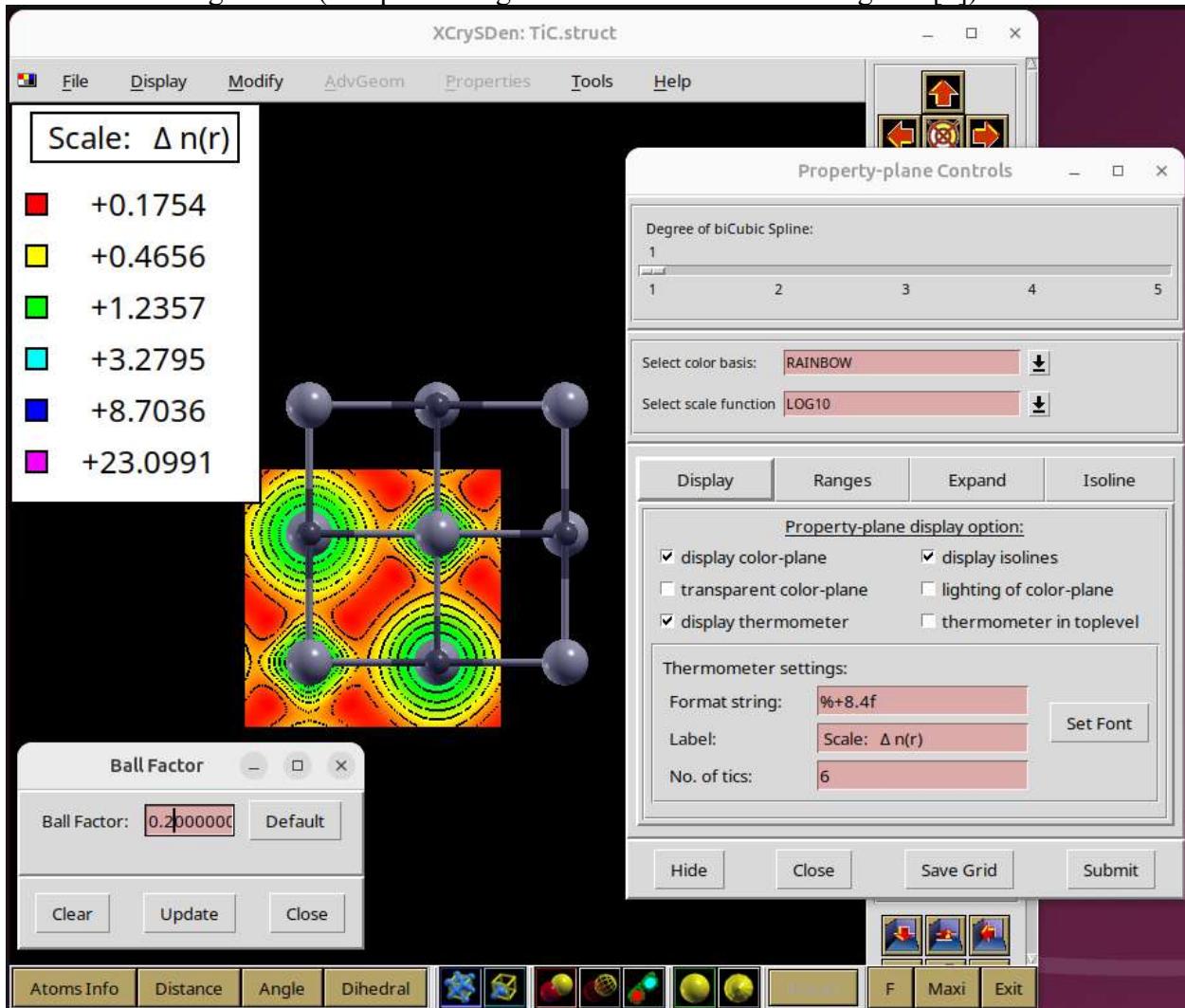
```

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”:

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

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.

We are in rho-plot mode

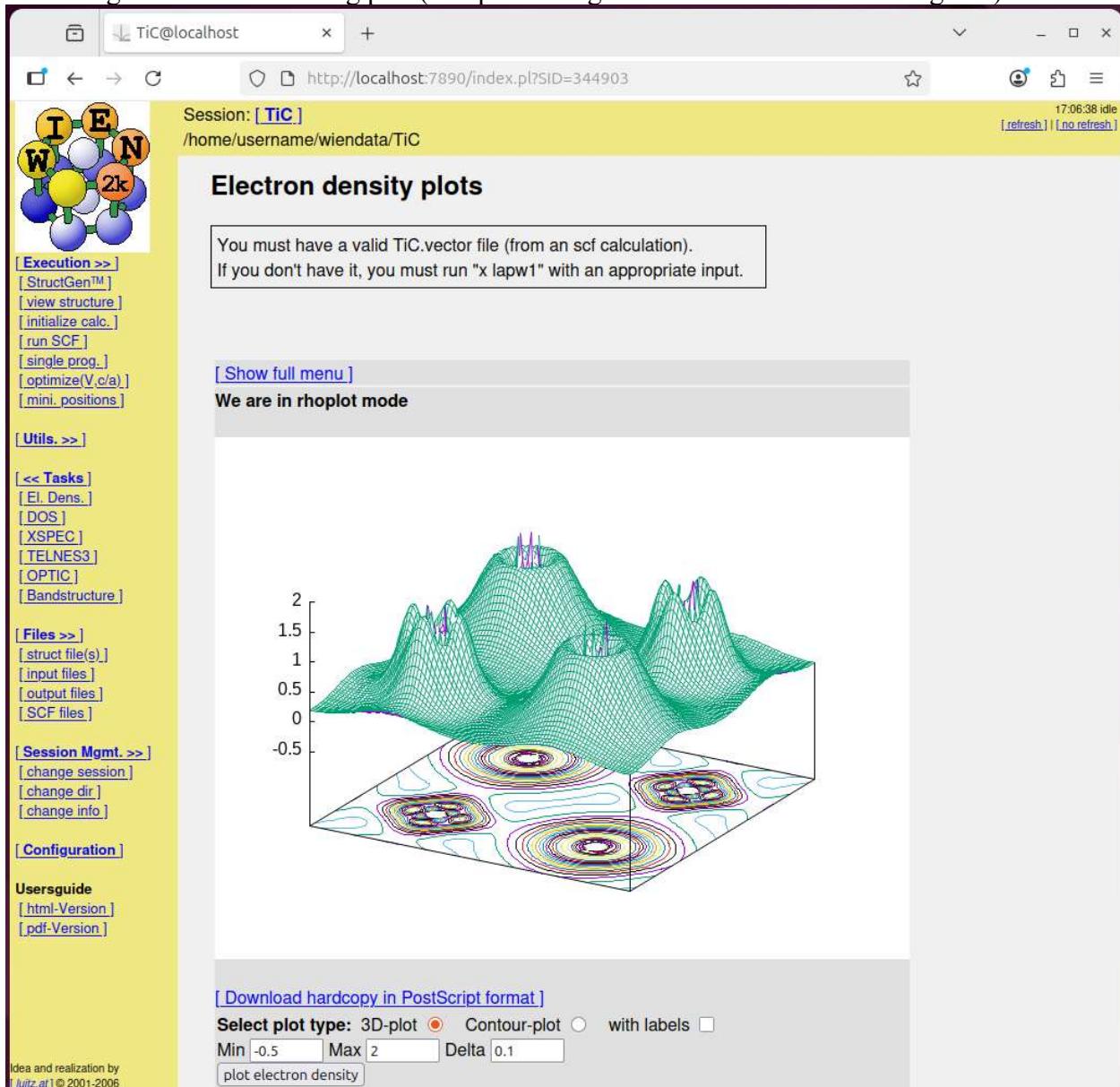
Select plot type: 3D-plot Contour-plot with labels

Min Max Delta

plot electron density

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2web

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”:

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

17:07:08 idle
[refresh] | [no refresh]

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:

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95. Click on “continue with DOS”:

The screenshot shows a web browser window for 'TiC@localhost' at 'http://localhost:7890/index.pl?SID=344903'. The session is labeled 'TiC' and the path is '/home/username/wiendata/TiC'. The time is 17:07:08 idle. The commandline is 'x lapw2 -qtl' and the program input is '""'. The output shows 'LAPW2 END' with statistics: 0.053u 0.022s 0:00.07 100.0% 0+0k 0+480io 0pf+0w.

A 'Continue with' button is present, with the 'continue with DOS' option highlighted by a mouse cursor. To the right, there is a DOS plot titled '2web' with a wavy line graph. The left sidebar contains a navigation menu with sections like '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' (with links to 'html-Version' and 'pdf-Version'), and a note '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
```

