

WIEN2k TiC Example

Fedora Linux 42

WIEN2k_24.1 (Release 1/8/2024)

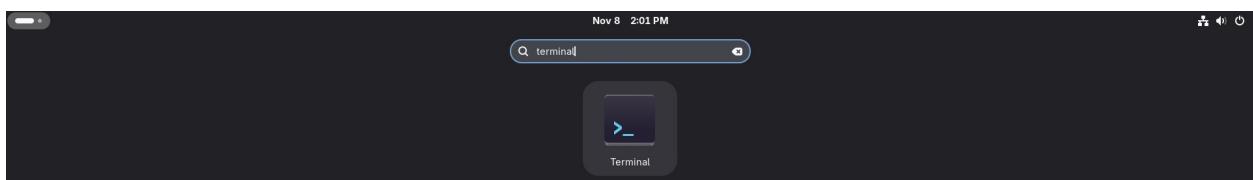
ifx version 2025.3.0

WIEN2k patches [1]: Makefile.orig.patch, SearchZ.patch, StorePot.patch, angle.patch, atom_read.patch, atom_write.patch, charge.patch, executor.patch, init_elast_lapw.patch, init_orb_lapw.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. Search terminal and click on Terminal to open:



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

```

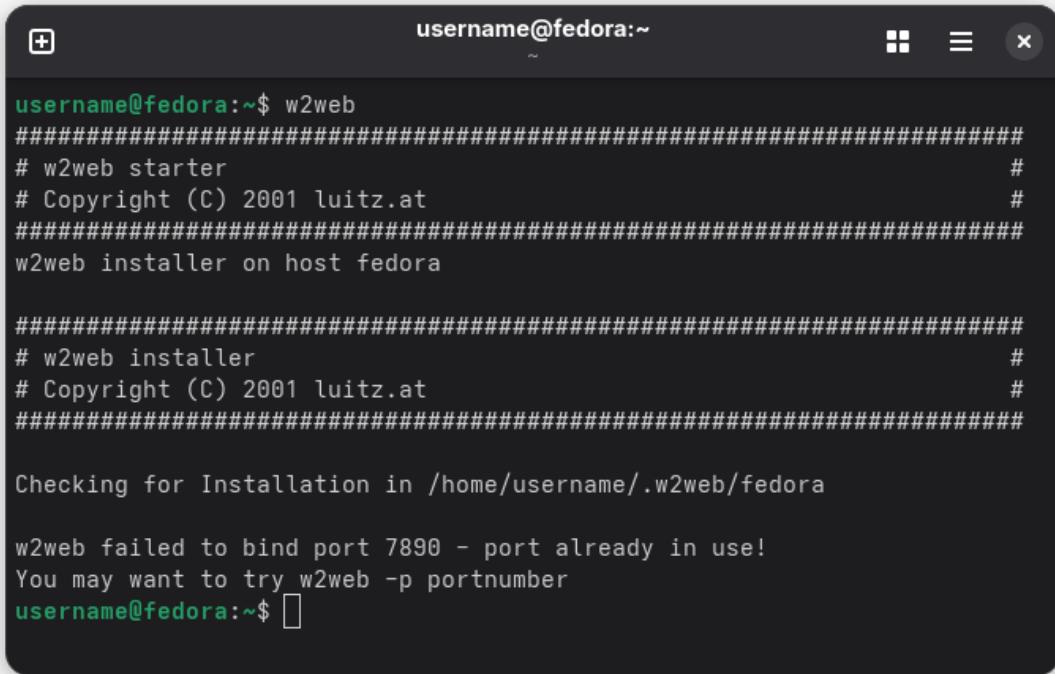
username@fedora:~$ w2web
#####
# w2web starter
# Copyright (C) 2001 luitz.at
#####
w2web installer on host fedora

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

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

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

If your w2web is already started, you will get:



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

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

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

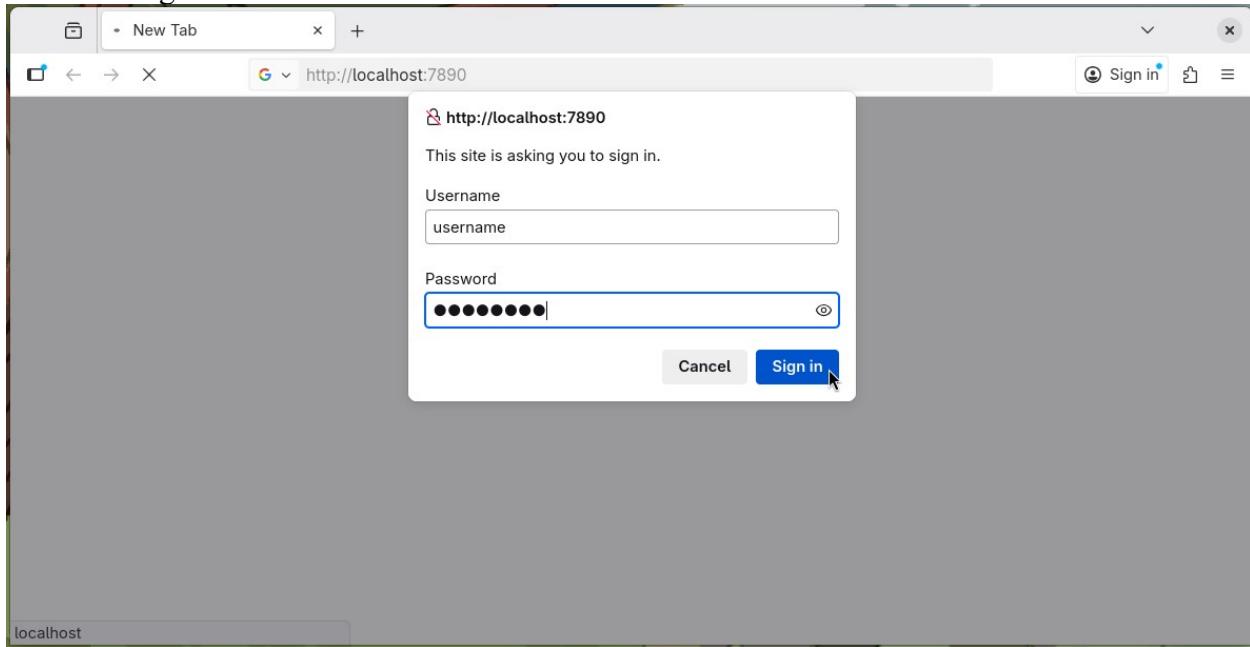
w2web failed to bind port 7890 - port already in use!
You may want to try w2web -p portnumber
username@fedora:~$ 
```

