

WIEN2k TiC Example

Ubuntu 24.04.2 LTS

WIEN2k_24.1 (Release 1/8/2024)

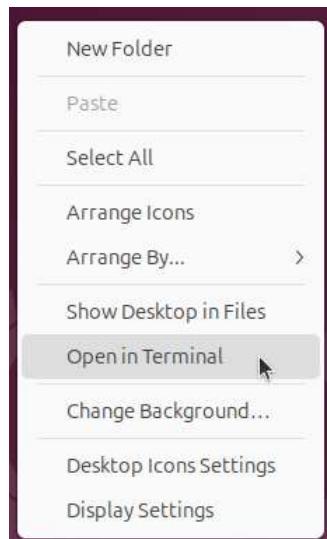
ifx version 2025.1.0

WIEN2k patches [1]: SearchZ.patch, angle.patch, atom_read.patch, charge.patch, executor.patch, x_lapw.patch

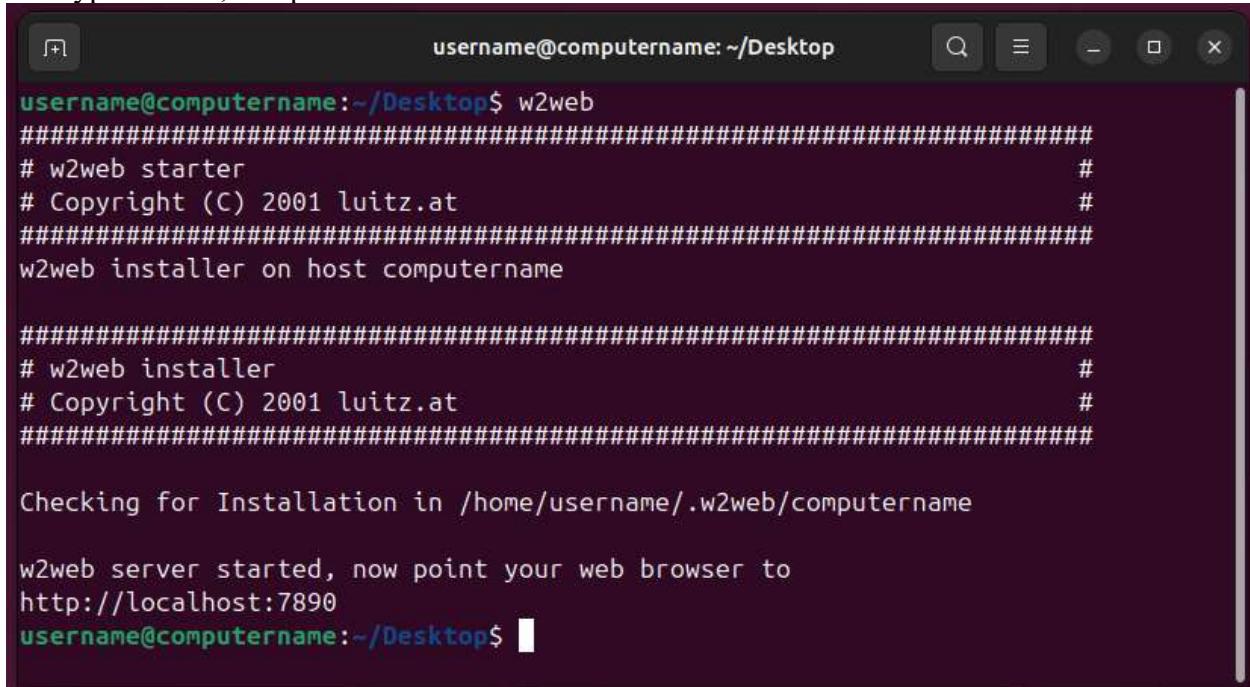
[1] <https://github.com/gsabo/WIEN2k-Patches/tree/master/24.1>

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:



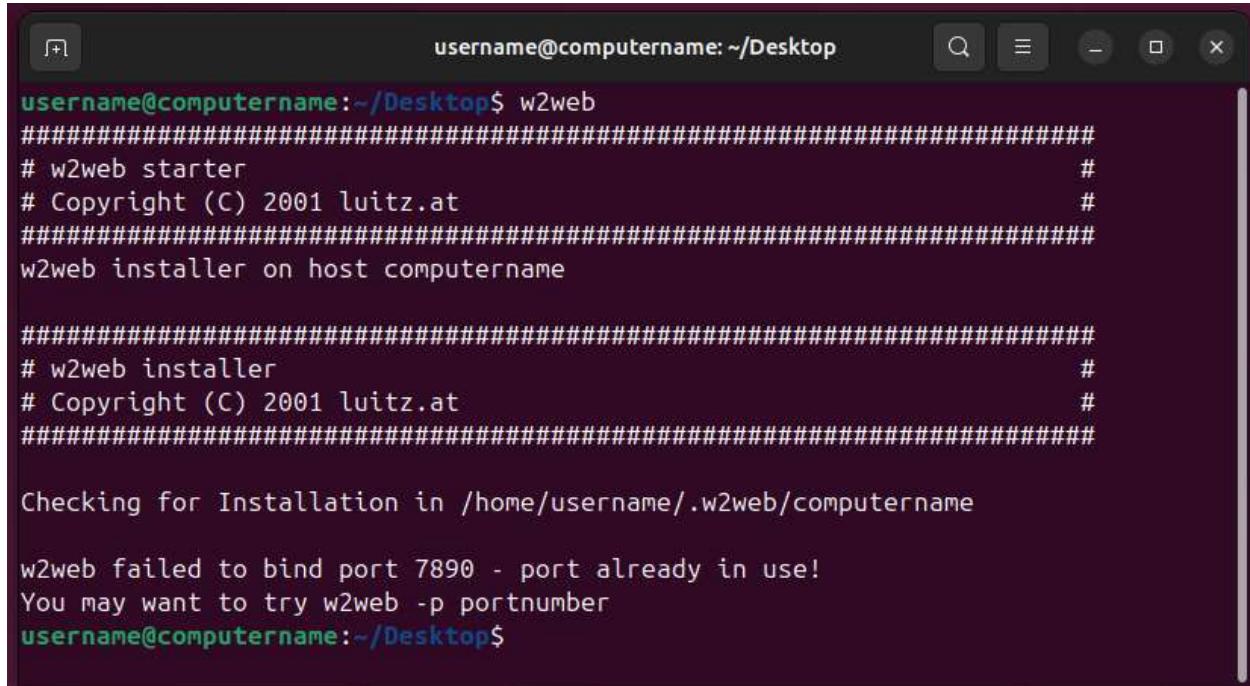
```
username@computername:~/Desktop$ w2web
#####
# w2web starter
# Copyright (C) 2001 luitz.at
#####
w2web installer on host computername

#####
# 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

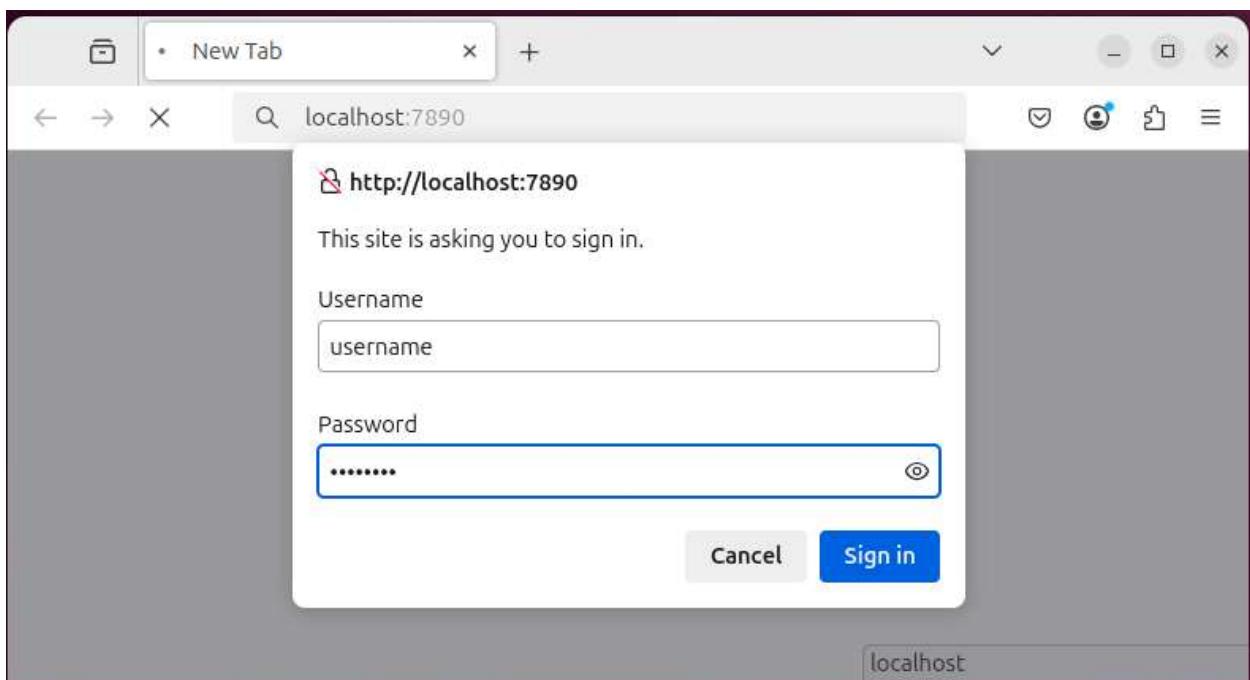
w2web failed to bind port 7890 - port already in use!
You may want to try w2web -p portnumber
username@computername:~/Desktop$
```

Open Firefox and login to w2web

3. Click on the Firefox icon to open Firefox:

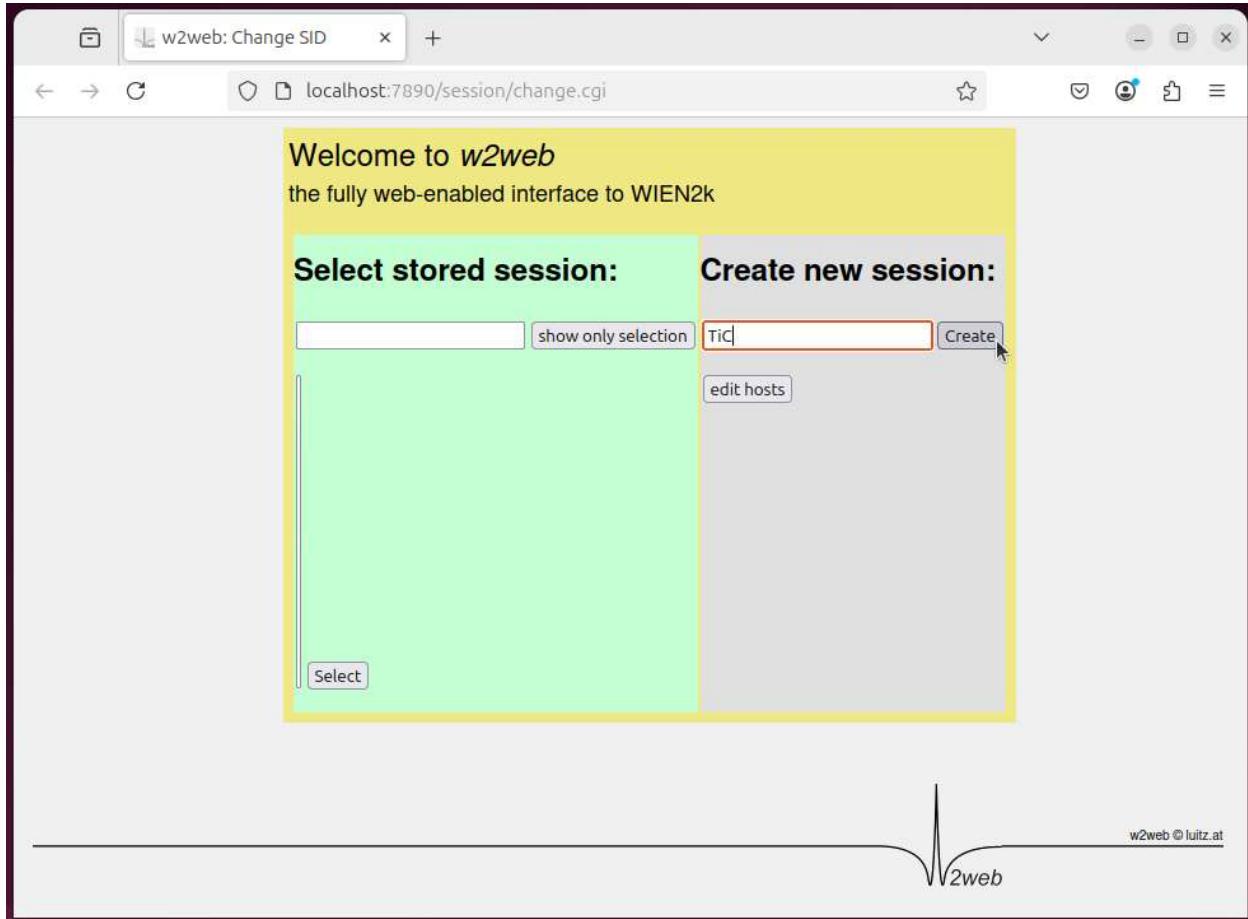


4. Enter url <http://localhost:7890>, type your w2web username and password, then click "Sign in" to login to w2web:

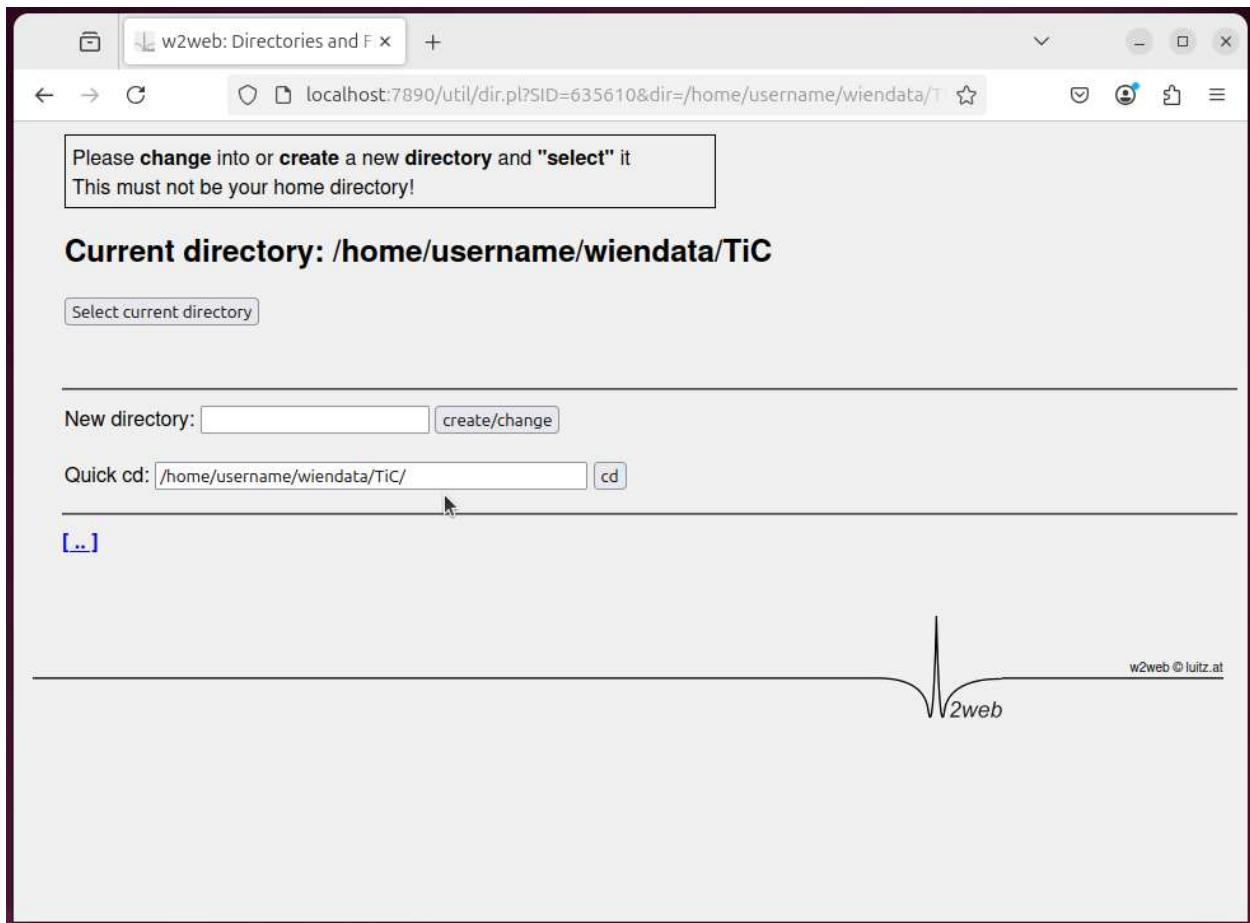


Create a new session (calculation)