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

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

Header from TiC.qtl:

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

Title

```
-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),KSP
0 1 tot           # atom, case=column in qtl-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
```

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

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

17:09:08 idle
[\[refresh\]](#) | [\[no refresh\]](#)

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

```
DOS for tetrahedra around K= -1
covered volume (%) 100.00000000000000
LEGAL END TETRA
0.010u 0.003s 0:00.01 100.0% 0+0k 0+624io 0pf+0w
```

Continue with

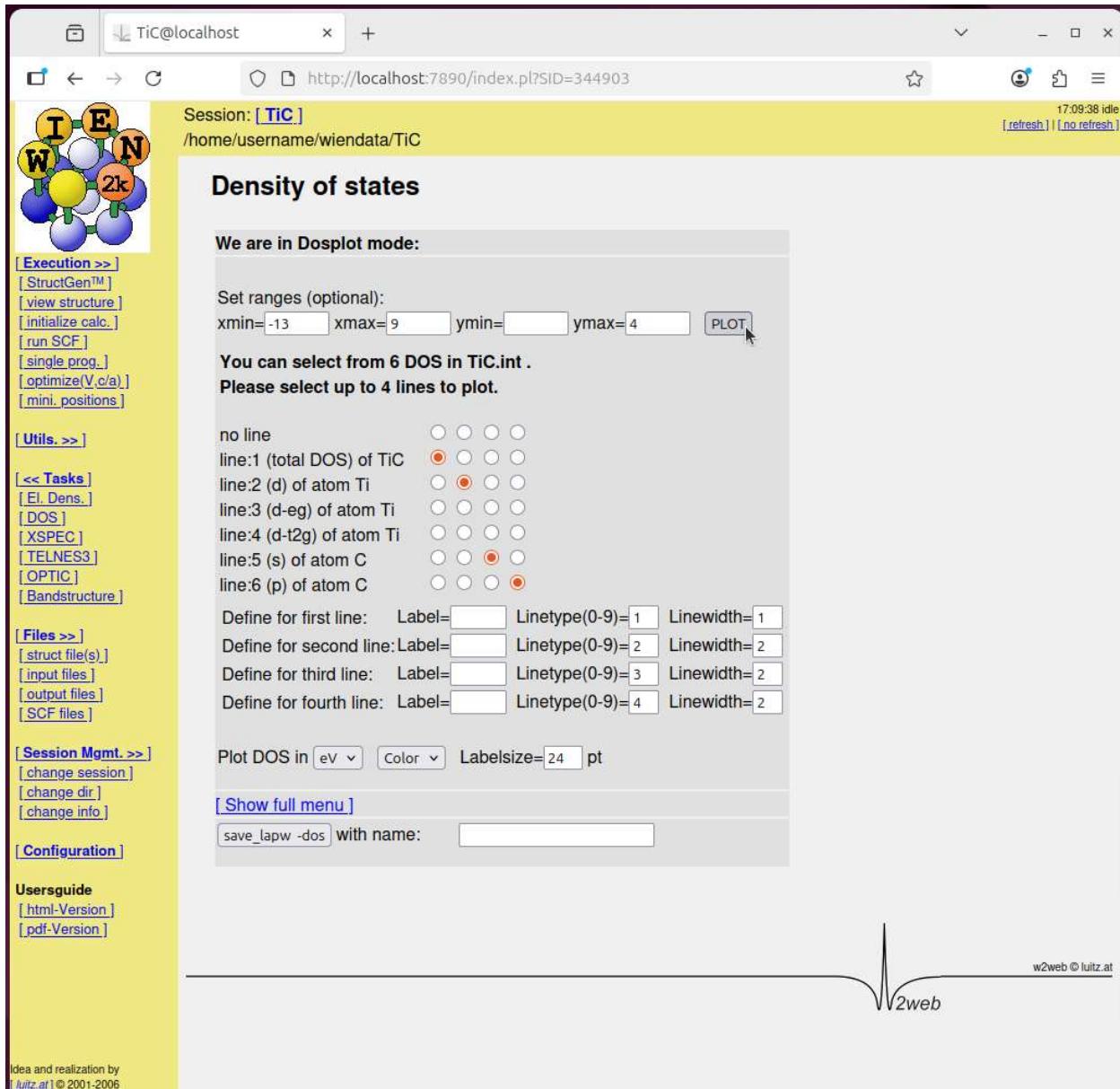
[continue with DOS](#)