Open Firefox and login to w2web

3. Click on the Firefox icon to open Firefox:

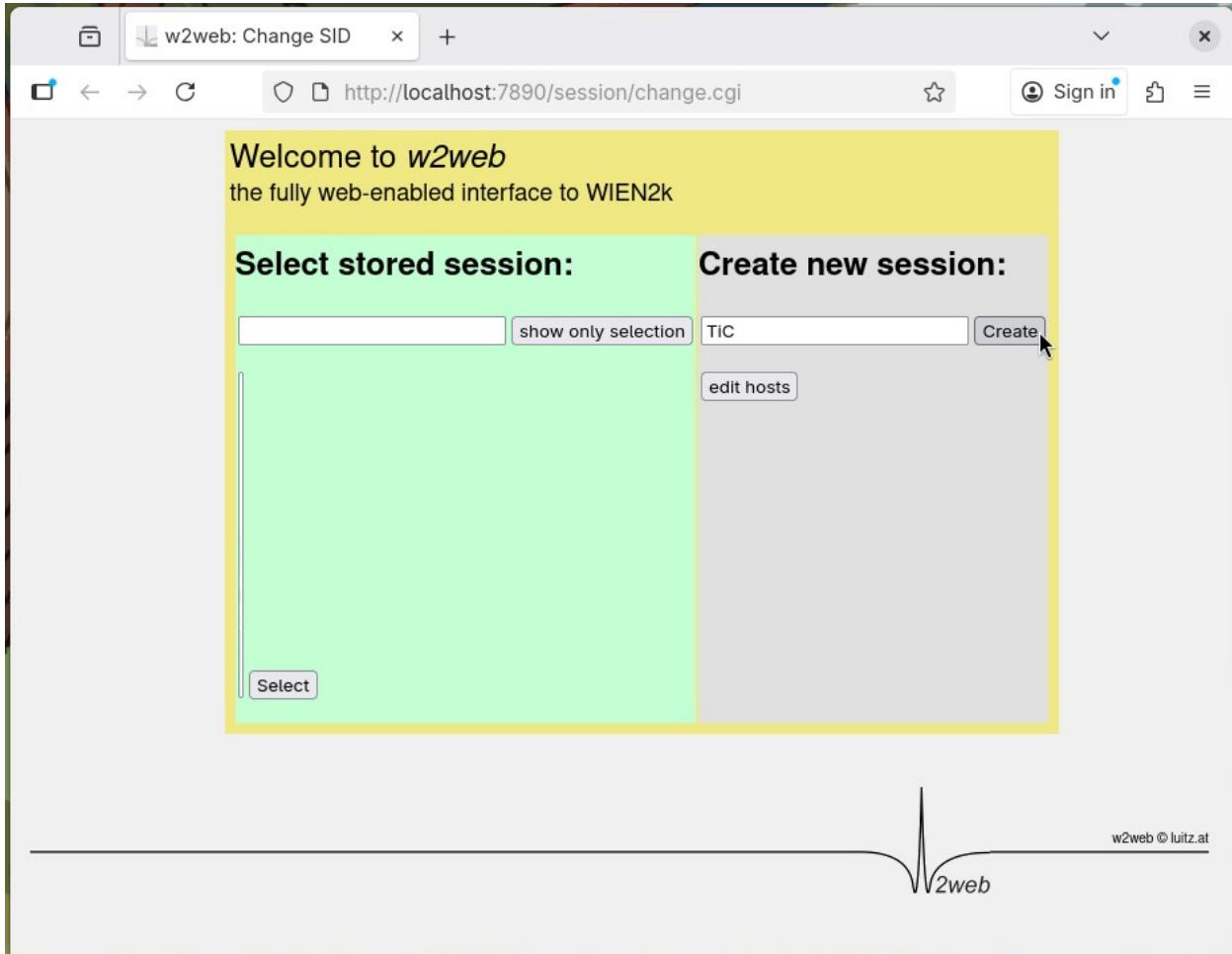


4. Enter url <http://localhost:7890>, type