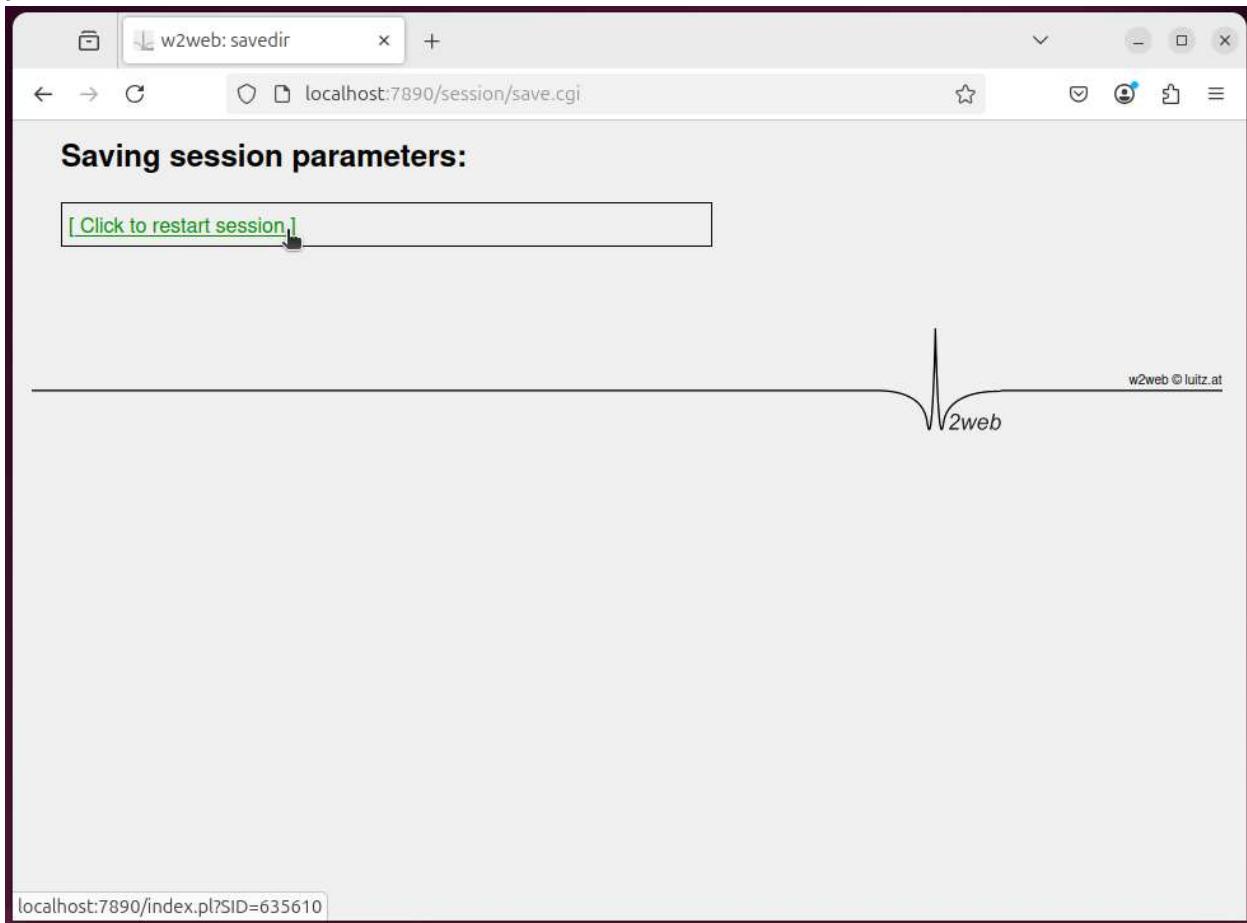
5. Enter “TiC” in the “Create new session:” box and then click the “Create” button:



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 URL "localhost:7890/index.pl?SID=635610". The page is titled "w2web, the fully web-enabled interface to WIEN2k". On the left, there is a sidebar with a molecular logo and various navigation links such as "Execution >>", "StructGen™", "view structure", "initialize calc.", "run SCF...", "single prog.", "optimize(V,c/a)", "mini_positions", "Utils. >>", "Tasks >>", "Files >>", "Session Mgmt. >>", "Configuration", and "Usersguide". The main content area shows session details: Session Name: TiC, Session ID: 635610, Directory: /home/username/wiendata/TiC, Last changed: Fri Apr 4 12:54:10 2025. It also lists comments with checkboxes for spin polarized calculation, AFM calculation, complex calculation (no inversion), and parallel calculation. A "Change session information" button is present. The bottom right corner features the "w2web" logo.

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:

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:

Alternatively:

Use cif2struct to convert a "cif" 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 (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]

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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=0.0000000 y=0.0000000 z=0.0000000 [remove] [split]
 [add position]

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

[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

w2web

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]

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

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

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 window has a title bar "Session: [TiC] /home/username/wiendata/TiC". It displays the following input fields:

- Title:** TiC
- Lattice:** F
- Type:** F
- Spacegroups from Bilbao Cryst Server:** A dropdown menu showing options P, F, B, CXY, CYZ, CXZ, R, H, and 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 (highlighted in red) with Z = 22.000 and RMT = 2.17. Buttons: [remove atom], [remove], [split], [add position].
 - Atom 2:** C (highlighted in red) with Z = 6.000 and RMT = 1.77. Buttons: [remove atom], [remove], [split], [add position].
- Number of symmetry operations:** generate
- Note:** You have to click "Save Structure" for changes to take effect!
- Buttons:** Save Structure, refresh, no refresh.

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" and is located at "/home/username/wiendata/TiC". The interface includes a sidebar with various navigation links and a main panel for inputting crystallographic parameters.

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

StructGen™

View only mode -->[edit STRUCT file]

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=2.0000
 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:

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; 0=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 Click here for more info.]" style="background-color: #ffffcc; border: 1px solid red; color: black; padding: 2px 10px; margin-right: 10px;"/>

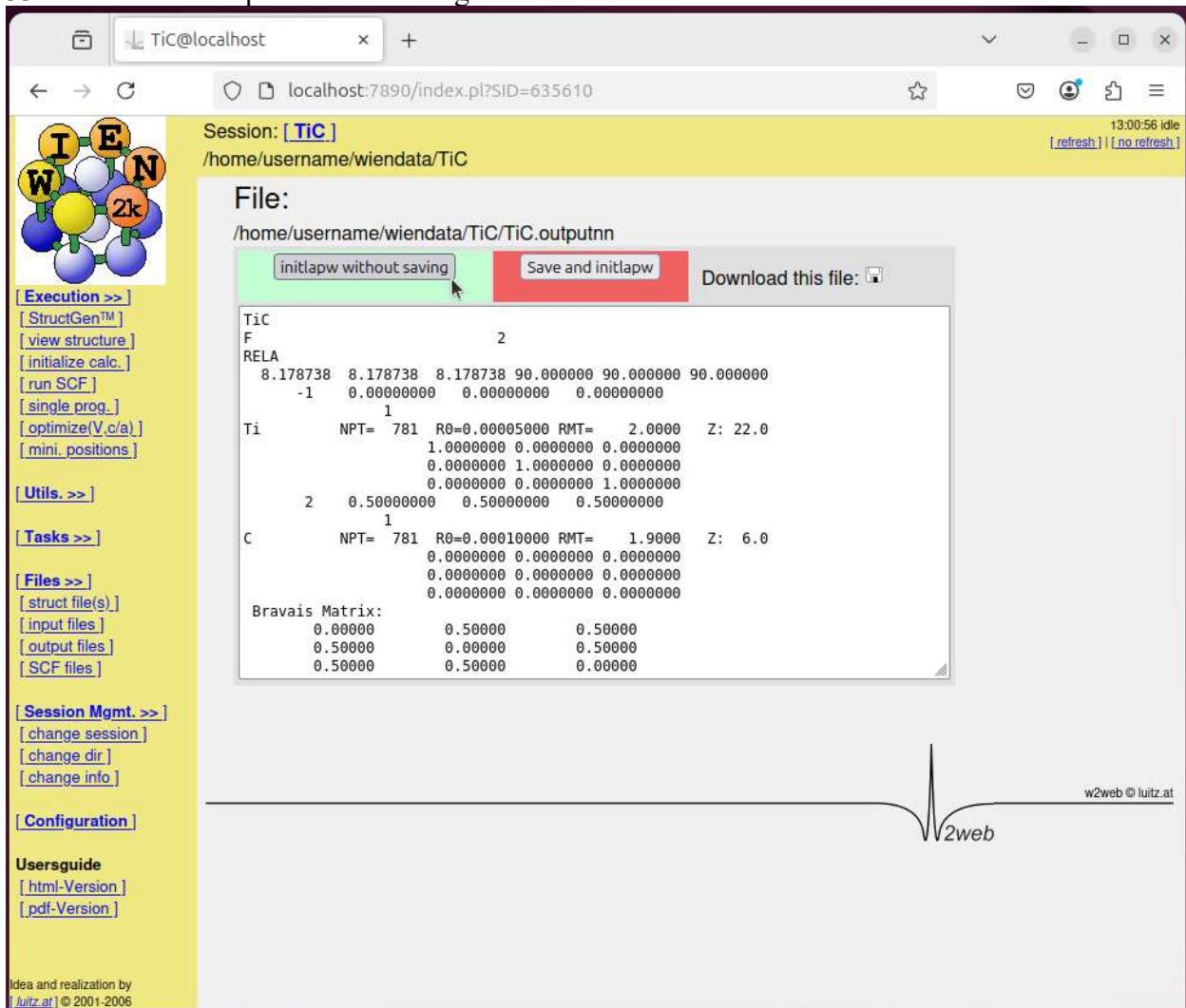
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30. By default 2 should be given in the box, click the “Execute!” button:

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 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 the value "2" and a button labeled "Execute!". In the bottom right corner, there is a small logo with the text "w2web © luitz.at" and "w2web". At the bottom of the page, there is a footer note: "Idea and realization by [luitz.at](#) © 2001-2006".

31. Click the “initlapw” button:

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



The screenshot shows a web browser window titled "TiC@localhost" displaying the output of a calculation. The URL is "localhost:7890/index.pl?SID=635610". The session name is "TiC". The output file is "/home/username/wiendata/TiC/TiC.outputnn".

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

Buttons at the top of the output area:

- initlapw without saving (highlighted)
- Save and initlapw
- Download this file:

The output text is as follows:

```

TiC
F          2
RELA
  8.178738  8.178738  8.178738  90.000000  90.000000  90.000000
    -1      0.00000000  0.00000000  0.00000000
              1
Ti      NPT= 781 R0=0.00005000 RMT=   2.0000   Z: 22.0
          1.0000000  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:
  0.0000000  0.5000000  0.5000000
  0.5000000  0.0000000  0.5000000
  0.5000000  0.5000000  0.0000000

```

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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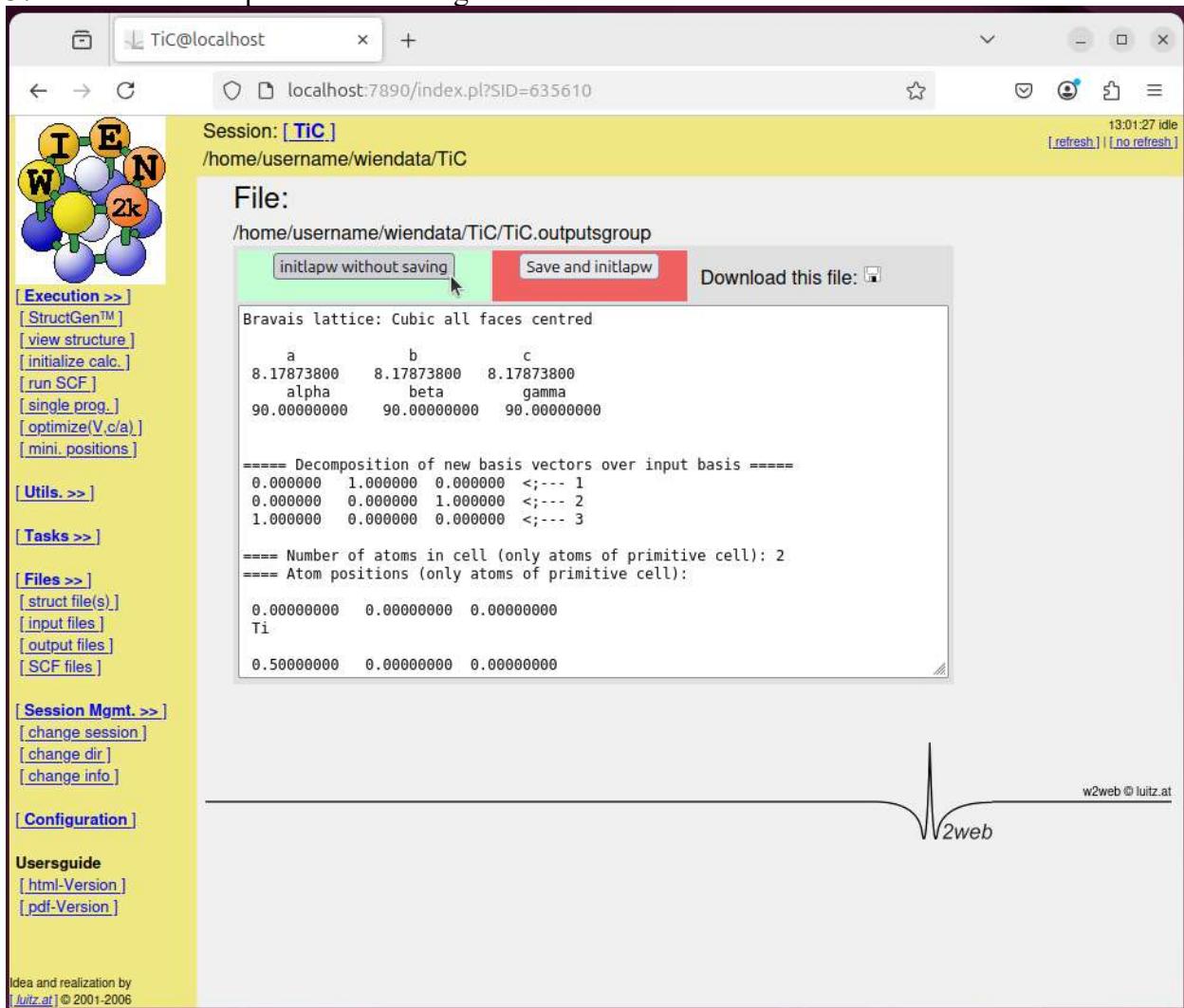
w2web © luitz.at

34. Click the “x sgroup” button

35. Click the “initlapw” button:

The screenshot shows a web browser window titled "TiC@localhost" with the URL "localhost:7890/index.pl?SID=635610". The page displays session information: "Session: [TiC.] /home/username/wiendata/TiC" and commandline: "x sgroup". It also shows "Program input is: """. Below this, resource usage is listed: "0.000u 0.001s 0:00.00 0.0% 0+0k 0+8io 0pf+0w". A "Continue with" section contains 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" and "w2web @ luitz.at". On the left side of the page, there is a sidebar with various navigation links under categories like "Execution >>", "Utils. >>", "Tasks >>", "Files >>", "Session Mgmt. >>", "Configuration", and "Usersguide". At the bottom left, there is a note: "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 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". The main content area shows a molecular model of TiC (Titanium Carbide) with atoms labeled Ti, C, W, E, N, and 2k. Below the model is a text box containing session output. At the top of this text box are three buttons: "initlapw without saving" (highlighted in green), "Save and initlapw" (in red), and "Download this file: ". The output text box contains the following data:

```

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

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

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
  
```

At the bottom right of the text box, there is a logo for "w2web" with the URL "w2web @ luitz.at".