w2web © iuitz.at

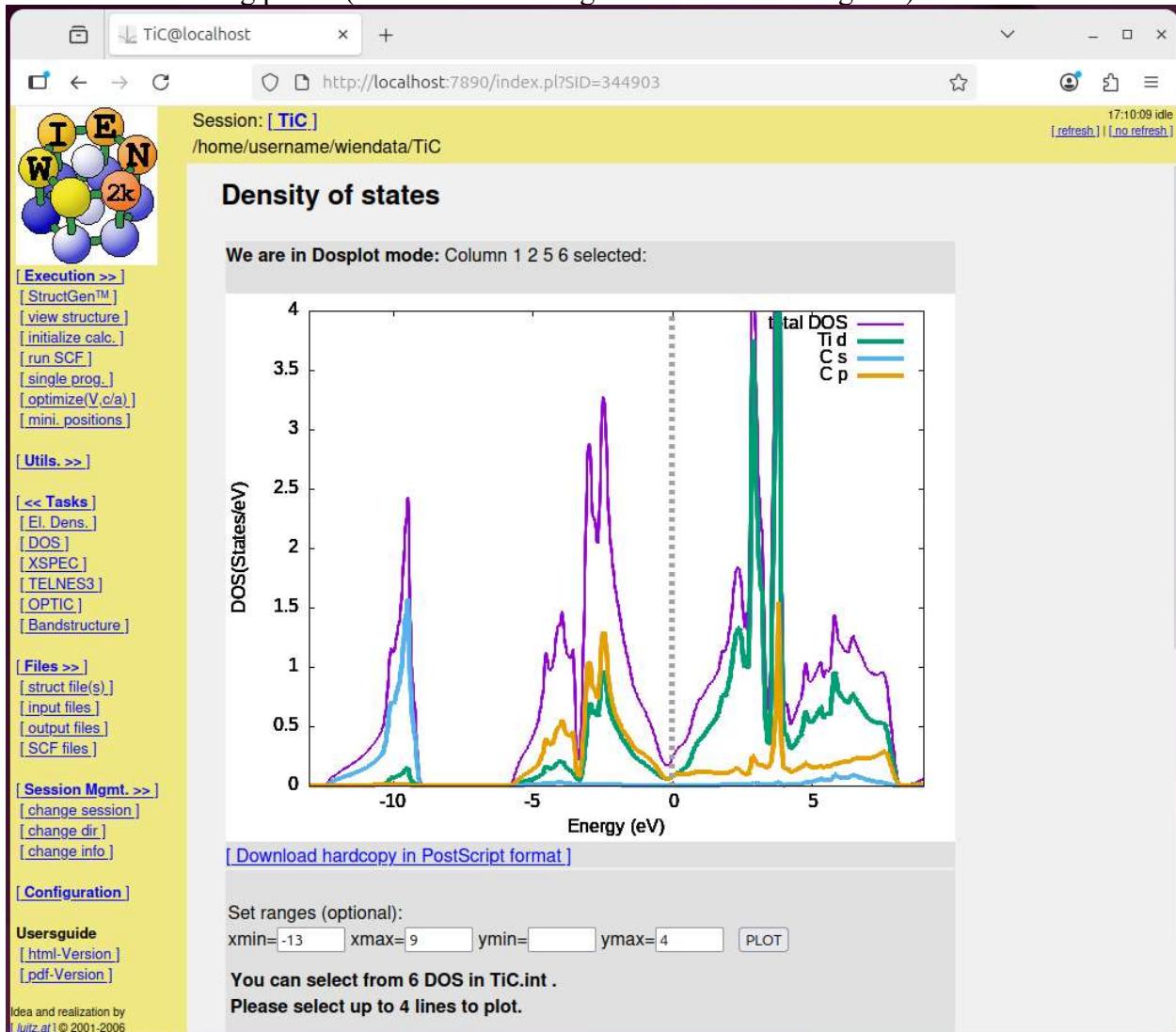
2web

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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”:

The screenshot shows the WiEN2Web software interface. On the left, there is a vertical sidebar with various menu items. The main area is titled "XSPEC" and contains several input fields and buttons. At the bottom, there is a plot of a single peak labeled "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]
- Idea and realization by [\[luitz.at\]](#) © 2001-2006

XSPEC

If you want to include states with higher energy

Edit in1

Calculate eigenvalues interactively

Calculate partial charges interactively

(specify input: atom, n and l of core state; broadening)

Calculate X-ray spectra interactively

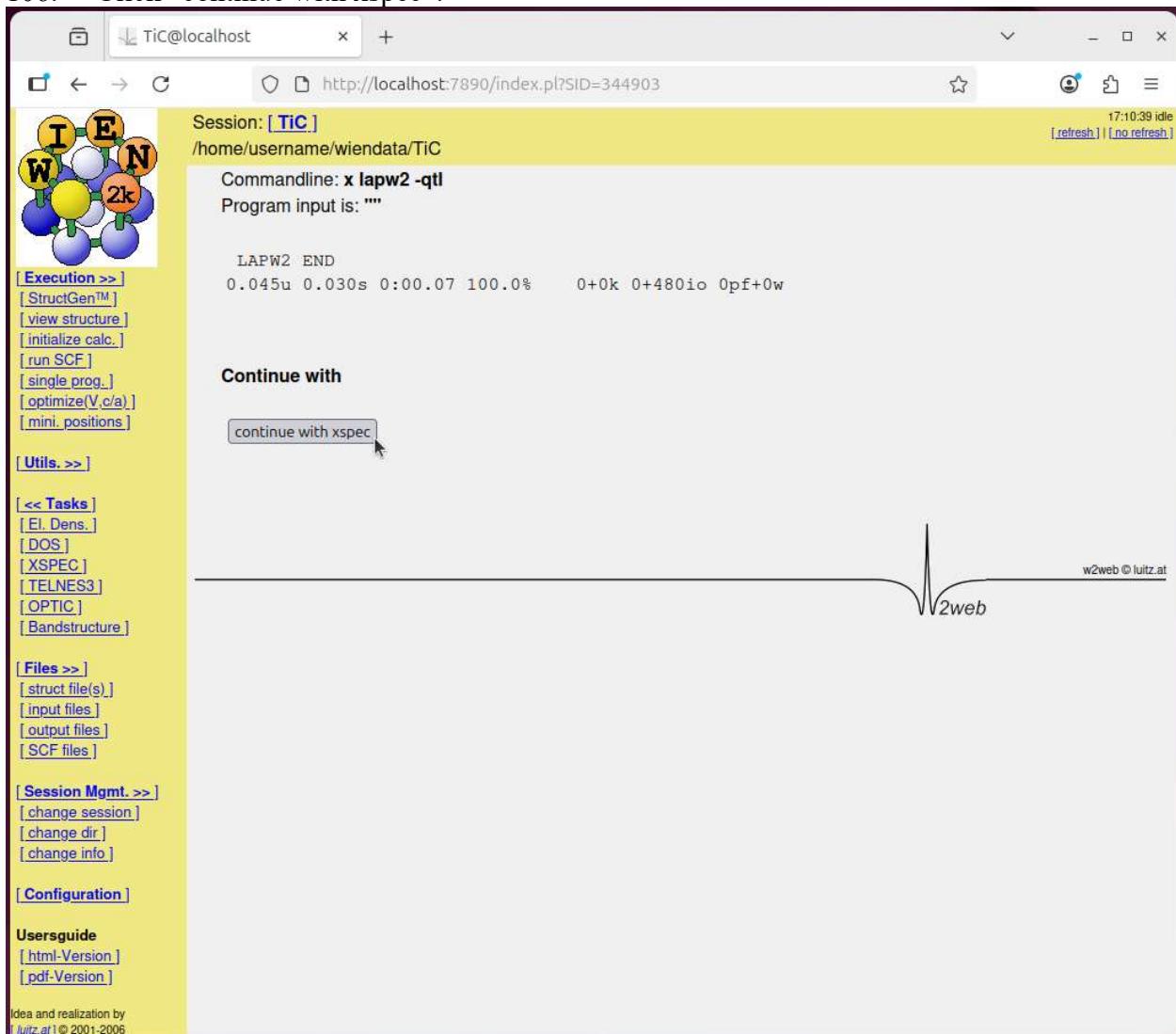
Plot XSPEC or download XSPEC ASCII files for plotting with your own plotting program

with name:

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2web

106. Click “continue with xspec”:



107. Click “x xspec”

108. Click “continue with xspec”:

Session: [TiC]
 /home/username/wiendata/TiC
 17:10:39 idle
 [refresh] | [no refresh]

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

```

Start INITXSPEC
INIT_XSPEC - done
0.000u 0.001s 0:00.00 0.0%      0+0k 0+16io 0pf+0w
Start TETRA
  covered volume (%) 100.00000000000000
  no broadening
  no broadening
  no broadening
  LEGAL END TETRA
0.005u 0.006s 0:00.01 0.0%      0+0k 0+304io 0pf+0w
Start TXSPEC
  1          850
  ABS  LC=          1  LL=          2
  angular multiplication factor W= 0.4000000000000000
  ABS  LC=          1  LL=          0
  angular multiplication factor W= 1.0000000000000000
TXSPEC DONE
0.032u 0.009s 0:00.04 75.0%      0+0k 0+360io 0pf+0w
Start LORENTZ
Lorentz done
0.008u 0.001s 0:00.00 0.0%      0+0k 0+56io 0pf+0w
> stop
> xspec done
0.062u 0.036s 0:00.09 100.0%     0+0k 0+768io 0pf+0w