your w2web username and password, then click “Sign in” to login to w2web:

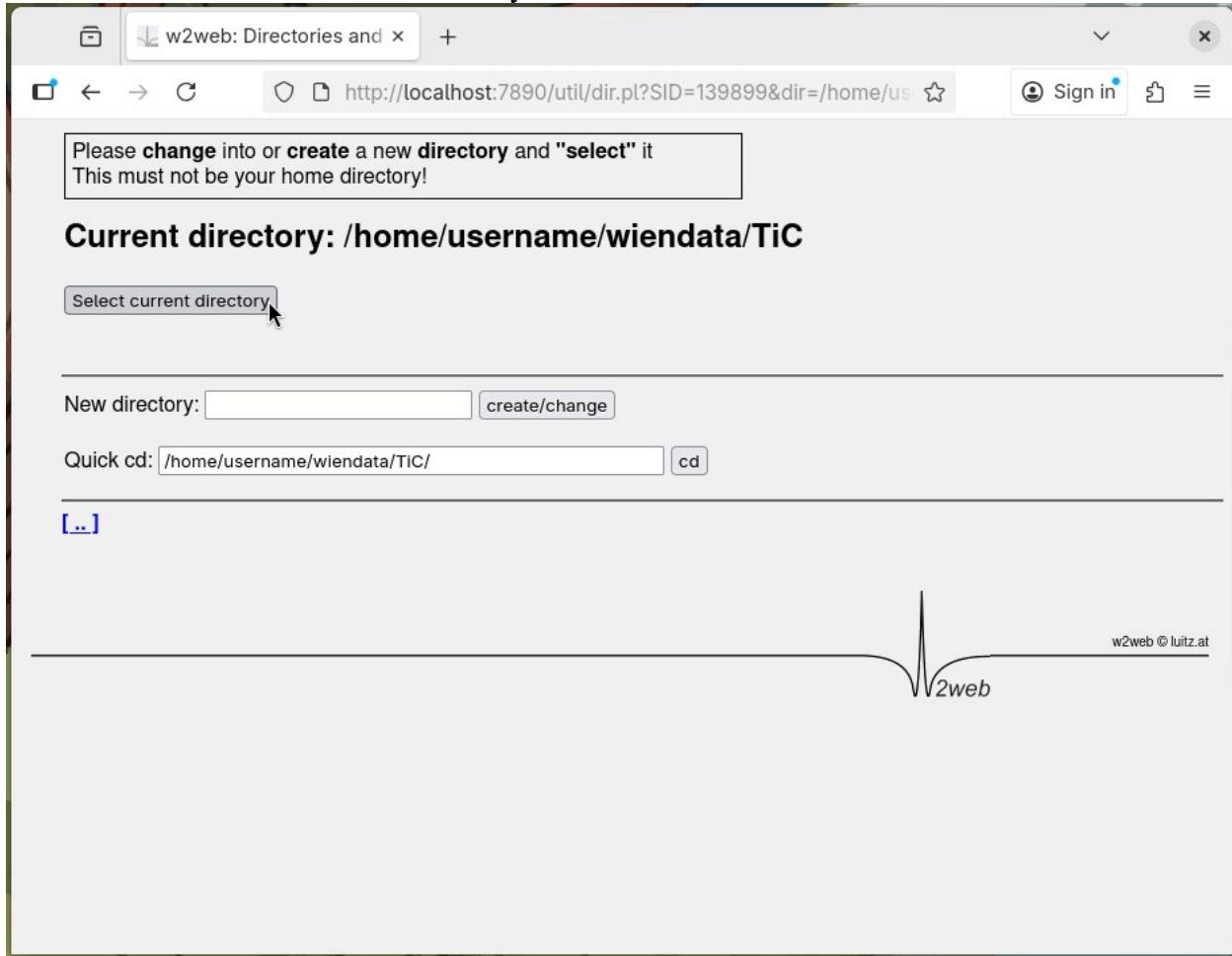


Create a new session (calculation)