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 options for using TEMP or TEMPS, setting k-points, and running dstart. A section titled 'Individual mode (phase 6)' provides instructions for antiferromagnets, self-generated structures, supercells, and surfaces. A prominent red box highlights a modal dialog box in the center. The dialog box contains the text: 'Use struct-file generated by sgroup? (Usually NO, unless WARNINGS appeared above)'. It has two buttons: 'Yes' and 'No'. The 'No' button is being pointed to by a mouse cursor.

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 named "TiC" with the path "/home/username/wiendata/TiC". The commandline entered is "x symmetry" and the program input is empty. A message indicates "SPACE GROUP CONTAINS INVERSION". Below this, there is a table of execution statistics:

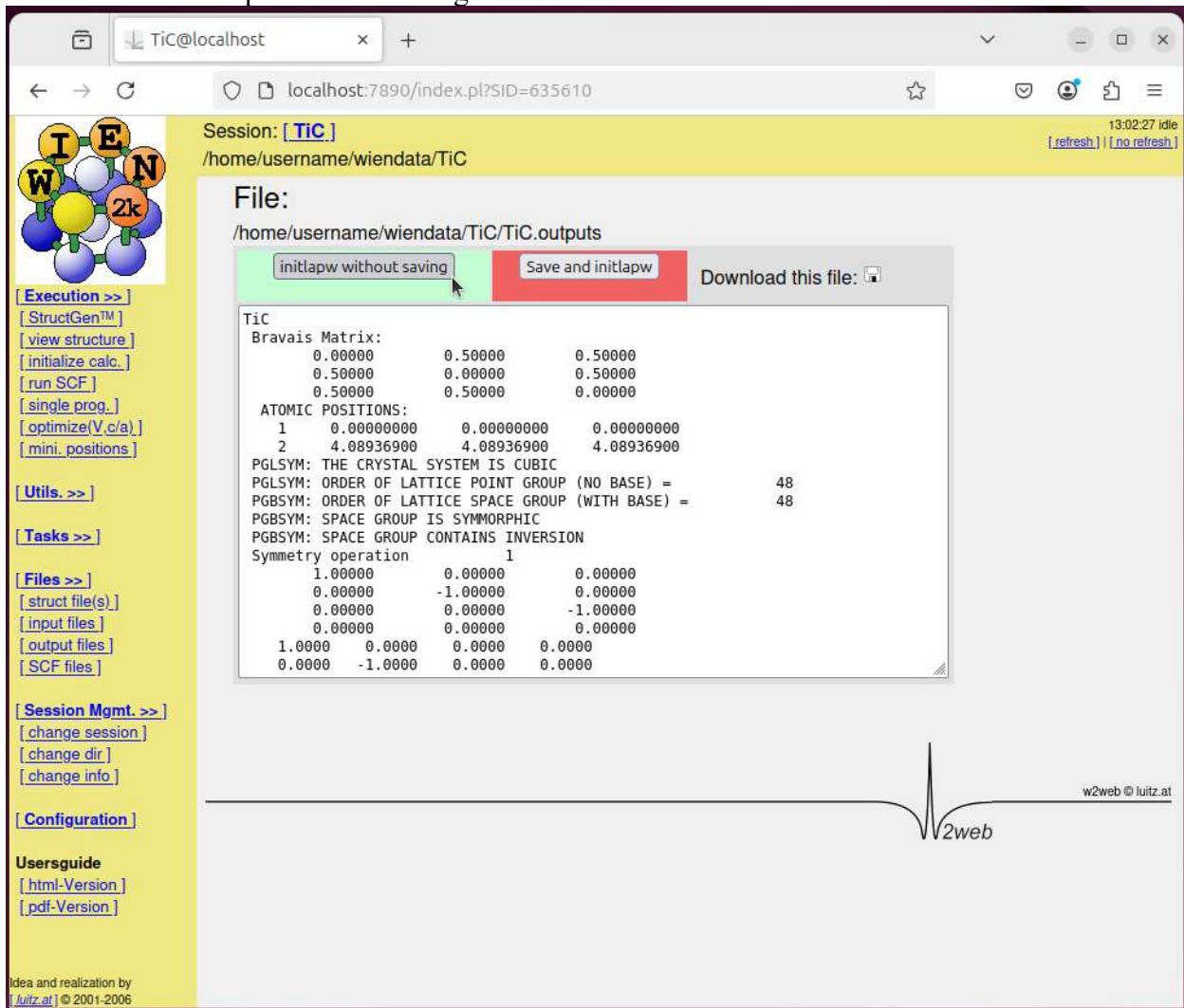
0.001u	0.005s	0:00.00	0.0%	0+0k	0+64io	0pf+0w
--------	--------	---------	------	------	--------	--------

On the right side of the page, there is a small graphic of a heart with the text "w2web © luitz.at" next to it. At the bottom left, there is a copyright notice: "Idea and realization by luitz.at © 2001-2006".

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]

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 working directory 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 right side of the interface features a logo for "w2web" with a stylized wave graphic.

43. Click the “instgen_lapw” button

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

The screenshot shows a web-based interface for the Wiendata software. The title bar says "TiC@localhost". The URL is "localhost:7890/index.pl?SID=635610". The session name is "TiC". The working directory is "/home/username/wiendata/TiC". A message at the top right says "instgen_lapw needs input" with a timestamp "13:02:57 idle". There is a refresh link "[refresh]" and a no-refresh link "[no refresh]".
On the left, there is a sidebar with various buttons:

- [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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The main panel displays the configuration for "instgen_lapw". It shows a molecular model of TiC with atoms labeled Ti, C, W, E, N, and 2k. The configuration options are:

Specify options for instgen_lapw
Chose 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!

At the bottom right, there is a small logo with the text "w2web" and "w2web @ luitz.at".

45. Click the “initlapw” button:

The screenshot shows a web browser window titled "TiC@localhost" with the URL "localhost:7890/index.pl?SID=635610". The session is named "TiC" and is located at "/home/username/wiendata/TiC". The commandline is "instgen_lapw -s -nm" and the program input is "u u". A molecular structure diagram is displayed on the left, showing atoms labeled Ti, C, E, N, W, and 2k. On the right, there is a "Continue with" section containing a button labeled "initlapw". The footer of the page includes a copyright notice: "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" with the URL "localhost:7890/index.pl?SID=635610". The page displays a molecular model of TiC with atoms labeled T, i, E, N, W, and 2k. 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 >>" (struct file(s), input files, output files, SCF files), "Session Mgmt. >>" (change session, change dir, change info), "Configuration", and "Usersguide" (html-Version, pdf-Version). The main content area shows the session information "Session: [TiC.] /home/username/wiendata/TiC" and a message "LSTART needs input". It includes a "Select Exchange Correlation Potential:" dropdown set to "PBE-GGA (Perdew-Burke-Ernzerhof 96)". Below it, a section titled "ENERGY to separate core and valence states:" asks "ALTERNATIVELY: specify charge localization (between 0.97 and 1.0) to select core state" with a text input field containing "-6.0" and a note "(recommended: -6.0 Ry)" followed by "(check how much core charge leaks out of MT-sphere)". A large "Execute!" button is visible. In the bottom right corner, there is a watermark "w2web © luitz.at" with a small logo.

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

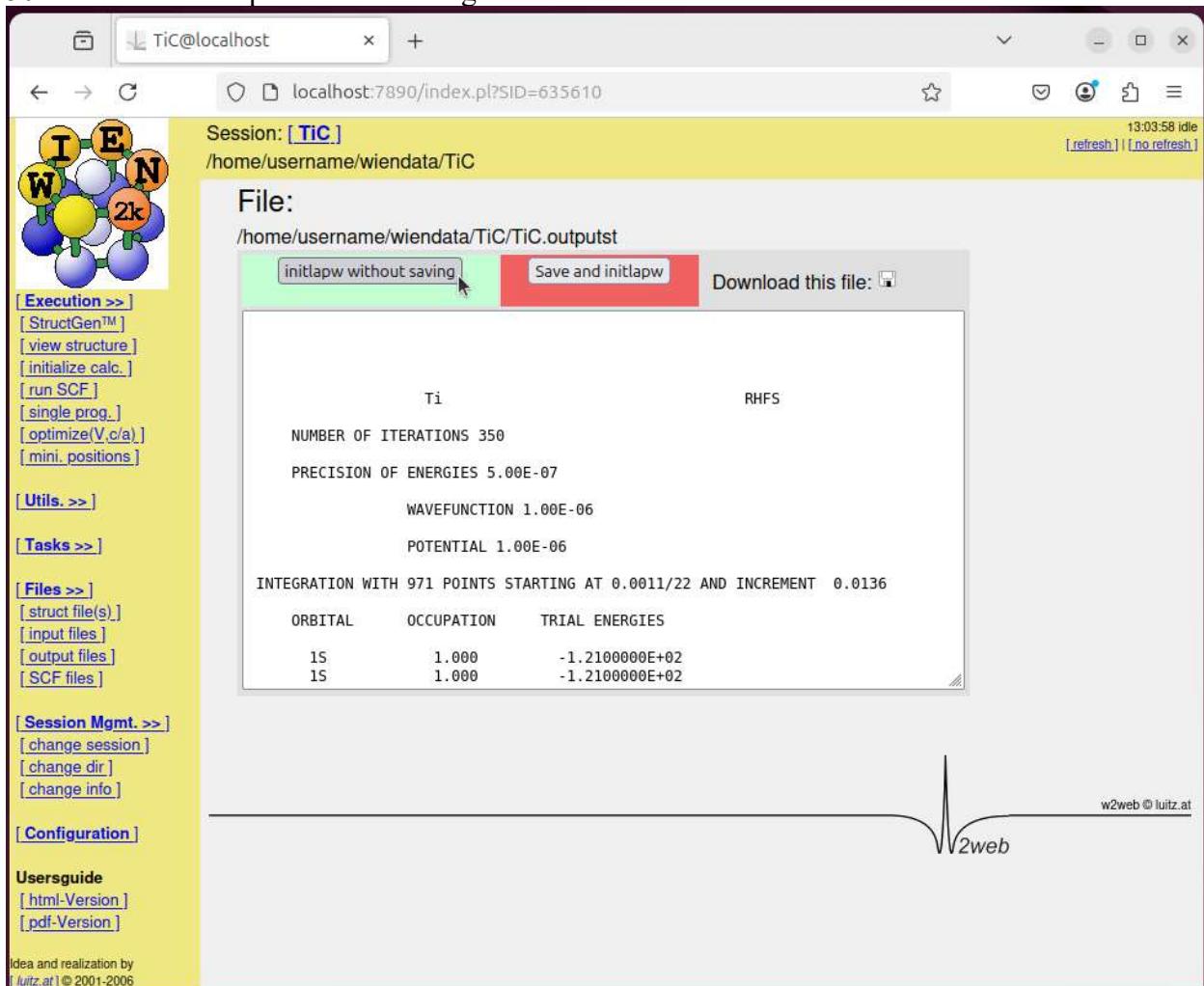
Atomic configuration for atom: C Z= 6.00					
	E-up (Ry)	E-dn (Ry)	Occupancy	q/sphere	core-state
1S	-20.092503	-20.092503	1.00	1.00	1.0000 T
2S	-1.010581	-1.010581	1.00	1.00	0.7309 F
2P*	-0.388826	-0.388826	0.50	0.50	0.6271 F
2P	-0.388183	-0.388183	0.50	0.50	0.6266 F

LSTART ENDS
 0.054u 0.002s 0:00.05 100.0% 0+0k 0+968io 0pf+0w

Continue with [initlapw](#)

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

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



The screenshot shows a web browser window titled "TiC@localhost" displaying a session for "TiC". The session path is "/home/username/wiendata/TiC". On the left, there is a sidebar with various buttons for execution, utilities, tasks, files, session management, configuration, and user guides. A molecular model of TiC is shown at the top left. The main content area displays the output of a calculation. At the top of the output area, there are three buttons: "initlapw without saving" (highlighted in green), "Save and initlapw" (in red), and "Download this file:". The output text includes:

```

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

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

initlapw without saving Save and initlapw Download this file: □

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

```

At the bottom right of the output area, there is a logo for "w2web" with the text "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 browser window for the Wiendata TiC application. The URL is `localhost:7890/index.pl?SID=635610`. The session name is `TiC`. The main area displays a molecular model of TiC and a text editor containing an input file. The text editor shows the following content:

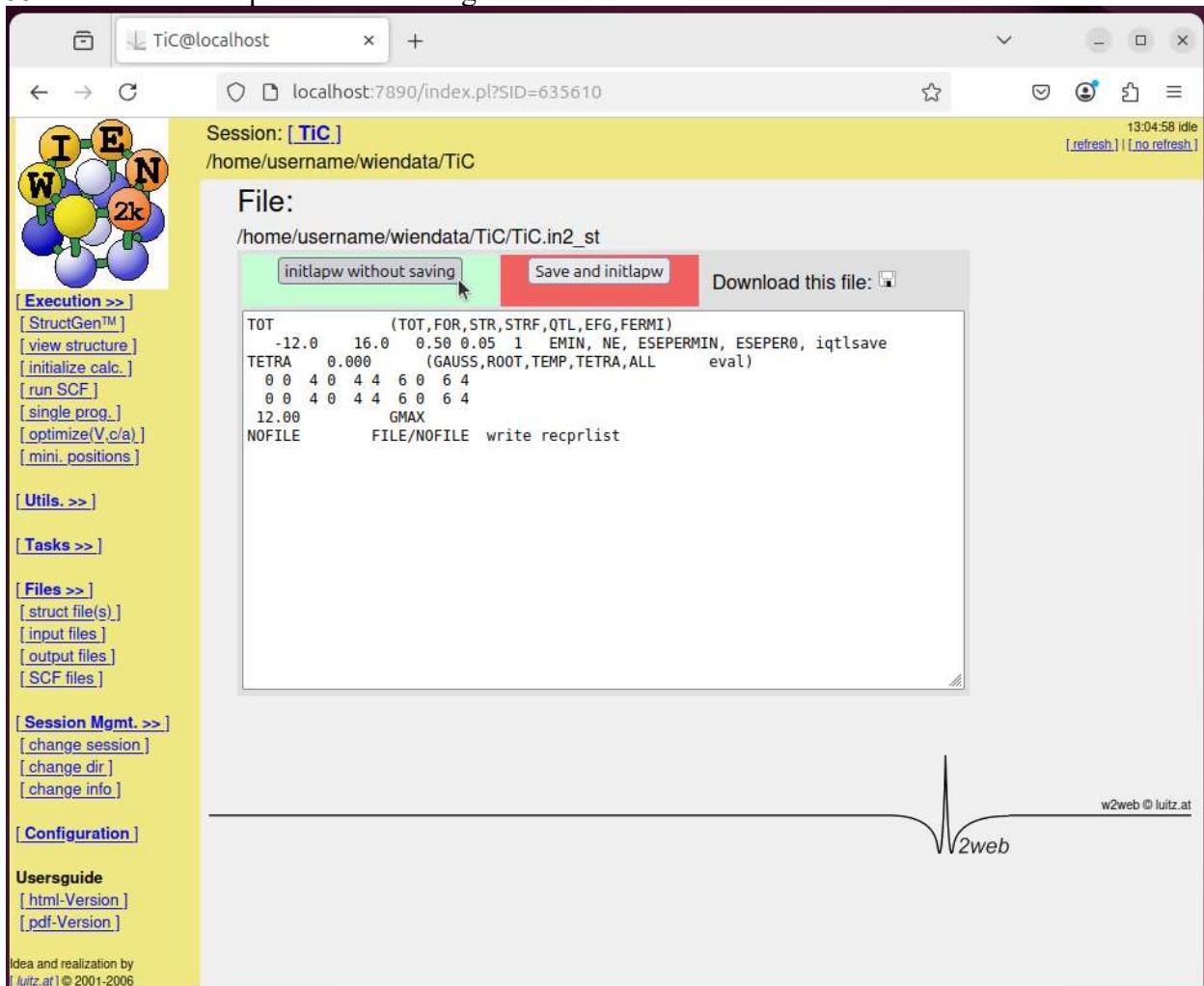
```

WFFIL EF= 0.50000      (WFFIL, WFPRI, ENFIL, SUPWE)
 7.00   10   4 ELPB 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

```

The 'Save and initlapw' button is highlighted with a red rectangle. On the left sidebar, there are several menu options under 'Execution >>', 'Files >>', 'Session Mgmt. >>', 'Configuration', and 'Usersguide'. At the bottom left, it says 'Idea and realization by [luitz.at](#) © 2001-2006'. The bottom right corner features a logo with the text 'w2web © luitz.at'.