```

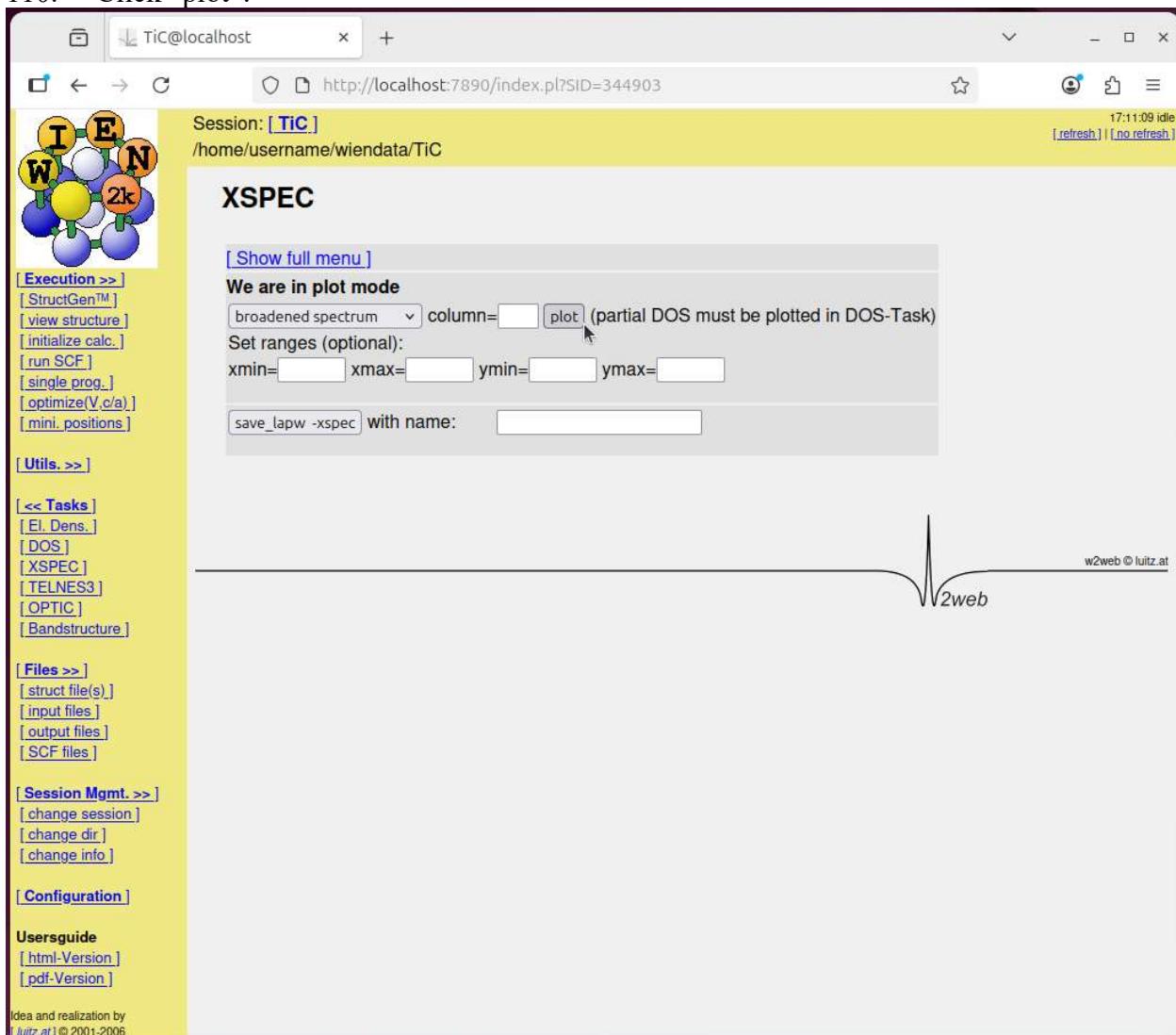
Continue with

continue with xspec

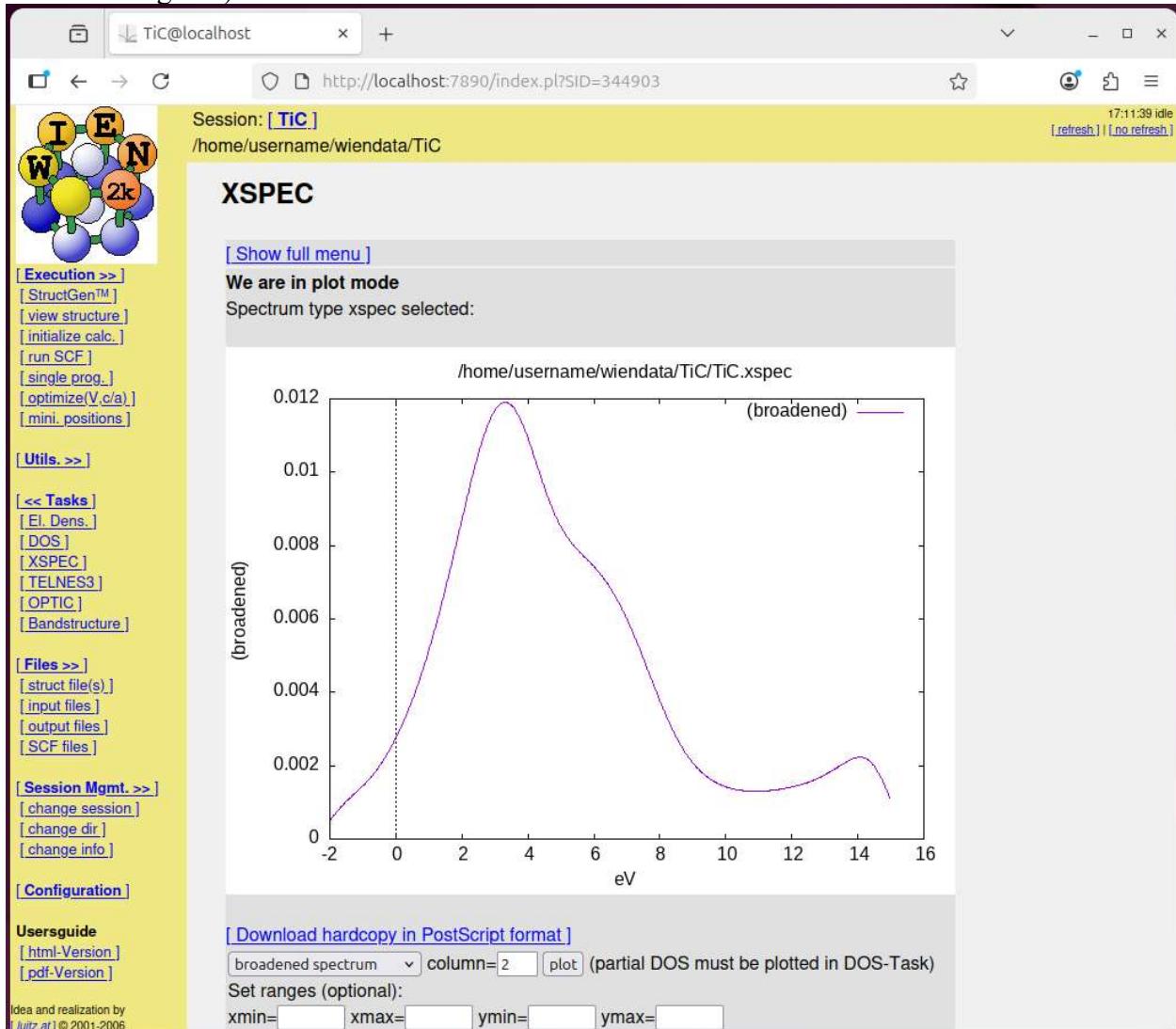
Idea and realization by
[Juiz.at](http://juiz.at) © 2001-2006