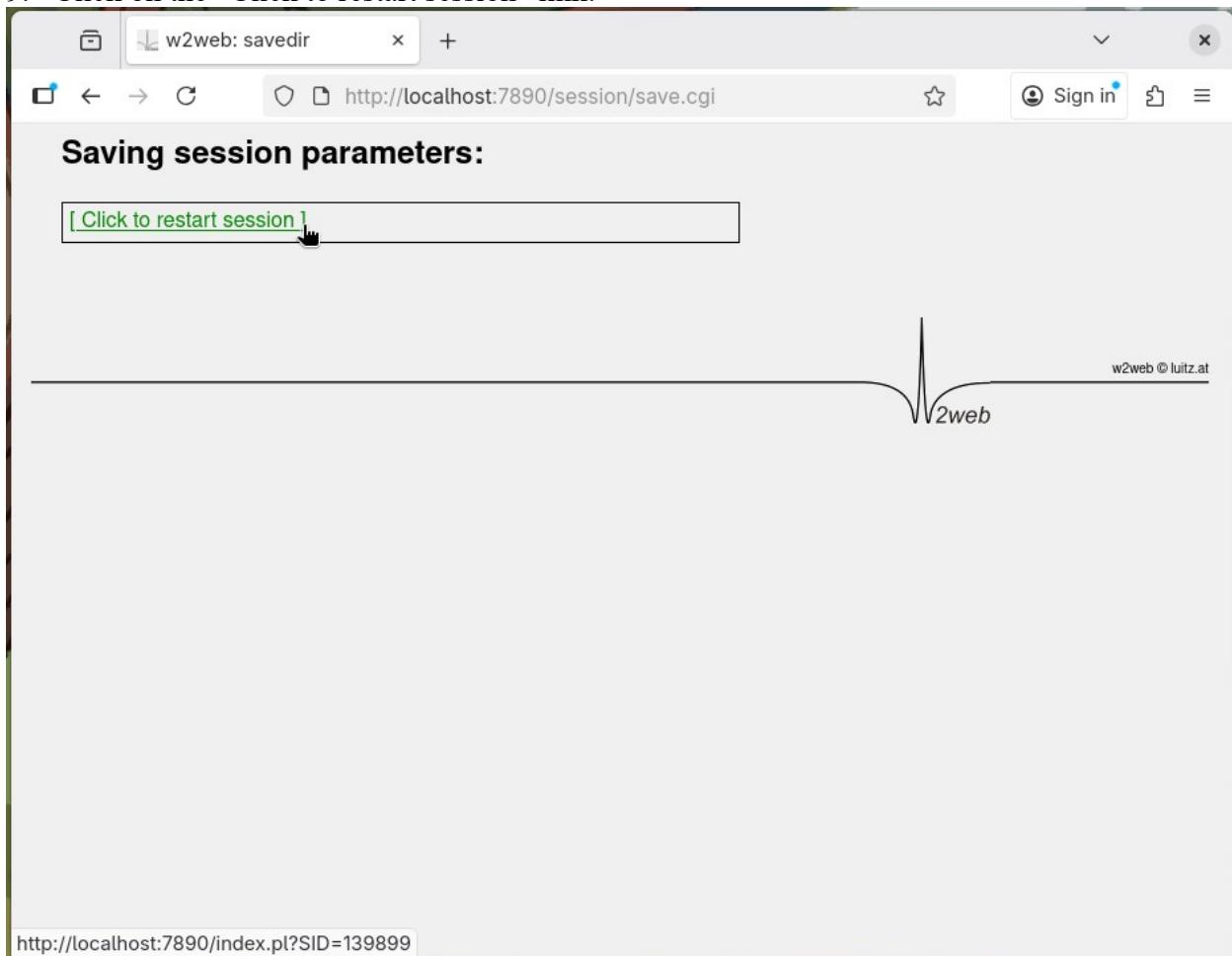
5. Enter “TiC” in the “Create new session:” box and then click the “Create” button:



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



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



10. The following window should appear:

TiC@localhost

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

16:03:39 idle
[refresh] | [no refresh]

w2web, the fully web-enabled interface to WIEN2k

Session Name: TiC
Session ID: 139899
Directory: /home/username/wiendata/TiC
Last changed: Sat Nov 8 16:03:29 2025
Comments:
 spin polarized calculation
 AFM calculation
 complex calculation (no inversion)
 parallel calculation

Change session information

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

[Utils. >>]

[Tasks >>]

[Files >>]
[struct file(s).]
[input files]
[output files]
[SCF files]

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

[Configuration]

Usersguide
[html-Version]
[pdf-Version]
Idea and realization by
[luitz.at] © 2001-2006

w2web © luitz.at
2web

Create the TiC structure for calculation

11. In the left menu, click on StructGen™ under Execution
12. The “Number of atoms” is 2, click the “Generate template” button:

The screenshot shows the StructGen™ web interface. On the left, there's a sidebar with various links for session management, utilities, tasks, files, and configuration. The main content area has a heading 'StructGen™'. It displays a molecular model of a TiC structure and a message: 'You do not have a TiC.struct file yet.' Below this, there's a text input field labeled 'Number of atoms:' containing '2' and a button labeled 'Generate template'. There are also sections for alternative conversion methods using 'cif2struct' and 'xyz2struct'.

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 for a session named "TiC".