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 [Jüttz.at](#) © 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 dstart interactively

No Yes

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" at the URL "localhost:7890/index.pl?SID=635610". The page displays a session configuration for "Session: [TiC.]". The "Number of k-points" field is set to "1000". Below it, there is a dropdown menu for "Shift k-mesh (if applicable)" with the option "Yes" selected. A note 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!)" followed by three empty input fields. At the bottom right of the main area, there is a watermark that says "w2web © luitz.at" with a small logo. On the left side of the page, there is a sidebar with various navigation links under categories like "Execution >>", "Utils. >>", "Tasks >>", "Files >>", "Session Mgmt. >>", "Configuration", and "Usersguide". At the very bottom of the sidebar, 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 "localhost:7890/index.pl?SID=635610". The session is identified as "Session: [TiC]" and the path is "/home/username/wiendata/TiC". The commandline is "x kgen" and the program input is "1000 1". The output window displays the following text:

```

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

```

The left sidebar contains a molecular structure icon and a list of buttons categorized by section:

- 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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A watermark "w2web" is visible at the bottom right of the page.

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 named "TiC". The URL is "localhost:7890/index.pl?SID=635610". The page content includes a molecular model of TiC and a table of data. A green button labeled "initlapw without saving" is highlighted with a mouse cursor. Other buttons include "Save and initlapw" and "Download this file:". The table data is as follows:

	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	7	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 sidebar on the left contains various navigation links such as "Execution >>", "Utils >>", "Tasks >>", "Files >>", "Session Mgmt. >>", "Configuration", and "Usersguide". The bottom of the sidebar also mentions "Idea and realization by luitz.at © 2001-2006". The footer of the page includes a logo for "w2web" and the text "w2web @ luitz.at".

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

TiC@localhost

localhost:7890/index.pl?SID=635610

Session: [TiC.]
 /home/username/wiendata/TiC
 Commandline: x dstart
 Program input is: ""

C T F
 DSTART ENDS
 0.785u 0.006s 0:00.79 98.7% 0+0k 0+368io 0pf+0w

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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13:06:59 idle
 [refresh.] | [no refresh.]

Continue with

initlapw

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 2web

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

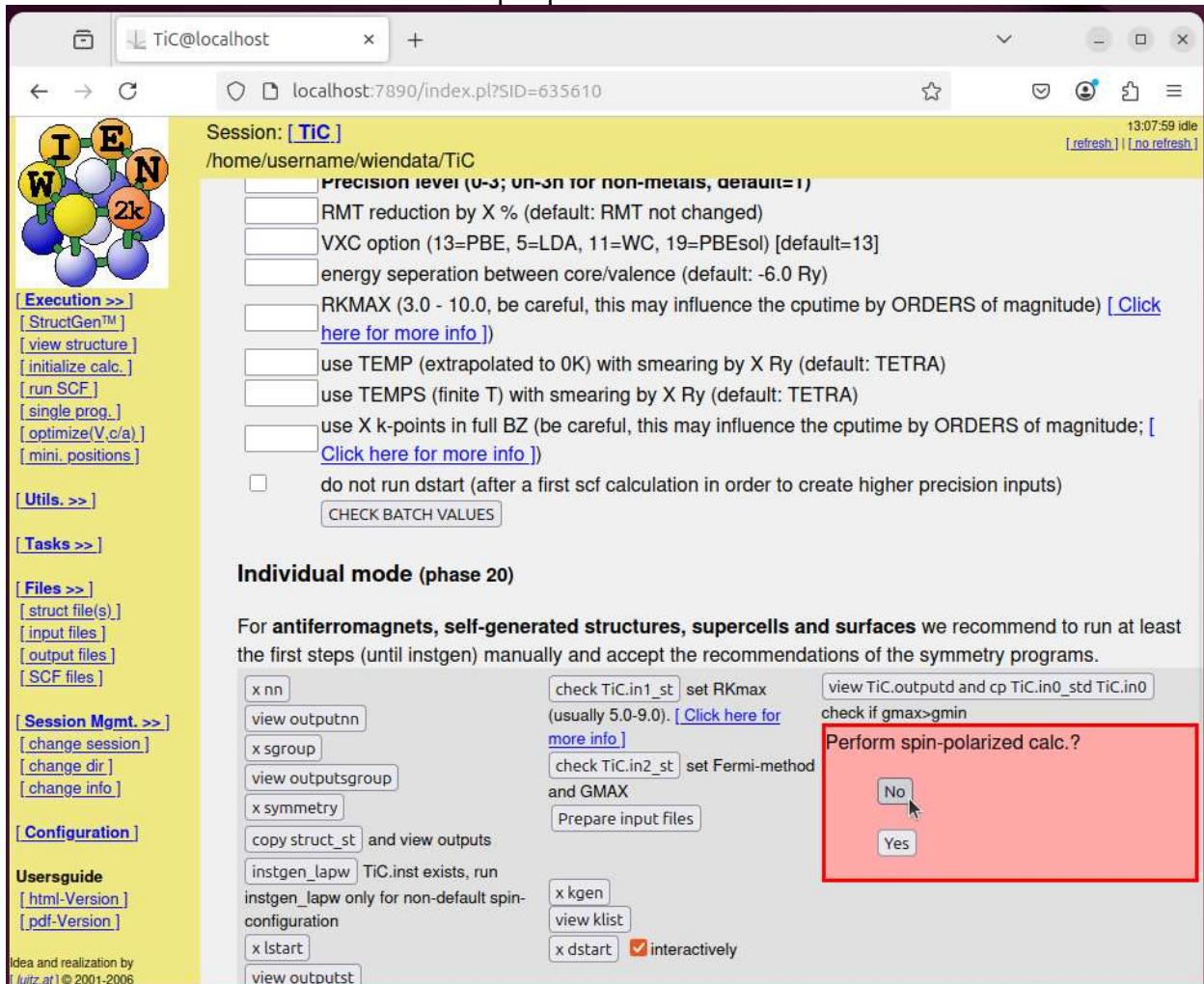
cutoff distance for superposition: 16.205
unitcell range: 4 4 4

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
  
```

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 w2web

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



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

The screenshot shows a web browser window for the TiC@localhost application. The URL is `localhost:7890/index.pl?SID=635610`. The page displays session configuration options and a summary of completed steps.

Session Configuration:

- Session: [TiC]
- /home/username/wiendata/TiC
- use TETRA (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.

Buttons and Links:

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

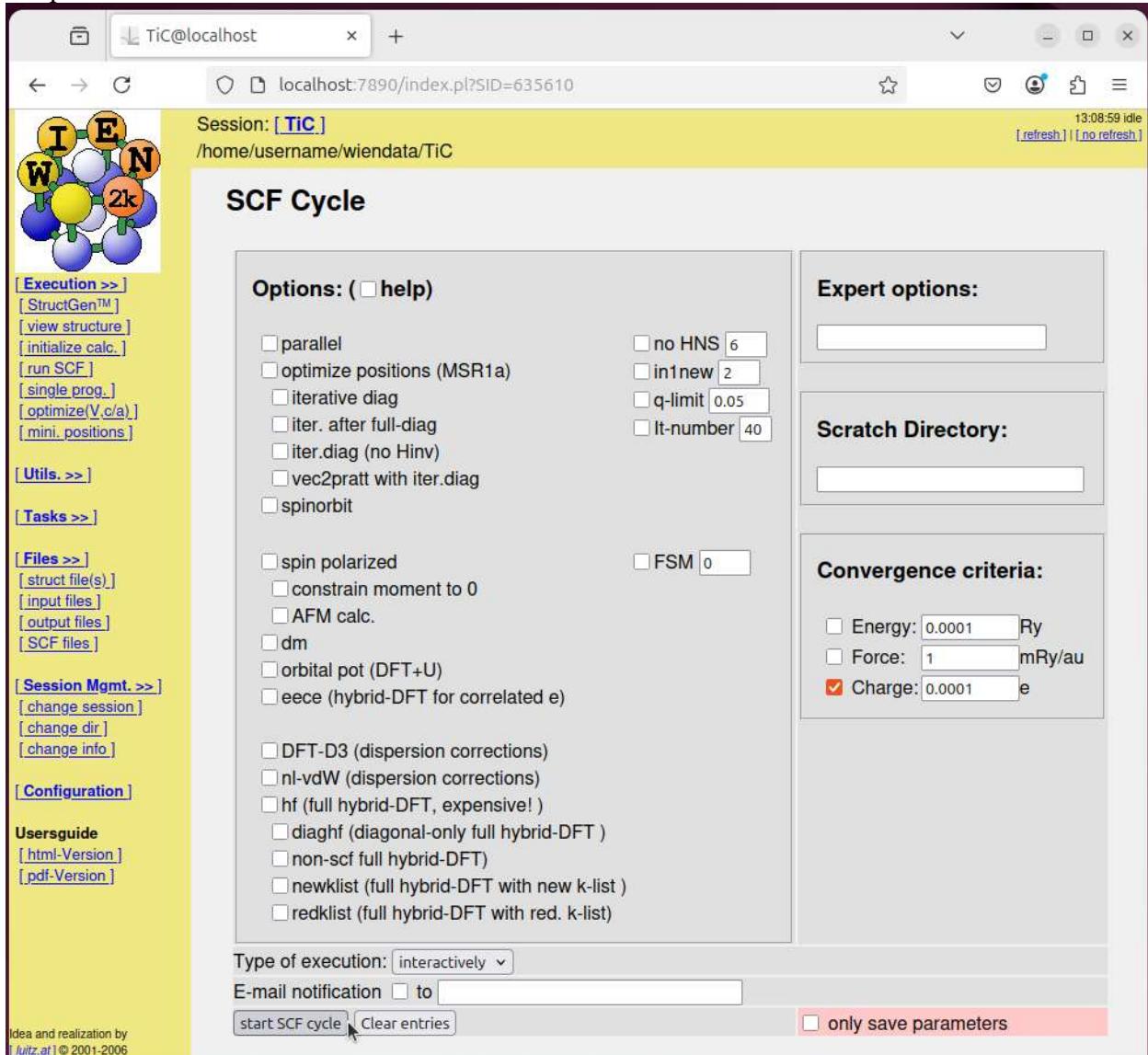
Initialization done:

[Continue with run SCF]

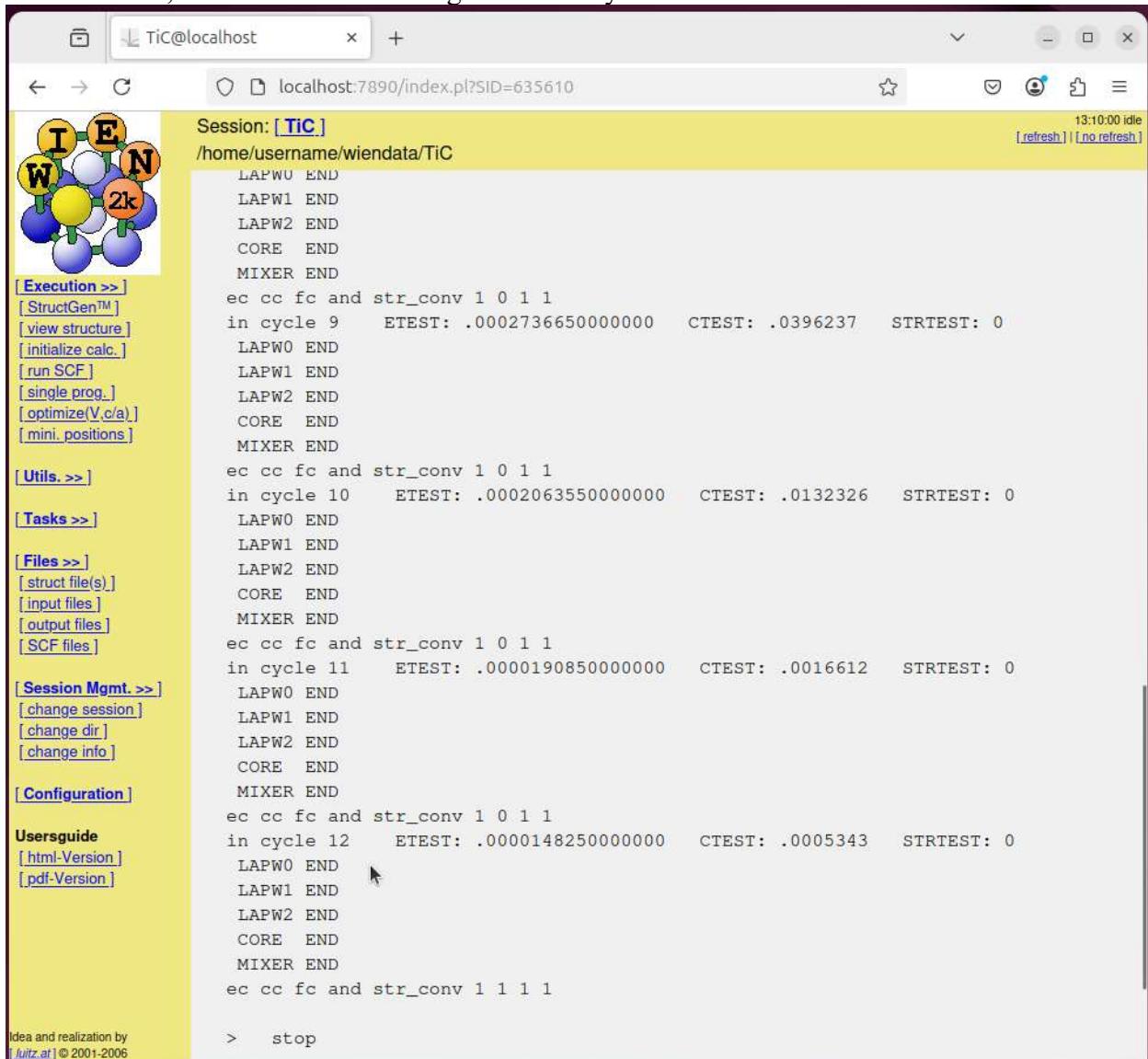
At the bottom left, the URL is `localhost:7890/exec/scf.pl?SID=635610`.

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:



```

Session: [TiC]
/home/username/wiendata/TiC
13:10:00 idle
[refresh] | [no refresh]