109. Click "plot"

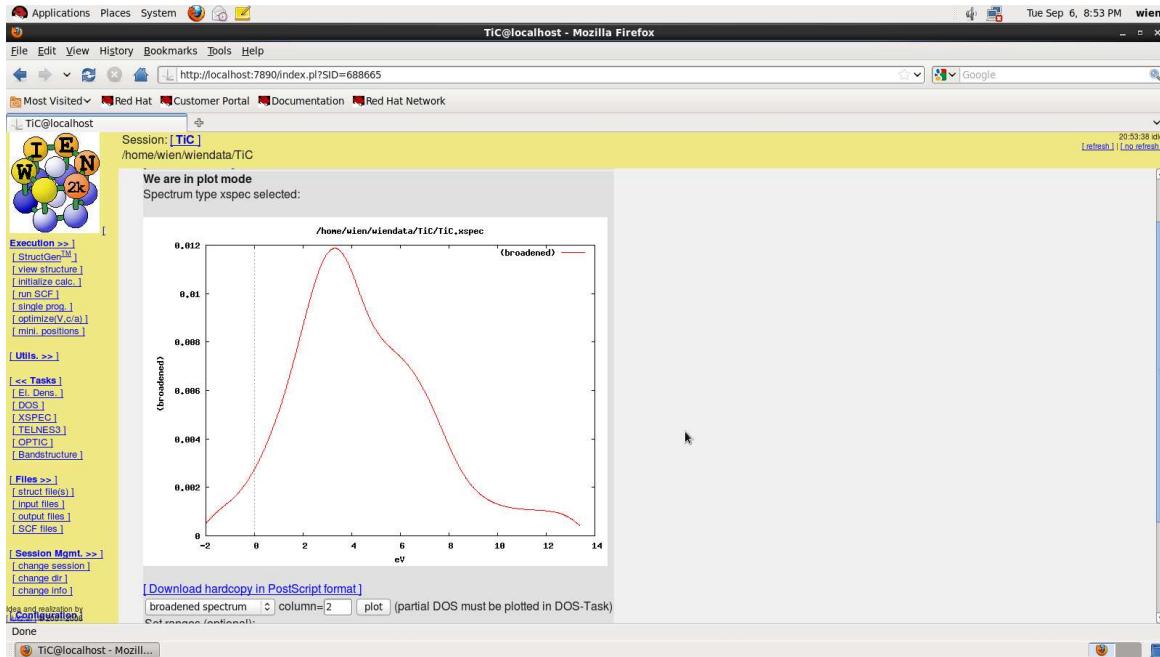
110. Click "plot":



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



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



Plot bandstructure

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

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

- [fcc] [create TiC.klist_band] [Brillouinzones from Bilbao Cryst Server]
- or [Generate k-mesh using XCrysden] (save klist as **TiC.klist_band**)
- x lapw1 -band Calculate Eigenvalues interactively

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

- x irrep Calculate irreducible representations so interactively

for band character plots only!

- x lapw2 -band -qtl Calculate partial charges ("qtl"-file) so interactively
- edit TiC.insp Insert correct EF
- x spaghetti Calculate bandstructure so interactively
- plot bandstructure Plot bandstructure or download Xmgrace files for plotting with xmgrace

save_lapw -band with name:

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114. Click on “x lapw1 -band”

115. Click “continue with bandstructure”:

The screenshot shows a web browser window for 'TiC@localhost' at 'http://localhost:7890/index.pl?SID=344903'. The session name is 'TiC'.

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

Commandline: **x lapw1 -band**
Program input is: ""

```
LAPW1 END
0.810u 0.327s 0:01.14 99.1%      0+0k 0+5976io 0pf+0w
```

Continue with

continue with bandstructure

A band structure plot is visible on the right, showing energy levels versus momentum. The plot is labeled '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]

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

Session: [TiC]
 /home/username/wiendata/TiC
 Commandline: x lapw2 -band -qtl
 Program input is: ""

```
LAPW2 END
0.095u 0.054s 0:00.15 93.3%      0+0k 0+1024io 0pf+0w
```

Continue with

[continue with bandstructure](#)

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2web

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118. Edit TiC.insp by clicking “edit TiC.insp”, change jatom to 1, jtype to 6, Fermi energy to 0.7425 (or could enter 0.7429563361 shown on the screen):

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

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

Header from TiC.qtl and possible FERMI energies:

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

/home/username/wiendata/TiC/TiC.scf: EF (TETRAH.M.) = 0.7429563361

```
### 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:

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

The screenshot shows a web browser window for 'TiC@localhost' at the URL <http://localhost:7890/index.pl?SID=344903>. The page displays a 3D ball-and-stick model of a crystal structure with atoms labeled I, E, N, W, and 2k. On the left, a vertical menu bar lists various options under categories like 'Execution >>', 'Utils. >>', 'Files >>', 'Session Mgmt. >>', and 'Configuration'. The main content area shows a command-line session:

```

Session: [TiC]
/home/username/wiendata/TiC
17:13:40 idle
[refresh] | [no refresh]

Commandline: x spaghetti
Program input is: ""