- Left Sidebar:** Contains a crystal structure visualization and a list of navigation links:
 - [<< Execution]
 - [StructGen™]
 - [view structure]
 - [initialize calc.]
 - [run SCF]
 - [single prog.]
 - [optimize(V,c/a)]
 - [mini_positions]
 - [command line]
 - [frozen phonons]
- Top Bar:** Shows the session name "TiC@localhost", the URL "http://localhost:7890/index.pl?SID=139899", and a "Sign in" button.
- Header:** Displays "Session: [TiC] /home/username/wiendata/TiC" and "StructEdit /home/username/wiendata/TiC".
- Main Area:**
 - StructGen™** title.
 - A message: "You have to click "Save Structure" for changes to take effect!"
 - Save Structure** button.
 - Title:** TIC
 - Lattice:** Type: P (selected from a dropdown menu)
 - P
 - F
 - B
 - CXY
 - CYZ
 - CXZ
 - R
 - H
 - 1_P1
 - Spacegroups from Bilbao Cryst Server**
 - Lattice parameters in Å**
 - a = 4.328
 - b = 4.328
 - c = 4.328
 - α = 90.000000
 - β = 90.000000
 - γ = 90.000000
 - Inequivalent Atoms: 2**
 - Atom 1:** Ti (highlighted) 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 (highlighted) 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** button (with a cursor icon).
- Bottom Left:** "Idea and realization by [lutz.at] © 2001-2006"

20. Click the “Save Structure” button

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

TiC@localhost

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

16:06:10 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 © iuitz.at

w2web

Execution

StructGen™

view structure

initialize calc.

run SCF

single prog.

optimize(V,c/a)

mini_positions

command line

frozen phonons

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=139899

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

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

16:06:10 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

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[luitz.at](#) © 2001-2006

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 a navigation tree and a "Session Mgmt. >>" section. The main area displays a 3D ball-and-stick model of a crystal structure with atoms labeled T, E, N, W, and 2k. Below the model, several buttons are listed: [<< Execution], [StructGen™], [view structure], [initialize calc.], [run SCF], [single prog.], [optimize(Vc/a)], [mini_positions], [command line], [frozen phonons]. Under "Tasks >>", there are buttons for [Files >>] (with sub-options like struct file(s), input files, output files, SCF files), [Session Mgmt. >>] (with sub-options like change session, change dir, change info), and [Configuration]. Under "Usersguide", there are links for [html-Version] and [pdf-Version]. At the bottom left, it says "Idea and realization by Jürgen Blaurock © 2001-2006".

The central workspace is titled "StructGen™" and contains the following information:

- You have to click "Save Structure" for changes to take effect!**
- Save Structure** button
- Title:** TiC
- Lattice:** F
- Type:** F
- Spacegroups from Bilbao Cryst Server:** P
- Lattice parameters in Å:**
 - a = 4.32800003862
 - b = 4.32800003862
 - c = 4.32800003862
 - α = 90.000000
 - β = 90.000000
 - γ = 90.000000
- Inequivalent Atoms: 2**
- Atom 1:** Ti
 - Pos 1: x = 0.00000000, y = 0.00000000, z = 0.00000000
 - [remove], [split], [add position]
- Atom 2:** C
 - 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!**
- Save Structure** button

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™ web interface for a TiC session. The left sidebar contains various execution and utility links. The main area displays the following input parameters:

- Title:** TiC
- Lattice:** F (selected from a dropdown menu)
- Type:** F (selected from a dropdown menu)
- Spacegroups from Bilbao Cryst Server:** A link to a list of spacegroups.
- Lattice parameters in Å:**
 - a = 4.32800003862
 - b = 4.32800003862
 - c = 4.32800003862
 - α = 90.000000
 - β = 90.000000
 - γ = 90.000000
- Inequivalent Atoms: 2**
- Atom 1:** Ti (labeled in red), Z = 22.000, RMT = 2.0000
Pos 1: X = 0.00000000, Y = 0.00000000, Z = 0.00000000
- Atom 2:** C (labeled in red), Z = 6.000, RMT = 1.9000
Pos 1: X = 0.50000000, Y = 0.50000000, Z = 0.50000000
- Number of symmetry operations:** generate
- View only mode --> [edit STRUCT file]**

At the bottom right, there is a logo for "w2web @ luitz.at" with a stylized wave graphic.

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 software interface. On the left, there is a sidebar with various menu items such as Execution, Utils, Tasks, Files, Session Mgmt., Configuration, and a Usersguide. The main area is titled "Initialize WIEN2k calculation". It has two sections: "Fast mode (recommended)" and "Individual mode (phase 1)".

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; On-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 (highlighted in red)

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

check if gmax>gmin

Perform spin-polarized calc.?

No

Yes

check TIC.in2_st set Fermi-method and GMAX

Prepare input files

x kgen

view klist

x dstart interactively

instgen_lapw TiC.inst needs to be generated by instgen_lapw

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

TiC@localhost

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

please specify nn-bondlength factor: (usually=2)

2

NN needs input

16:08:42 idle
[refresh] || [no refresh]

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2web

[<< Execution]
[StructGen™]
[view structure]
[initialize calc.]
[run SCF]
[single prog.]
[optimize(V,c/a)]
[mini_positions]
[command line]
[frozen phonons]

[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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[luitz.at] © 2001-2006

31. Click the “initlapw” button:

The screenshot shows a web-based graphical user interface for a molecular simulation session named 'TiC'. The interface includes a sidebar with various navigation links such as 'Execution', 'Tasks >>', 'Files >>', 'Session Mgmt. >>', and 'Configuration'. A large molecular model of TiC is displayed on the left, featuring atoms labeled 'Ti' (yellow), 'C' (orange), and 'W' (blue). The main workspace displays command-line output for a calculation involving a 'nn' bond length factor. The output shows details for atom pairs (1,2) and (2,1) with RMT values of 2.00000 and 1.90000 respectively, and a sum of 3.90000. It also lists NN DISTANCE values of 4.08937 and 4.08937. The session status bar at the top right indicates 'idle' with a timestamp of '16:08:42' and refresh/no-refresh options.