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

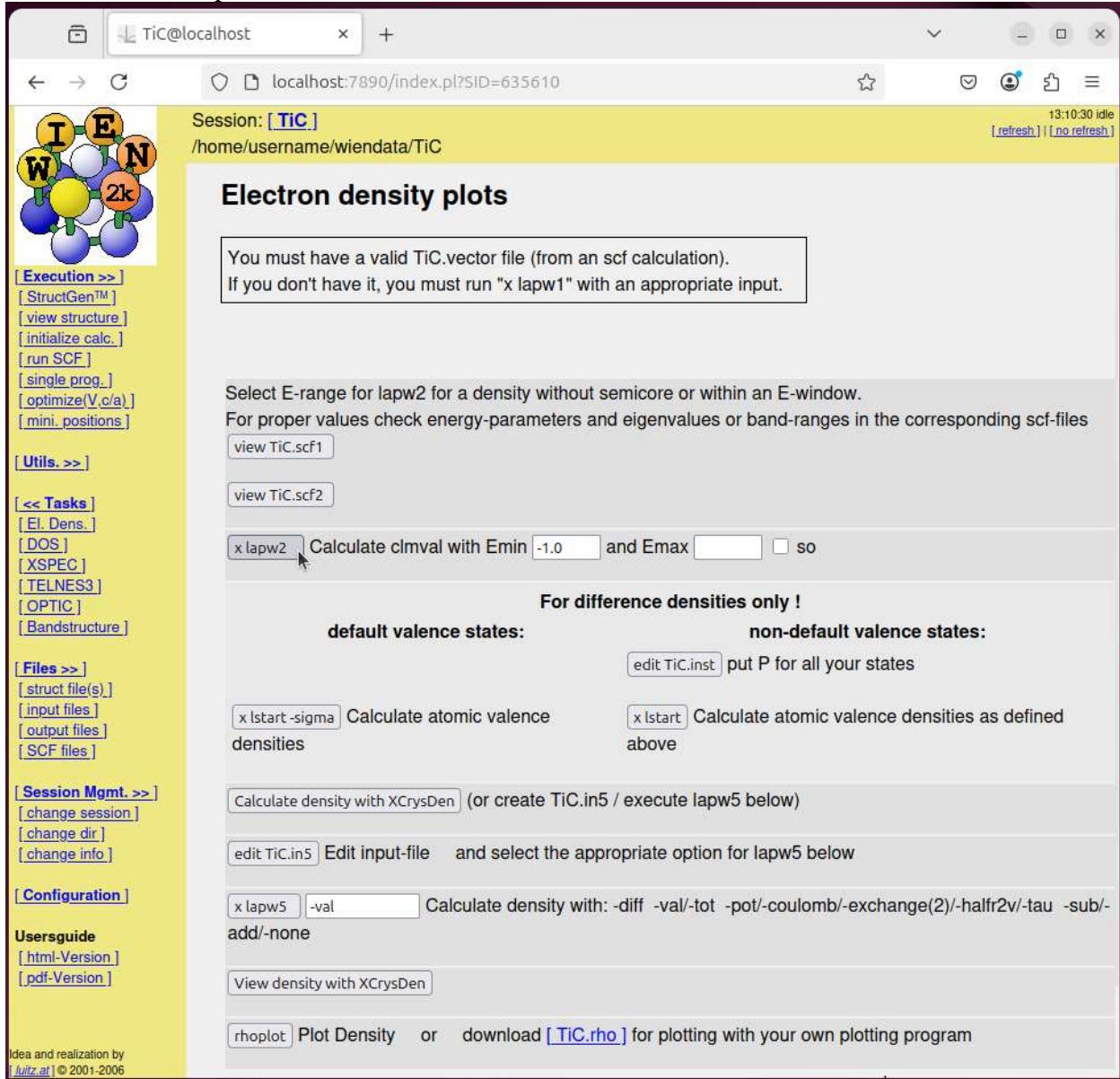
```

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[fritz.at] © 2001-2006

Plot electron density

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

72. Click the “x lapw2” button with Emin -1.0:



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

The screenshot shows a web browser window for `TiC@localhost` at port 7890. The session is titled `TiC` and is located at `/home/username/wiendata/TiC`. The commandline used was `x lapw2 -emin -1.0`. The program input is empty. The LAPW2 calculation has ended successfully with the following statistics:
LAPW2 END
0.131u 0.137s 0:00.26 100.0% 0+0k 0+520io 0pf+0w

In the center, there is a "Continue with" section containing a button labeled "continue with electron density". To the right of this section is a small logo featuring a stylized wave or peak with the text "w2web" below it.

The left sidebar contains a navigation menu with the following sections and links:

- Execution >>**
 - [StructGen™]
 - [view structure]
 - [initialize calc.]
 - [run SCF]
 - [single prop.]
 - [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 left, there is a copyright notice: "Idea and realization by [luitz.at] © 2001-2006".

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 a web browser window for the WIEN2k session 'TiC@localhost'. The URL is 'localhost:7890/index.pl?SID=635610'. The session name 'Session: [TiC]' is displayed above the code editor. The code editor contains the following input file content:

```

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: □

```

The 'Save and continue with electron density' button is highlighted with a red box. The code in the editor is:

```

-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|DIF|OVER; ADD|SUB or blank
ANG VAL NODEBUG   # ANG|ATU; VAL|TOT; DEBUG|NODEBUG
ORTHO             # optional: ORTHO|NONORTHO plotting directions

```

The left sidebar contains various navigation links such as 'Execution >>', 'Utils. >>', 'Files >>', 'Session Mgmt. >>', 'Configuration', and 'Usersguide'. The bottom left corner credits 'Idea and realization by luitz.at © 2001-2006'.

77. Click the “x lapw5” button

78. Click the “continue with electron density” 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. Session details include "Session: [TiC.]", "Commandline: x lapw5 -val", and "Program input is: """. Below this, log output shows "TOT changed to VAL in TiC.in5" and "DIFF changed to RHO in TiC.in5". A timestamp "0.084u 0.007s 0:00.09 88.8% 0+0k 0+880io 0pf+0w" is also present. A "Continue with" section contains a button labeled "continue with electron density", which is being clicked by a cursor. The right side of the interface features a logo for "w2web © luitz.at" with a stylized wave graphic.

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”

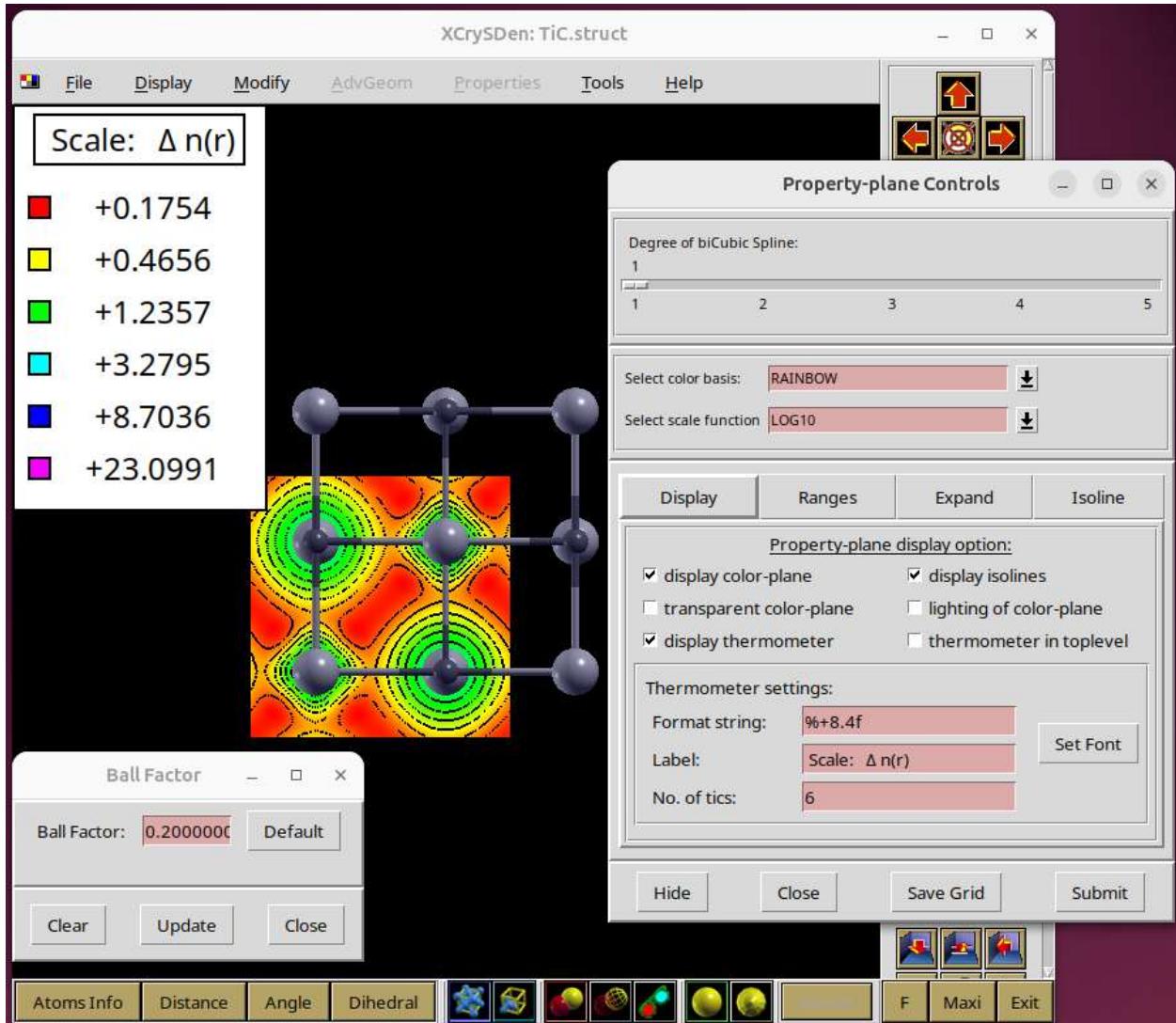
83. Click the “Submit” button

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”:

The screenshot shows a web browser window titled "TiC@localhost" with the URL "localhost:7890/index.pl?SID=635610". The session is identified as "Session: [TIC] /home/username/wiendata/TiC". The time "13:16:06 idle" and refresh/no refresh buttons are visible in the top right.

The main content area is titled "Electron density plots". A message box states: "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." Below this, there is a "Show full menu" link and a note "We are in rhoplot mode".

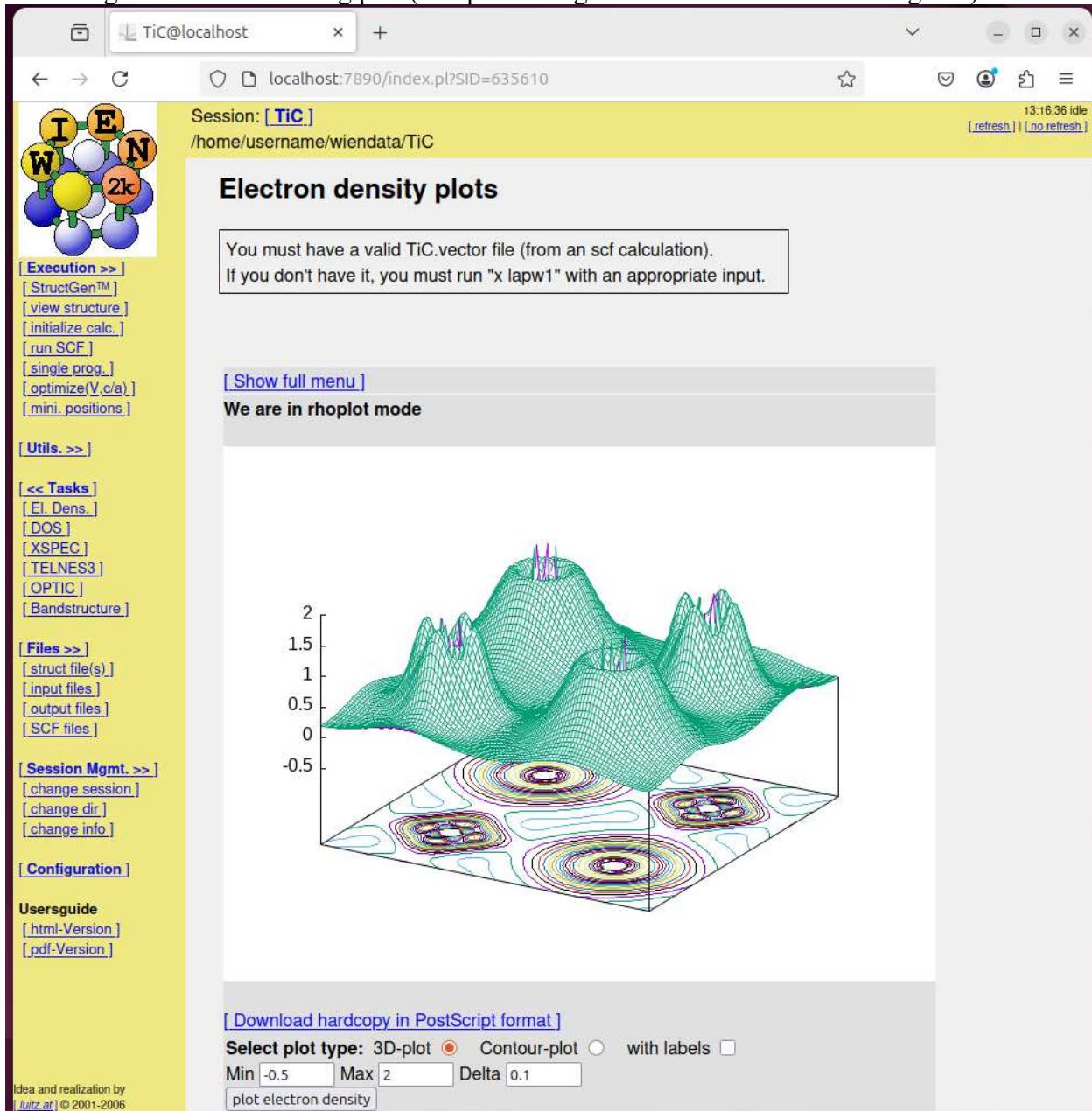
A "Select plot type:" section includes radio buttons for "3D-plot" (selected), "Contour-plot", and "with labels", and a checkbox for "Delta 0.1". Input fields for "Min" (-0.5), "Max" (2), and "Delta" (0.1) are present. A button labeled "plot electron density" is highlighted with a cursor.

The bottom right corner features a watermark "w2web © luitz.at" and "w2web".

The left sidebar contains a navigation tree with sections like "Execution >>", "StructGen™", "view structure", etc., under "Tasks"; "El. Dens.", "DOS", "XSPEC", "TELNES3", "OPTIC", "Bandstructure" under "Files >>"; "Session Mgmt. >>", "Configuration"; and "Usersguide" with links to "html-Version" and "pdf-Version".

At the bottom left, a footer notes "Idea and realization by [luitz.at] © 2001-2006".

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.ing` 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

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

`save_lapw -dos` with name:

Idea and realization by [Juiz.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](#)

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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]

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 the Wienda software interface. On the left is a sidebar with various buttons for execution, structure generation, viewing, initializing calculations, running SCF, single programs, optimization, mini positions, utilities, tasks, density calculations, DOS, XSPEC, TELNES3, OPTIC, and bandstructure analysis. Below these are buttons for files, session management, configuration, and users' guide. At the bottom, there is a note about the realization of the software.

The main window title is "TiC@localhost". The address bar shows "localhost:7890/index.pl?SID=635610". The session name is "Session: [TiC] /home/username/wiendata/TiC". The file path is "/home/username/wiendata/TiC/TiC.int".

The content of the file is:

```

File: /home/username/wiendata/TiC/TiC.int
continue with DOS without saving Save and continue with DOS Download this file: □
Header from TiC.qml:
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 qml-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

```

A red box highlights the "Save and continue with DOS" button. The footer of the window includes the text "w2web © iuitz.at" and "w2web".

98. Click “Save and continue with DOS”

99. Click “x tetra”

100. Click “continue with DOS”:

TiC@localhost

localhost:7890/index.pl?SID=635610

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

13:20:39 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 0.004s 0:00.01 100.0% 0+0k 0+624io 0pf+0w
```

Continue with

continue with DOS

w2web © luitz.at

w2web

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.]