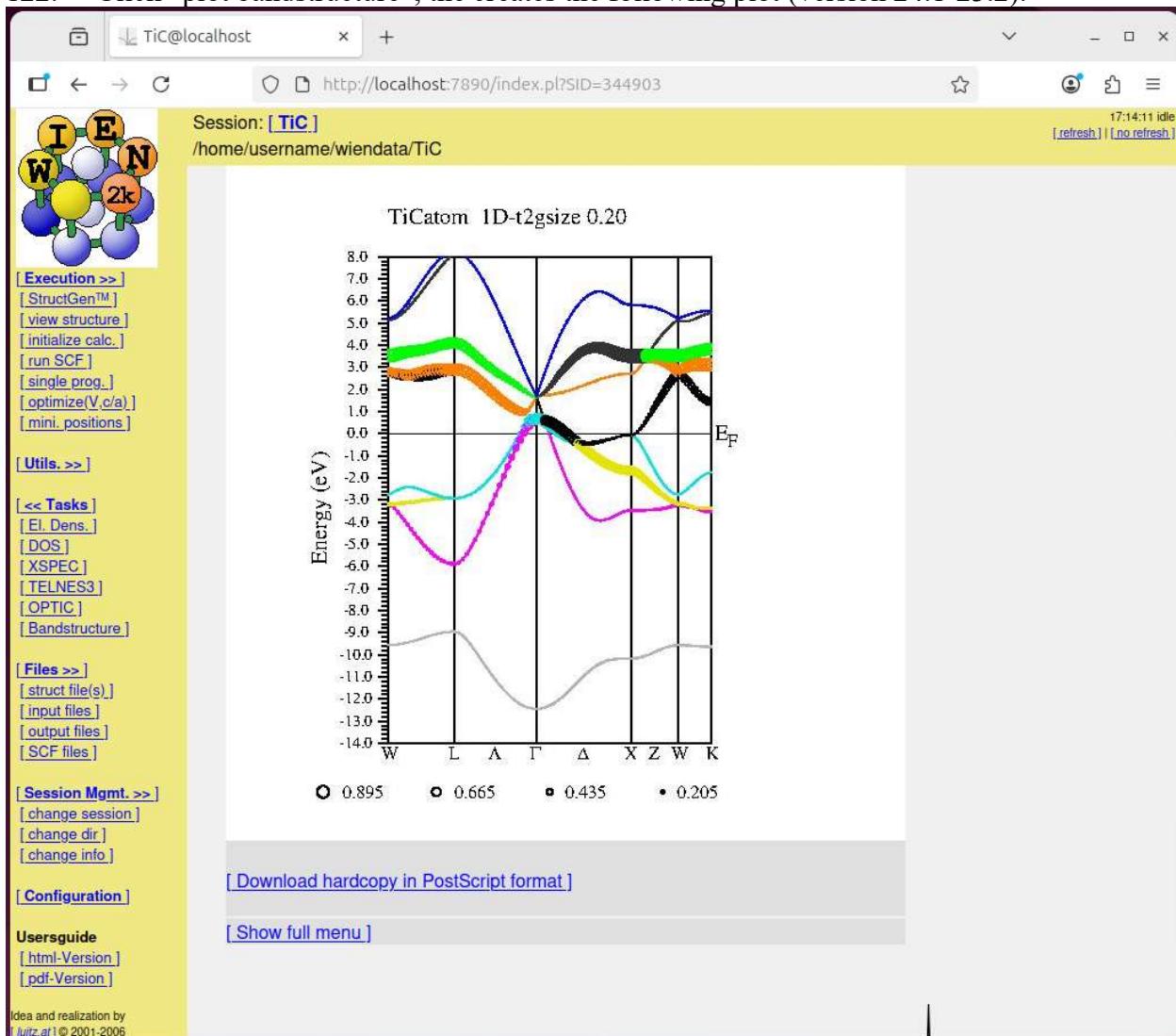
SPAGH: Read band energy from case.output1
      number of k-points read in case.vector=           111
SPAGH END
0.010u 0.005s 0:00.01 100.0%   0+0k 0+624io 0pf+0w