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

16:08:42 idle
[refresh] | [no refresh]

Commandline: x nn
Program input is: "2 "

```
specify nn-bondlength factor: (usually=2) [and optionally dlimit, dstmax (a
1.d-5, 20)]
dfac,DSTMAX: 2.0000000000000000 20.000000000000000
iix,iyy,iiz 5 5 5 40.893690000000000
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

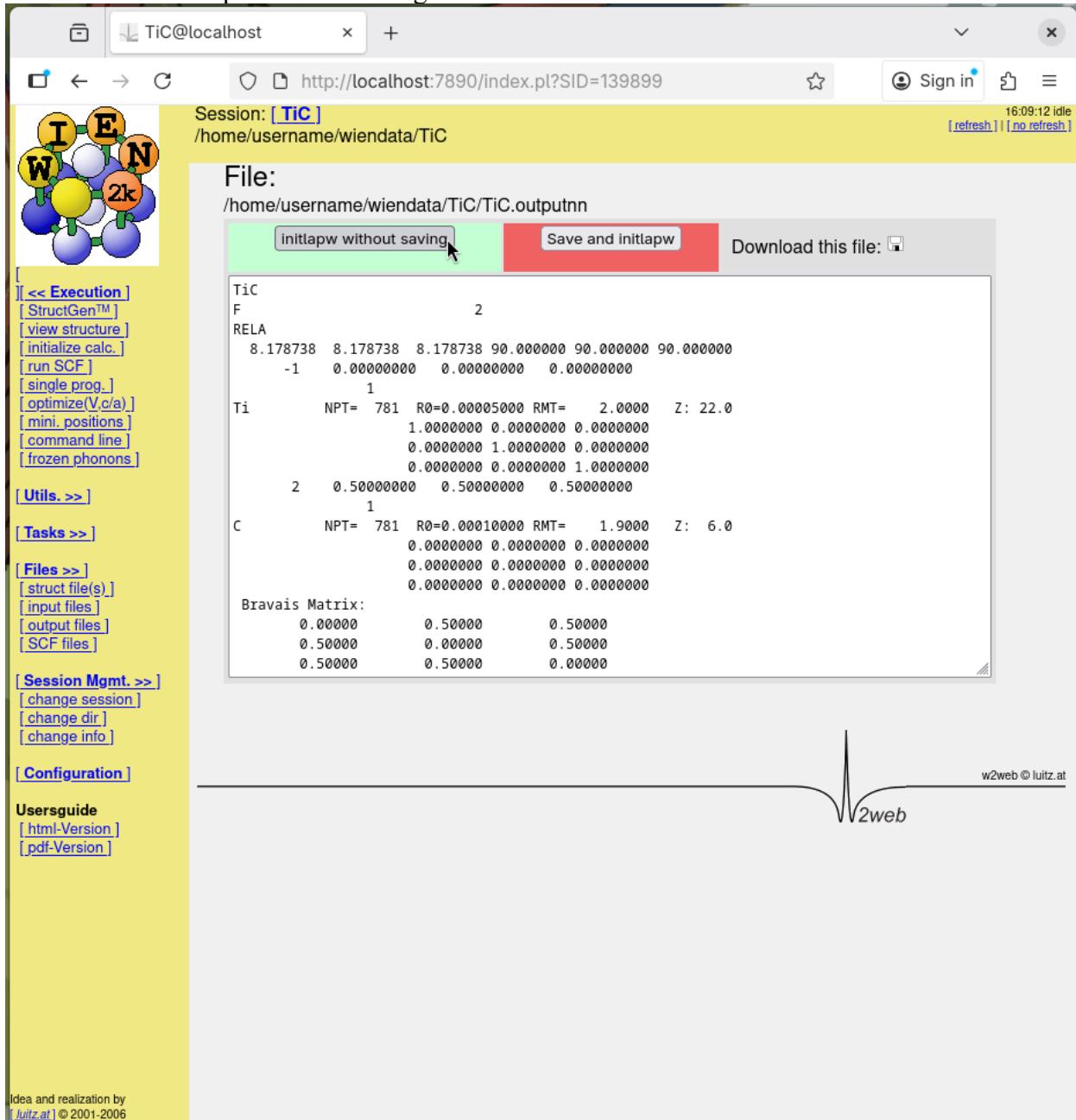
ATOM 2 C ATOM 1 Ti
RMT( 2)=1.90000 AND RMT( 1)=2.00000
SUMS TO 3.90000 LT. NN-DIST= 4.08937
NN ENDS
0.002u 0.004s 0:00.00 0.0% 0+0k 0+32io 0pf+0w
```