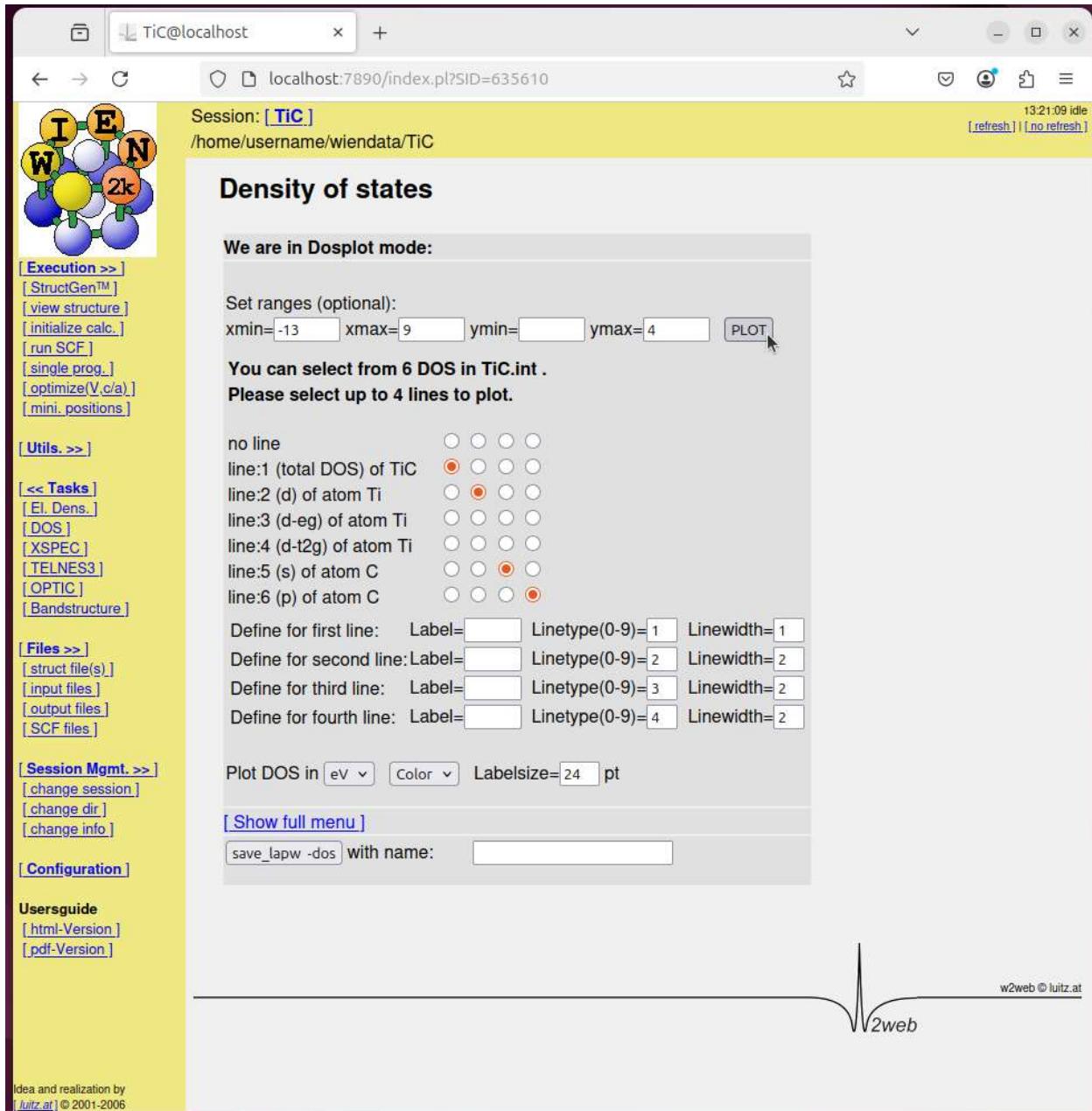
Configuration

Usersguide

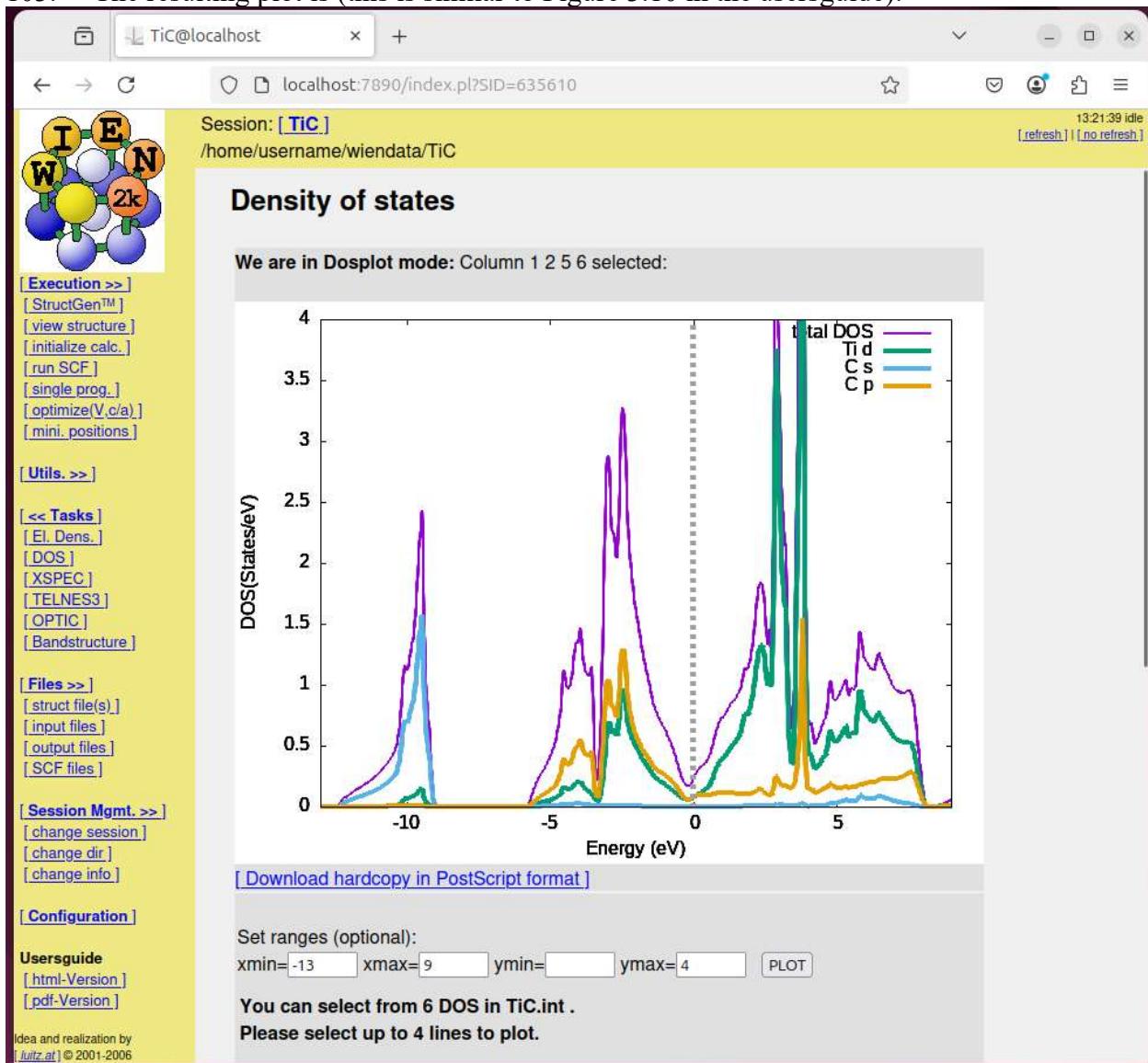
- [html-Version.]
- [pdf-Version.]

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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”:

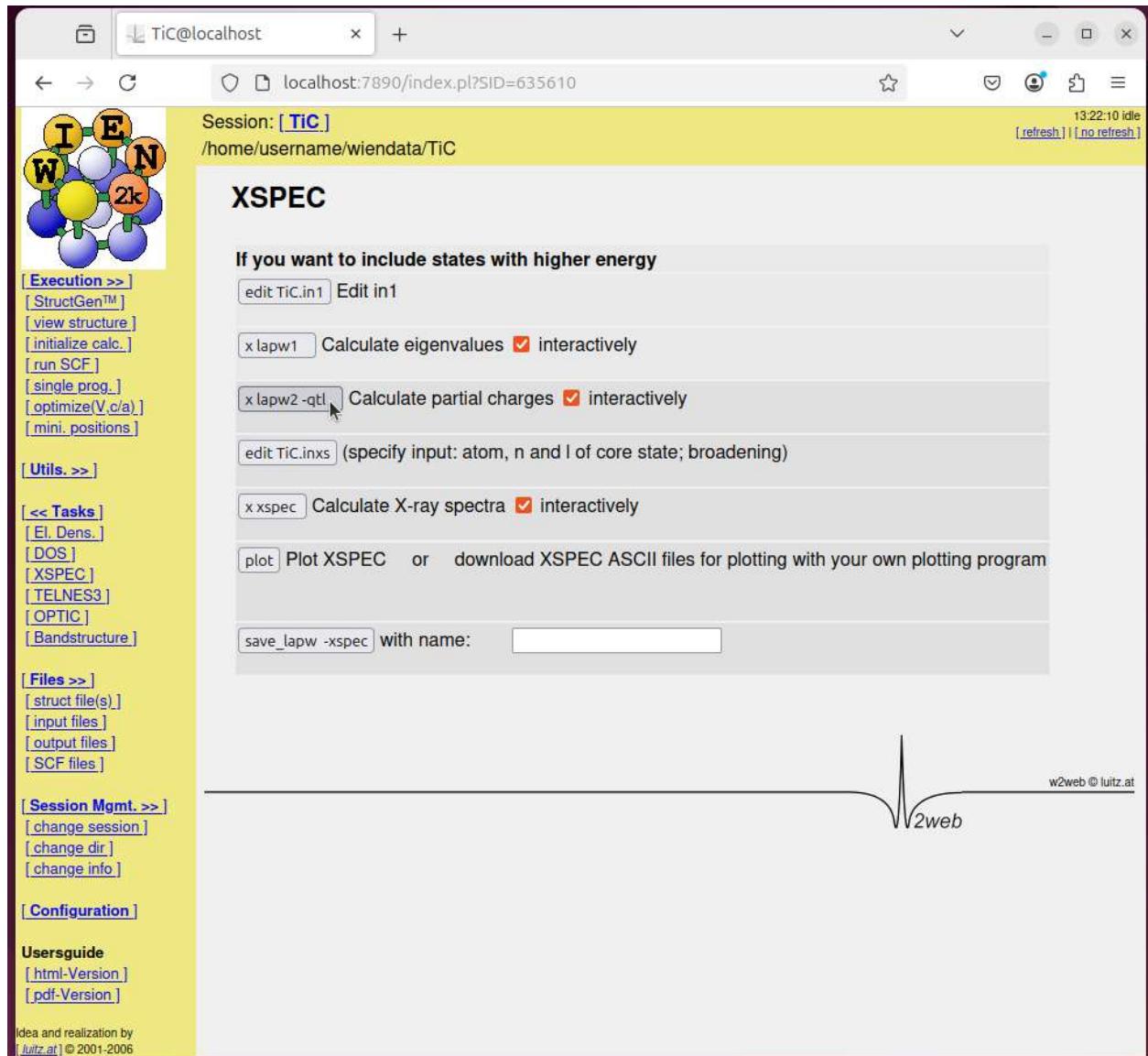


103. The resulting plot is (this is similar to Figure 3.10 in the usersguide):



Plot x-ray spectra

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



106. Click “continue with xspec”:

The screenshot shows a web browser window for 'TiC@localhost' at port 7890. The session is named 'TIC' and is located at '/home/username/wiendata/TiC'. The commandline is 'x lapw2 -qtl' and the program input is ''. The LAPW2 END section shows statistics: 0.036u 0.037s 0:00.07 85.7% 0+0k 0+480io 0pf+0w. Below this, there is a 'Continue with' section containing a button labeled 'continue with xspec'. A mouse cursor is hovering over this button. On the right side of the page, there is a small logo with the text 'w2web @ luitz.at' and '2web' below it. The left sidebar contains various navigation links under categories like Execution, Utils., Tasks, Files, Session Mgmt., Configuration, and Usersguide.

Session: [TIC]
/home/username/wiendata/TiC
13:22:10 idle
[refresh] | [no refresh]