Continue with
  continue with bandstructure

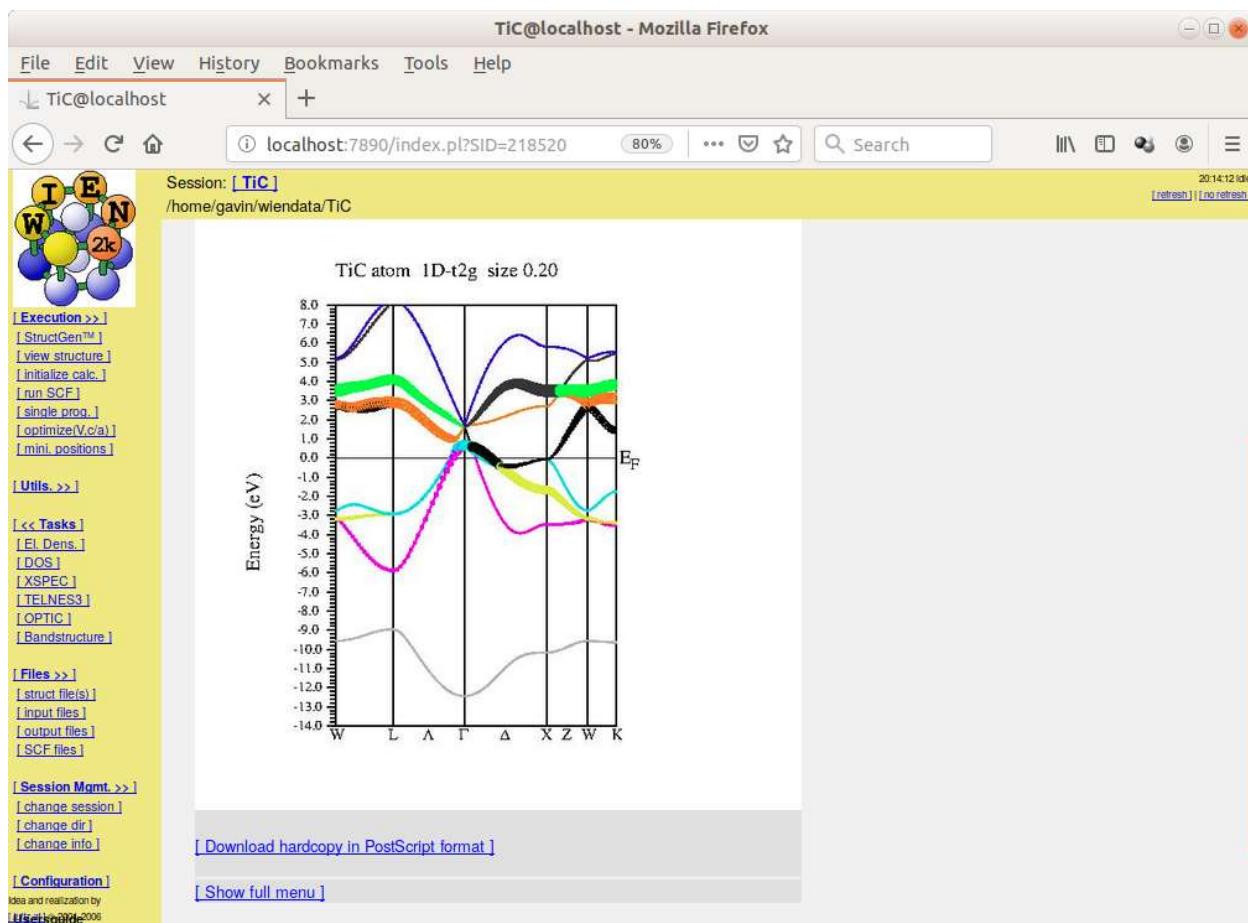
```

A mouse cursor is hovering over the 'continue with bandstructure' button. The bottom right corner of the page features a small logo with the text 'w2web © iuitz.at' and '2web'.

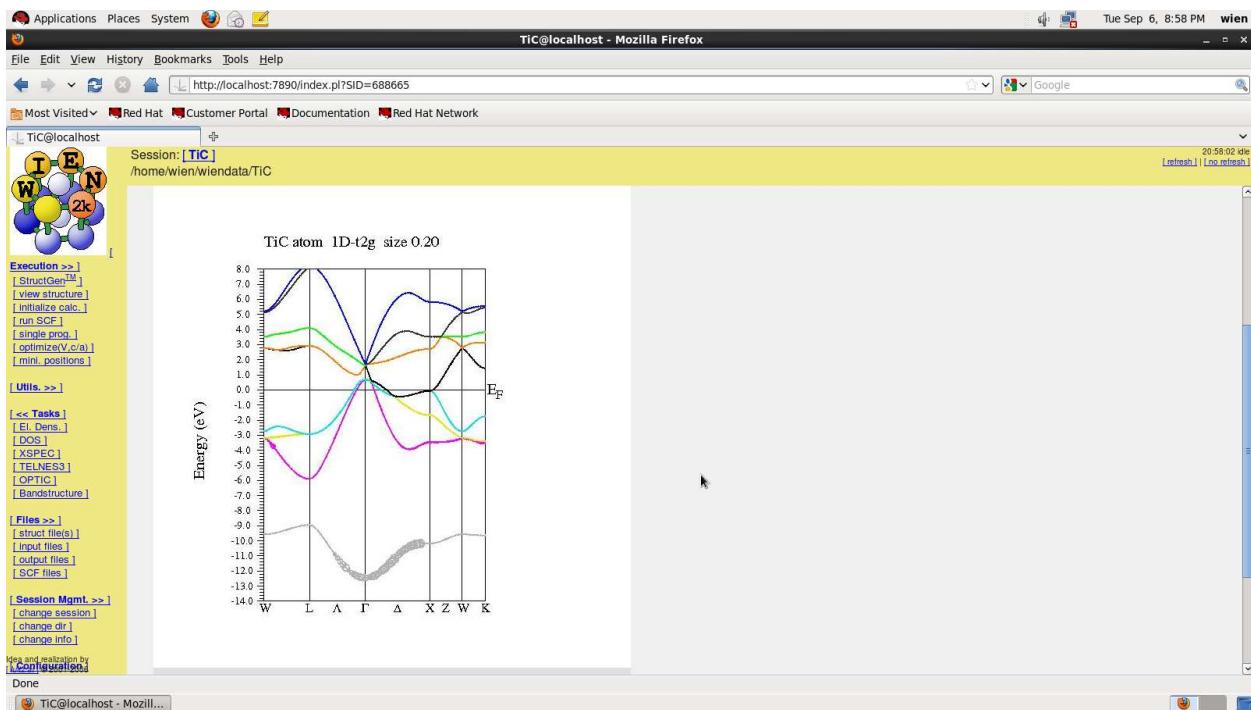
122. Click “plot bandstructure”, the creates the following plot (version 24.1-23.2):



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



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

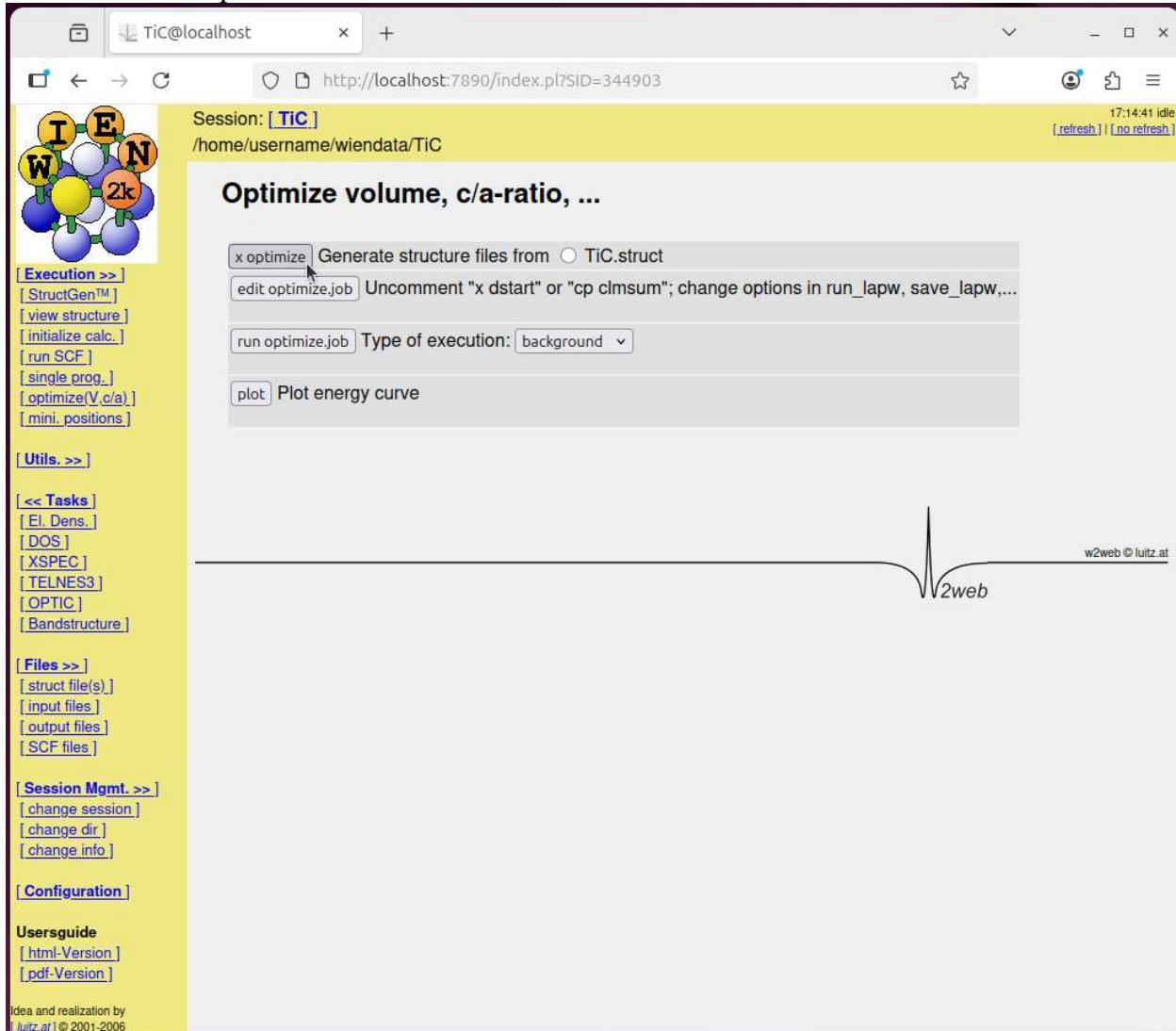


Plot volume optimization

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

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

124. Click “x optimize”:



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

126. Click “Execute!”:

The screenshot shows a web browser window titled "TiC@localhost" with the URL "http://localhost:7890/index.pl?SID=344903". The session name is "TiC" and the path is "/home/username/wiendata/TiC". The status bar indicates "17:15:11 idle" and "optimize needs input".

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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2web

127. Click “continue with optimizer”:

The screenshot shows a web-based graphical user interface for a computational chemistry application named TiC. The title bar indicates the session is 'TiC' at 'localhost:7890'. The main area displays a 3D ball-and-stick model of a molecule with atoms labeled T, C, N, E, W, and 2k. Below the model is a list of optimization steps, each consisting of a command and a resulting structure file name. The steps are:

- 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
0.000u 0.002s 0:00.00 0.0% 0+0k 0+248io 0pf+0w

On the left side, there is a sidebar with various menu items under sections like 'Execution >>', 'Tasks', 'Files >>', 'Session Mgmt. >>', and 'Configuration'. At the bottom of the sidebar, it says 'Idea and realization by Jutz.at © 2001-2006'. In the bottom right corner of the main content area, there is a button labeled 'Continue with' and 'continue with optimizer'.

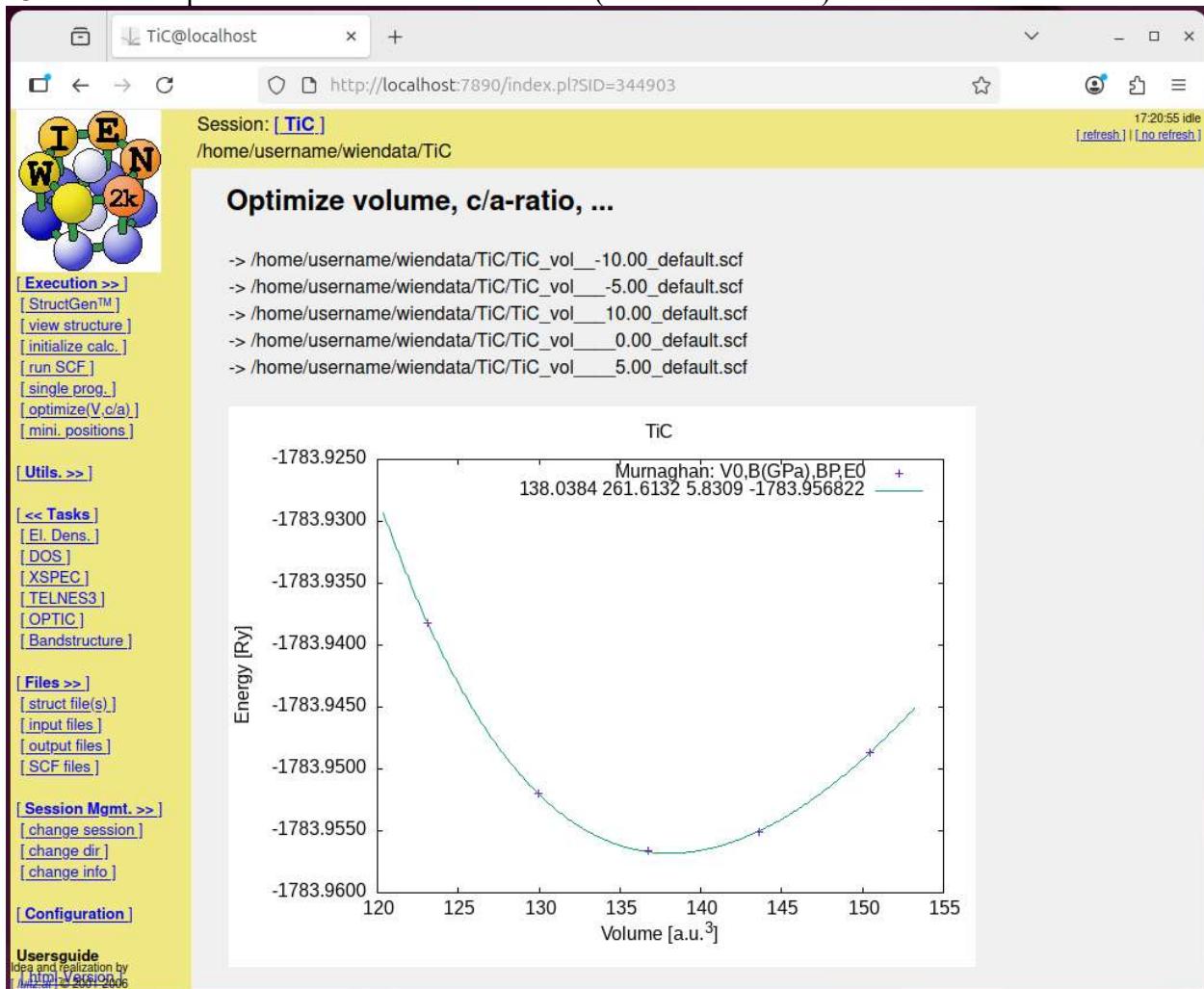
128. Click “run optimize.job”

129. Click “continue with optimizer”:

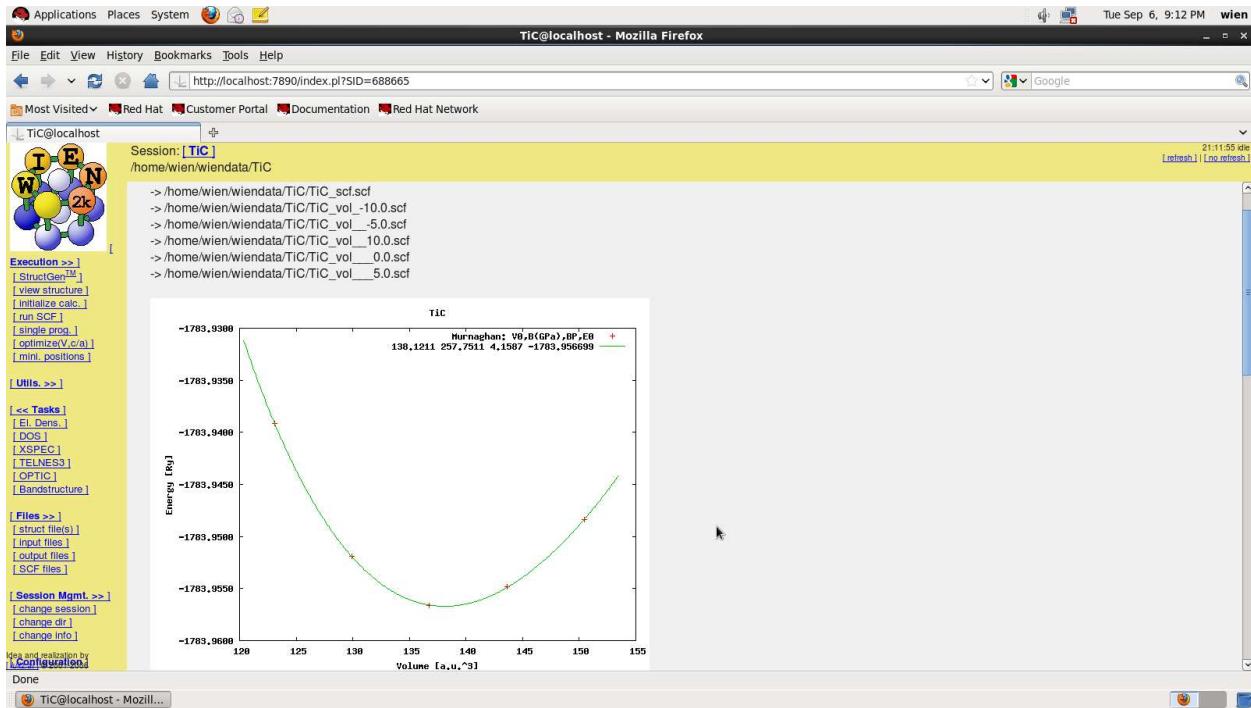
The screenshot shows a web browser window for the TiC application. The URL is `http://localhost:7890/index.pl?SID=344903`. The session name is `TiC`. The command line is `/home/username/wiendata/TiC` and the program input is `""`. A note says `cd /home/username/wiendata/TiC; echo '' | ./optimize.job >/home/username/wiendata/TiC/STD`. There is a link to `[View STDOUT]` to monitor progress. Below it, there is a button labeled `Continue with` and a sub-button labeled `continue with optimizer`, which is highlighted with a mouse cursor. On the left, there is a sidebar with various menu items under categories like `Execution`, `StructGen™`, `view structure`, etc. At the bottom of the sidebar, it says `Idea and realization by [Juiz.at] © 2001-2006`. The right side of the interface has a decorative footer with the text `w2web © iuitz.at` and a small logo.

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.