Continue with

[initlapw](#)

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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 <http://localhost:7890/index.pl?SID=139899>. The session is named **TiC**. The left sidebar contains a molecular logo and links for execution, utilities, tasks, files, session management, and configuration. The main content area displays the **File:** [/home/username/wiendata/TiC/TiC.outputnn](#). The file content is as follows:

```

TiC
F
RELA
  8.178738  8.178738  8.178738  90.000000  90.000000  90.000000
    -1      0.0000000   0.0000000   0.0000000
          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      0.5000000   0.5000000   0.5000000
          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:
  0.0000   0.50000   0.50000
  0.50000  0.00000   0.50000
  0.50000   0.50000   0.00000

```

At the top of the content area, there are three buttons: **initlapw without saving** (highlighted), **Save and initlapw**, and **Download this file:**.

34. Click the “x sgroup” button

35. Click the “initlapw” button:

The screenshot shows a web browser window titled "TiC@localhost" with the URL "http://localhost:7890/index.pl?SID=139899". The session name is "TiC" and the path is "/home/username/wiendata/TiC". The commandline is "x sgroup" and the program input is empty. Resource usage is shown as 0.000u 0.001s 0:00.00 0.0% CPU, 0+0k 0+8io 0pf+0w memory.

Execution Options:

- [<< Execution]
 - [StructGen™]
 - [view structure]
 - [initialize calc.]
 - [run SCF]
 - [single prog.]
 - [optimize(V,c/a)]
 - [mini_positions]
 - [command line]
 - [frozen phonons]
- [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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Continue with

Initlapw button (highlighted with a cursor)

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V2web

36. Click the “view outputsgroup” button

37. Click the “initlapw without saving” button:

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
90.0000000	90.0000000	90.0000000

===== 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):

0.0000000	0.0000000	0.0000000	Ti
0.5000000	0.0000000	0.0000000	

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2web

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

The screenshot shows the TiC@localhost web interface. On the left, there's a sidebar with various links like 'Execution', 'StructGen™', 'view structure', etc. The main content area has a yellow header bar with session information. Below it, there's a section for specifying precision levels and a 'CHECK BATCH VALUES' button. Under 'Individual mode (phase 6)', there are several buttons for file operations. A prominent red box highlights a modal dialog titled 'Use struct-file generated by sgroup? (Usually NO, unless WARNINGS appeared above)'. Inside this dialog, there are two buttons: 'Yes' and 'No'. The 'No' button is highlighted with a mouse cursor.

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; On-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 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 **check TIC.in1_st** set RKmax (usually 5.0-9.0). [[Click here for more info](#)]

view outputnn **view TIC.outputnd and cp TIC.in0_std TIC.in0**
x sgroup **check TIC.in2_st** set Fermi-method and GMAX
view outputsgroup **Prepare input files**

sgroup found: 225 (F m -3 m)

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

No **Yes**

x kgen **x symmetry**
view klist **copy struct_st** and view outputs
x start **interactively**