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

LAPW2 END
0.036u 0.037s 0:00.07 85.7% 0+0k 0+480io 0pf+0w

Continue with

continue with xspec

w2web @ luitz.at
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

107. Click “x xspec”

108. Click “continue with xspec”:

The screenshot shows a web browser window titled "TiC@localhost" with the URL "localhost:7890/index.pl?SID=635610". The page displays session output for a calculation named "TIC". The output includes command-line entries like "x xspec", session details, and various calculation steps such as INITXSPEC, TETRA, TXSPEC, and LORENTZ. At the bottom of the session log, there is a "Continue with" section containing a button labeled "continue with xspec".

```

Session: [ TIC ]
/home/username/wiendata/TIC
13:22:40 idle
[ refresh. ] | [ no refresh. ]

Commandline: x xspec
Program input is: ""

Start INITXSPEC
INIT_XSPEC - done
0.000u 0.002s 0:00.00 0.0%      0+0k 0+16io 0pf+0w
Start TETRA
covered volume (%)    100.000000000000
no broadening
no broadening
no broadening
LEGAL END TETRA
0.007u 0.005s 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
0.034u 0.007s 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

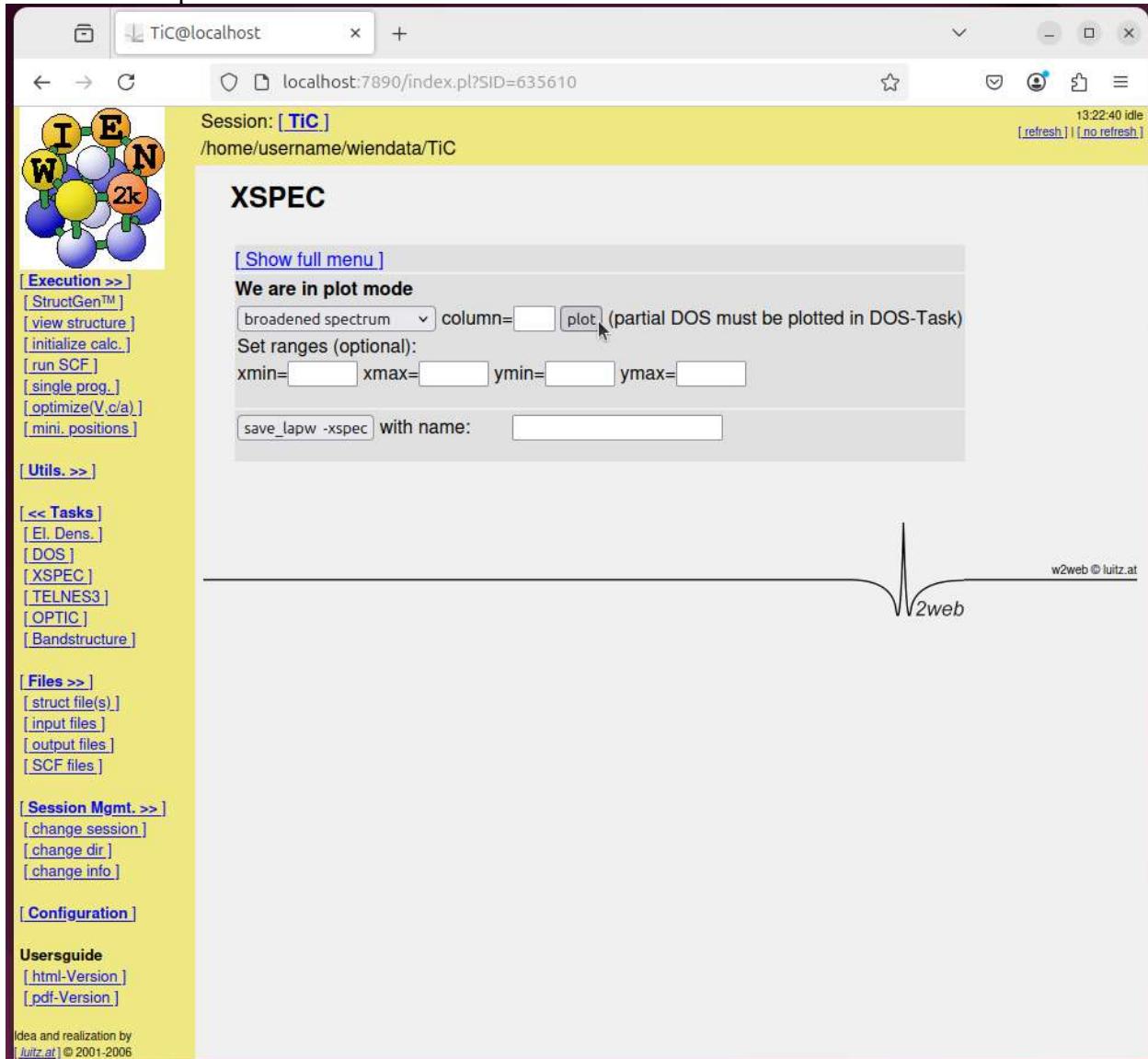
> stop
> xspec done
0.066u 0.034s 0:00.10 90.0%      0+0k 0+768io 0pf+0w

Continue with
  continue with xspec

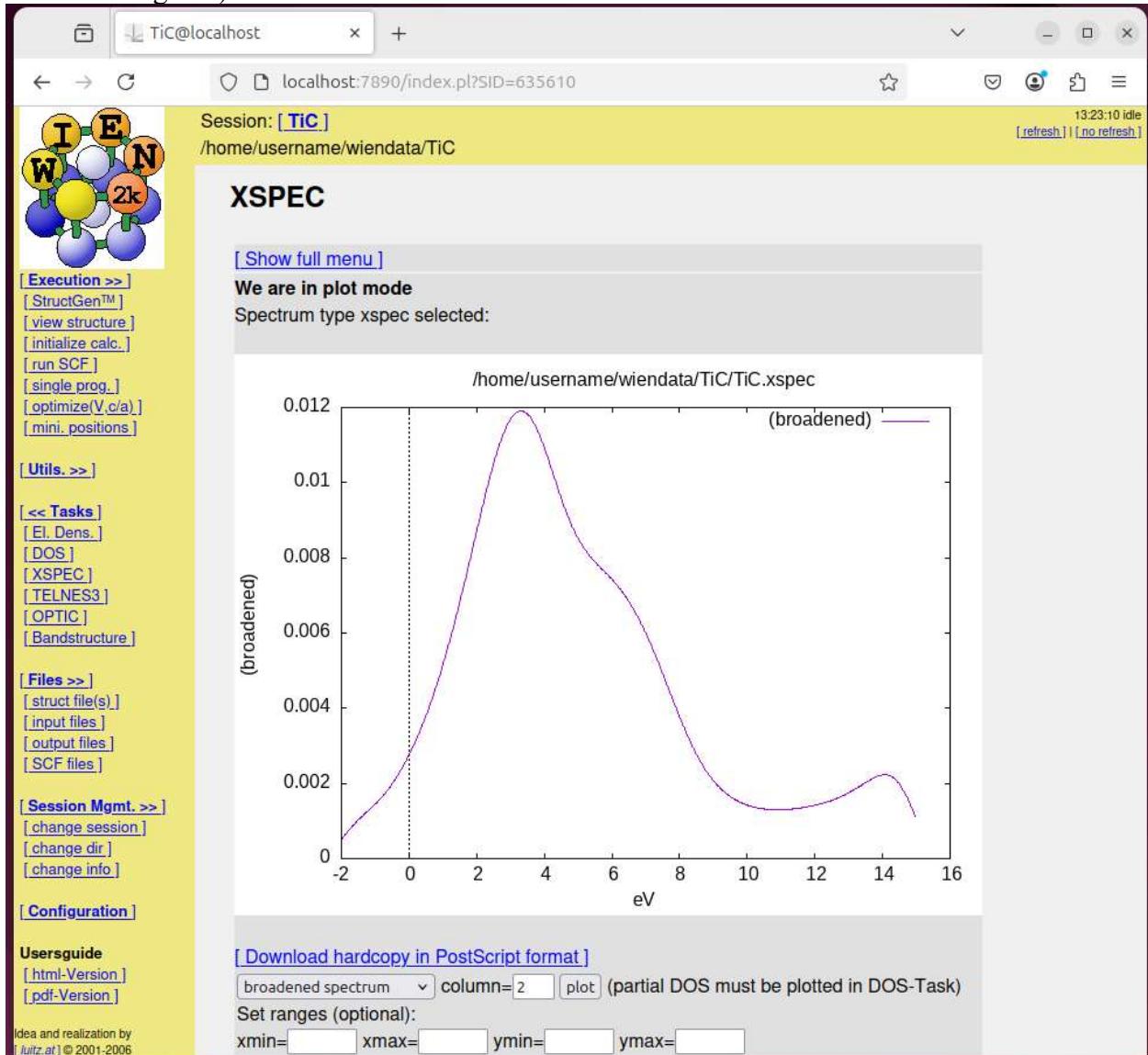
```

109. Click "plot"

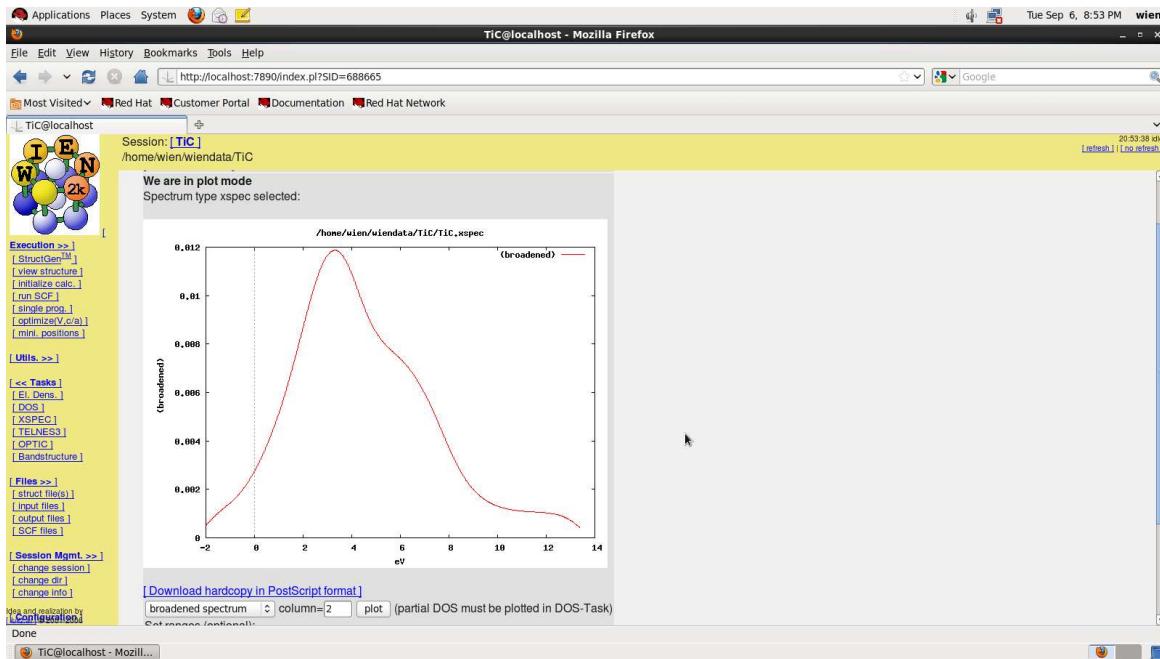
110. Click "plot":



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



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



Plot bandstructure

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

The 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:

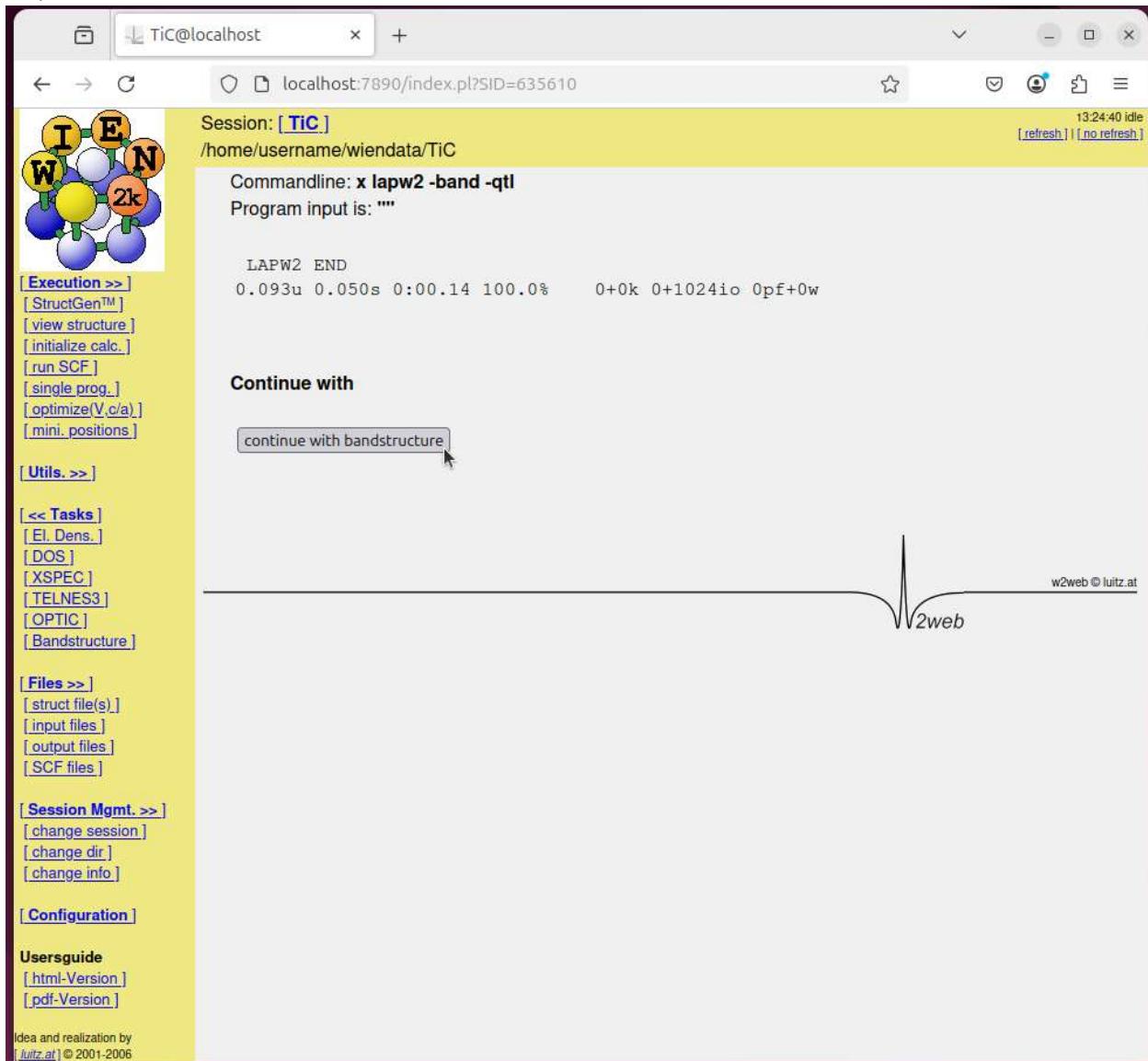
w2web © luitz.at

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 session is titled '[TIC]' and the path is '/home/username/wiendata/TiC'. The commandline is 'x lapw1 -band' and the program input is ''. The output shows 'LAPW1 END' with statistics: 0.816u 0.290s 0:01.11 99.0% 0+0k 0+5976io 0pf+0w. Below this, there is a 'Continue with' 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 peak labeled '2web'. On the left side of the page is a sidebar with various navigation links such as 'Execution >>', 'StructGen™', 'View structure', etc.

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 0.7429563359 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.)= 0.7429563359
  
```

```

### 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, ical, size of heavier plotting
  
```

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

Line switch:

w2web © luitz.at

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 the following text:

```

SPAGH: Read band energy from case.output1
number of k-points read in case.vector=      111
SPAGH END
0.008u 0.006s 0:00.01 0.0%      0+0k 0+624io 0pf+0w

```

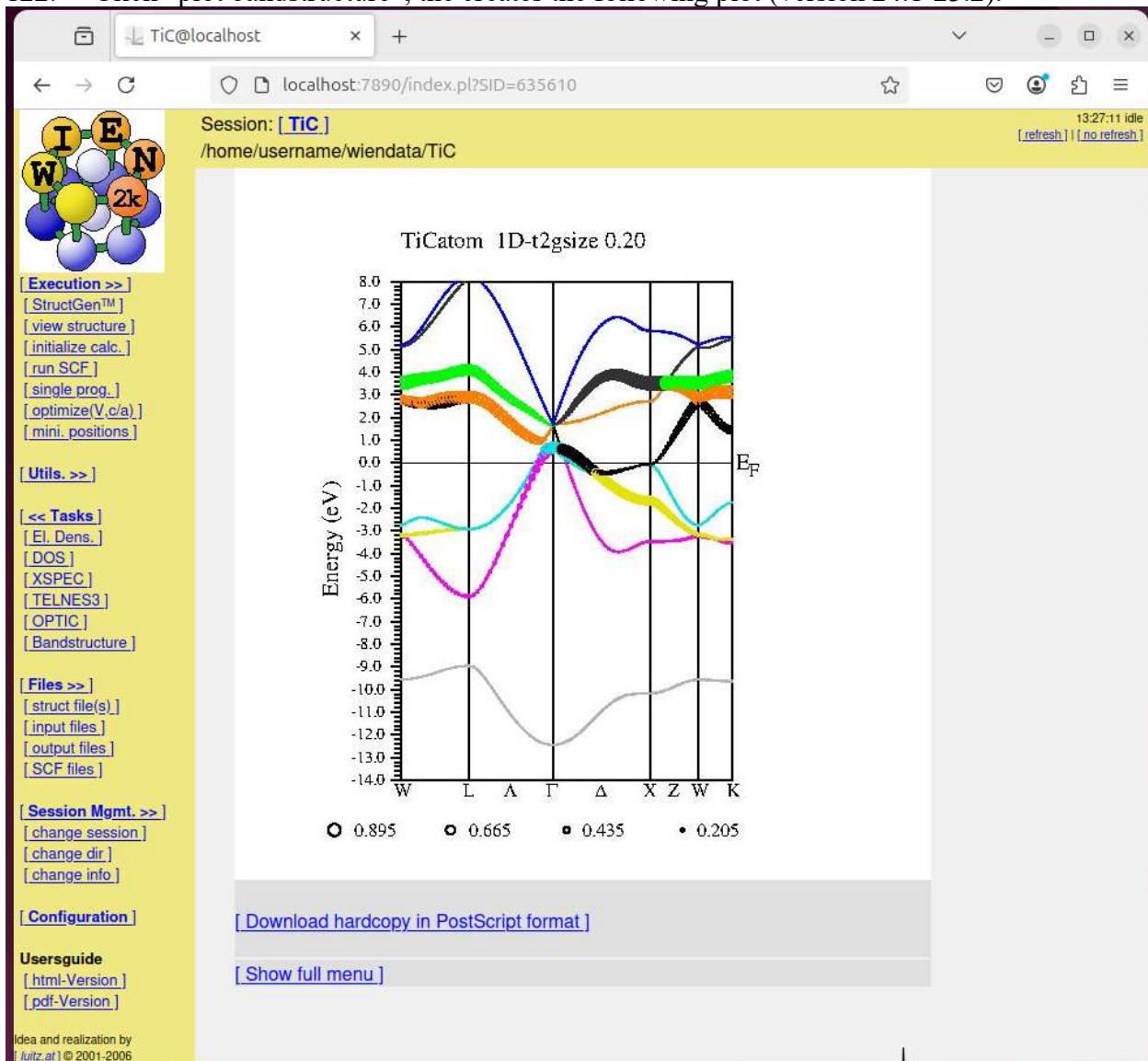
Below the output, there is a section titled **Continue with** containing a button labeled **continue with bandstructure**. A cursor arrow points towards this button. To the right of the button, there is a small logo with the text "w2web" and "w2web @ luitz.at".

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

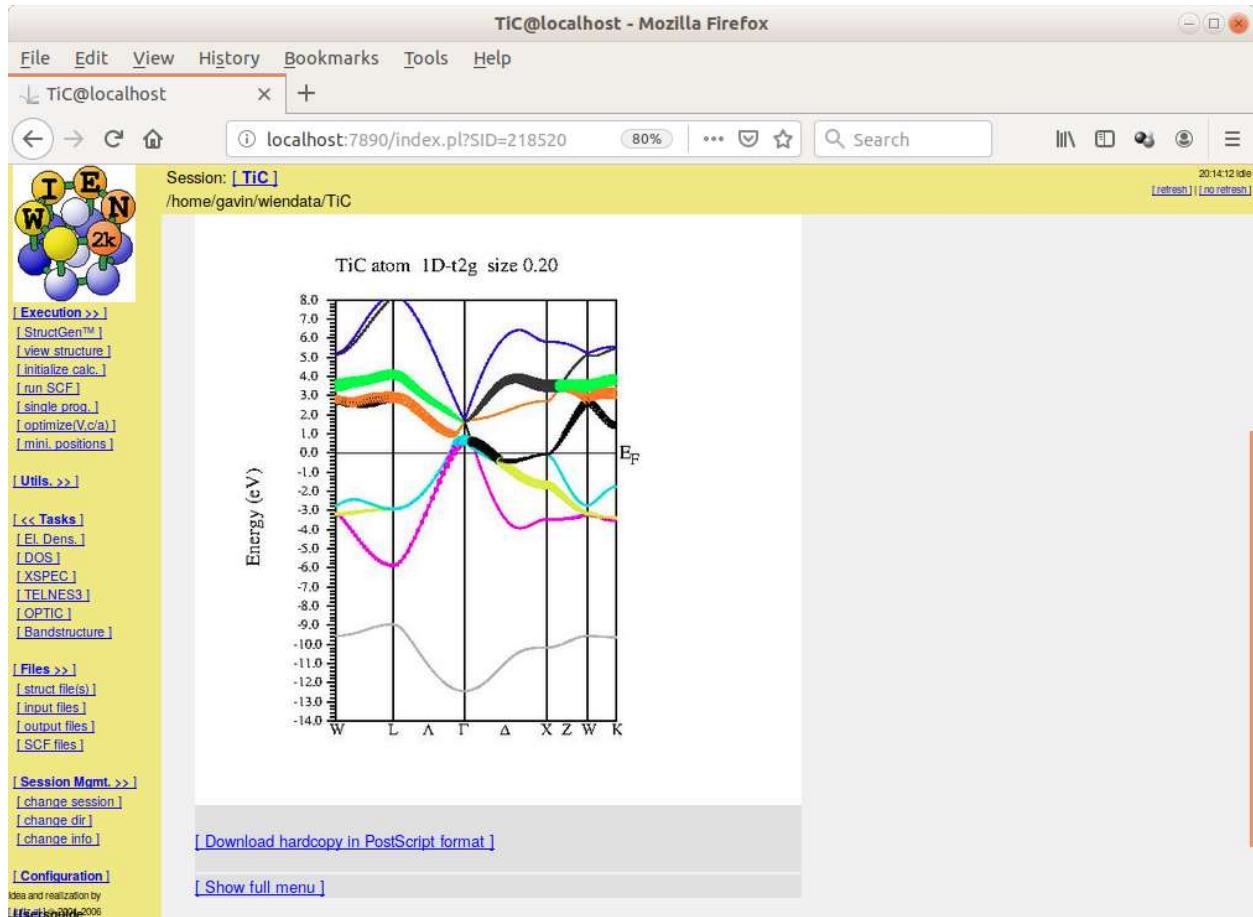
- Execution >>**
 - [StructGen™]
 - [view structure]
 - [Initialize calc.]
 - [run SCF.]
 - [single prog.]
 - [optimize(V_c/a)]
 - [mini_positions.]
- Utils. >>**
 - [<< Tasks]
 - [El. Dens.]
 - [DOS]
 - [XSPEC]
 - [TELNES3]
 - [OPTIC]
 - [Bandstructure]
- Files >>**
 - [struct file(s.)]
 - [input files]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

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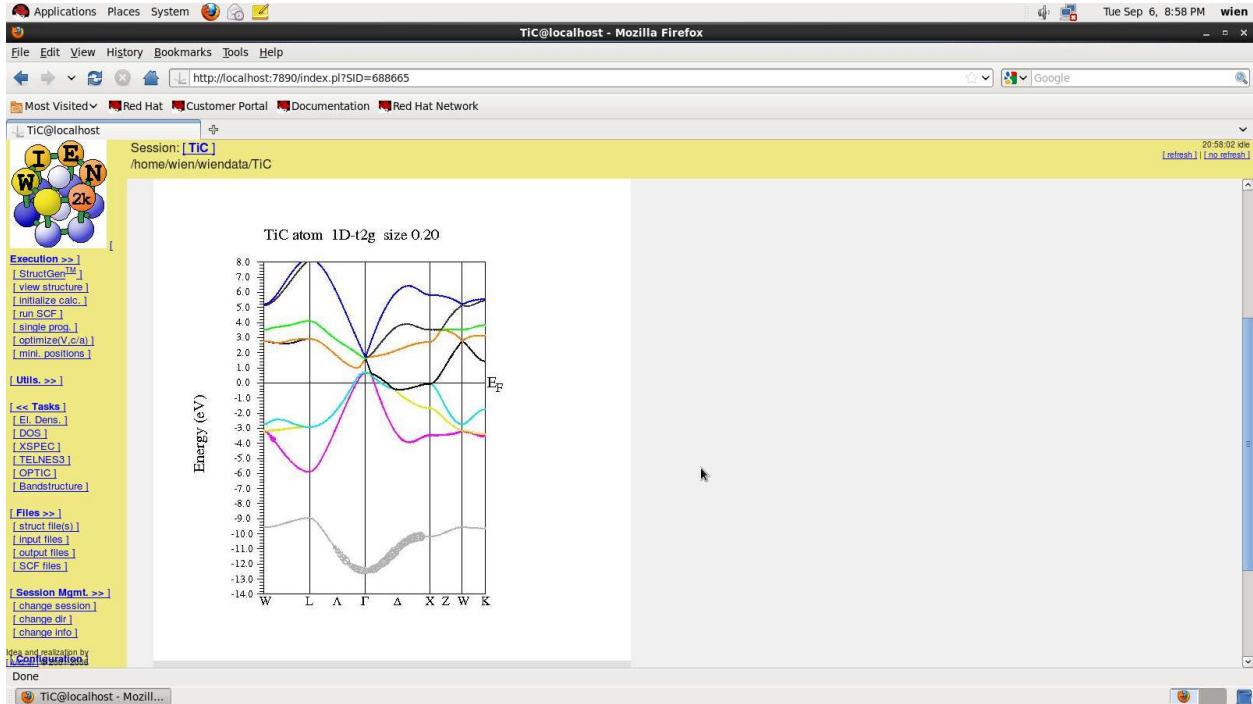
122. Click “plot bandstructure”, the creates the following plot (version 24.1-23.2):



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 is a vertical sidebar with a molecular structure icon at the top. Below it is a list of menu items grouped by category: Execution, Utils., Tasks, Files, Session Mgmt., Configuration, and Usersguide. Under Execution, the 'optimize(V,c/a)' option is highlighted. The main window title is 'TiC@localhost' and the URL is 'localhost:7890/index.pl?SID=635610'. The title bar also shows the session name 'Session: [TiC]' and the path '/home/username/wiendata/TiC'. The status bar at the top right indicates '13:28:42 idle' and has links for '[refresh]' and '[no refresh]'. The central area is titled 'Optimize volume, c/a-ratio, ...'. It contains 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 plot area, there is a signature 'w2web' with a small logo. The bottom left corner of the main window contains the text 'Idea and realization by luitz.at © 2001-2006'.

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
 13:29:12 idle
 [refresh] | [no refresh]

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”:



TiC@localhost localhost:7890/index.pl?SID=635610

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

13:29:12 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]

 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

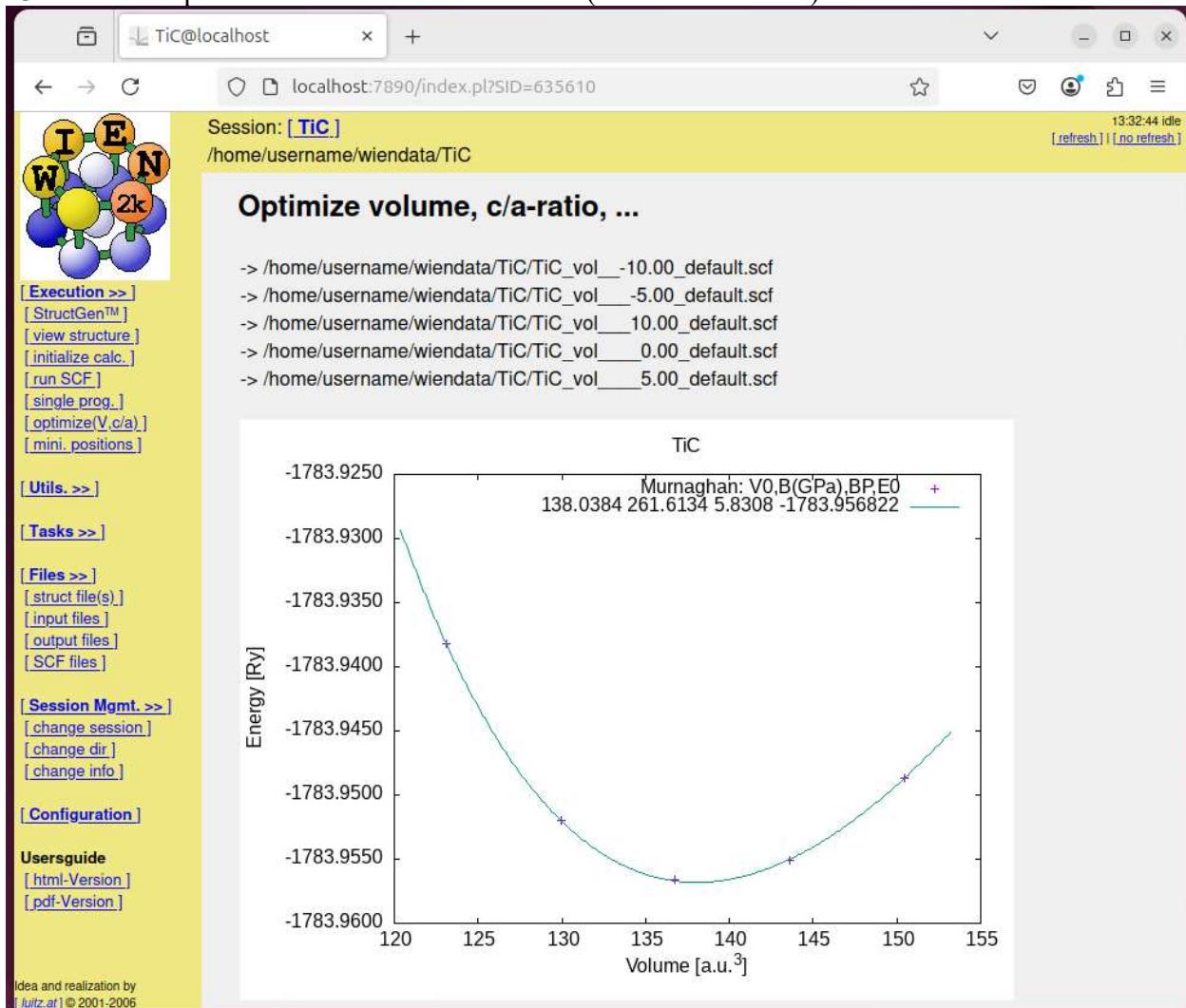
Idea and realization by
[Jürgen Atz](#) © 2001-2006

128. Click “run optimize.job”

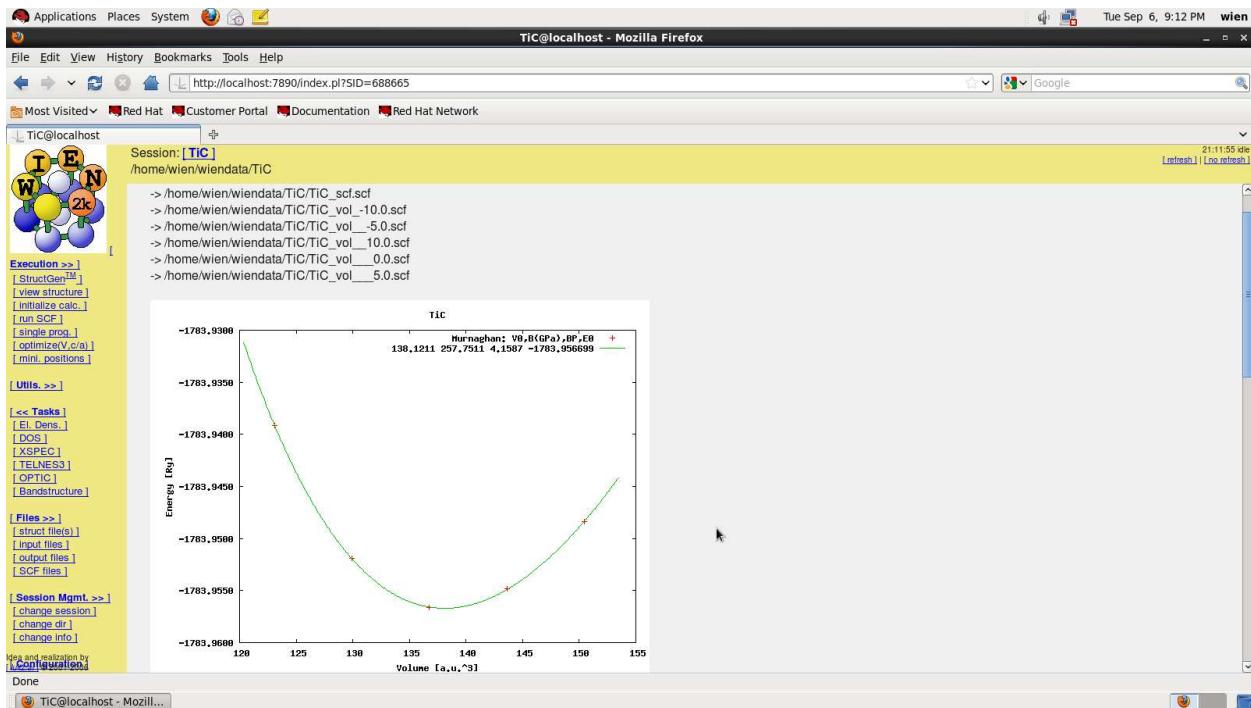
129. Click “continue with optimizer”:

The screenshot shows a web browser window with the URL `localhost:7890/index.pl?SID=635610`. The page title is "TiC@localhost". The main content area displays a session titled "Session: [TiC]" with the path "/home/username/wiendata/TiC". It shows a command line entry: "Commandline: ./optimize.job" and "Program input is: """. Below this, a link "[View STDOUT]" is provided to monitor the progress of the command. A button labeled "Continue with" has a mouse cursor hovering over it. The right side of the interface features a logo with the text "w2web @ luitz.at" and "w2web". On the left side, there is a sidebar with various navigation links grouped under sections like "Execution >>", "Tasks >>", "Files >>", "Session Mgmt. >>", "Configuration", and "Usersguide". At the bottom left of the sidebar, there is a note: "Idea and realization by [luitz.at] © 2001-2006".

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



Could compare to the differences in versions 11.1-13.1:



132. TiC example has been completed.