instgen_lapw TiC.inst needs to be generated by instgen_lapw

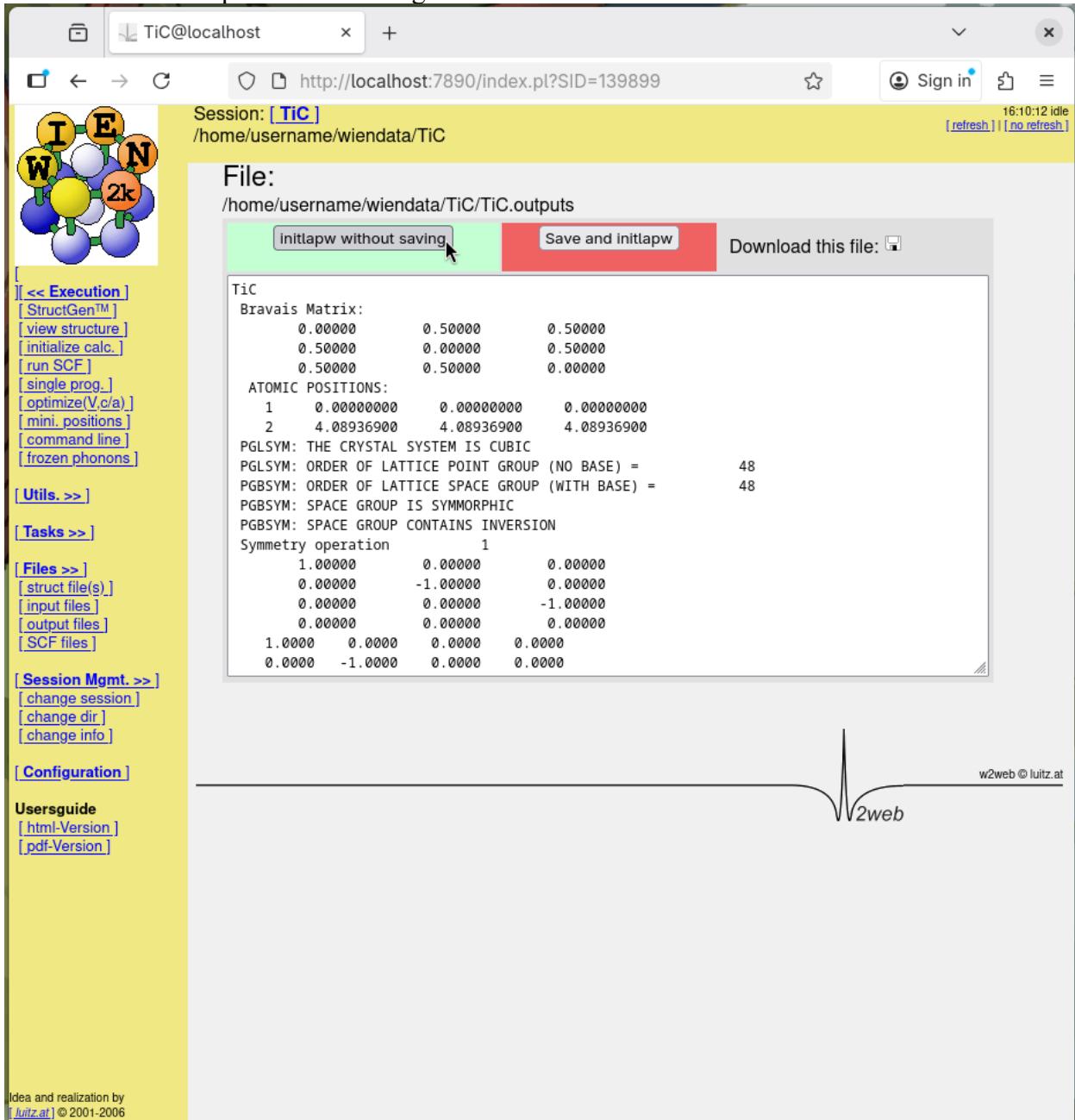
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39. Click the “x symmetry” button

40. Click the “initlapw” button:

The screenshot shows a web browser window titled "TiC@localhost" with the URL "http://localhost:7890/index.pl?SID=139899". The session is identified as "TiC" at "/home/username/wiendata/TiC". The commandline is set to "x symmetry" and the program input is empty. A message indicates that the space group contains inversion. Below this, there is a "Continue with" section containing a button labeled "initlapw" which has a mouse cursor hovering over it. On the left side of the interface, there is a sidebar with various navigation links such as "Execution", "StructGen™", "view structure", "initialize calc.", etc. At the bottom of the sidebar, there are links for "Session Mgmt.", "Configuration", and "Usersguide". The footer of the page includes a copyright notice for "luitz.at" from 2001-2006.

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



The screenshot shows a web browser window for the WiEN2k software. The title bar says "TiC@localhost". The address bar shows "http://localhost:7890/index.pl?SID=139899". The session name is "TiC" and the path is "/home/username/wien2k/TiC". The status bar at the top right says "16:10:12 idle [refresh] || [no refresh]".

File:
 /home/username/wien2k/TiC/TiC.outputs

Buttons at the top of the output area:

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

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]
 - [command line]
 - [frozen phonons]
- [Utils. >>]
- [Tasks >>]
- [Files >>]
 - [struct file(s)]
 - [input files]
 - [output files]
 - [SCF files]
- [Session Mgmt. >>]
 - [change session]
 - [change dir]
 - [change info.]
- [Configuration]
- Usersguide
 - [html-Version]
 - [pdf-Version]

Bottom footer:

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2web

43. Click the “instgen_lapw” button

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

The screenshot shows a web-based graphical user interface for a computational chemistry application. The title bar reads "TiC@localhost". The URL in the address bar is "http://localhost:7890/index.pl?SID=139899". The session name is "TiC" and the path is "/home/username/wiendata/TiC". The status bar at the top right shows "16:10:42 idle [refresh] || [no refresh]".

Main Panel Content:

- Session Information:** Session: [TiC], /home/username/wiendata/TiC
- Message:** instgen_lapw needs input
- Section:** Specify options for instgen_lapw
- Configuration:** 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 Configuration:**
 - atom 1: Ti
 - atom 2: C
- Buttons:** Execute! (highlighted with a mouse cursor)

Left Sidebar (Navigation):

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

Bottom Footer:

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

45. Click the “initlapw” button:

The screenshot shows a web browser window for 'TiC@localhost' at 'http://localhost:7890/index.pl?SID=139899'. The session is labeled 'TiC' and the path is '/home/username/wiendata/TiC'. The commandline is 'instgen_lapw -s -nm' and the program input is '"u u"'. The message area indicates '2 Atoms found: with labels Ti C' and 'generate atomic configuration for atom 1 : Ti' and 'generate atomic configuration for atom 2 : C'. Below this, there is a 'Continue with' section containing a 'initlapw' button, which is highlighted with a mouse cursor. To the right of the button, there is a logo for 'w2web' with the text 'w2web © luitz.at'. On the left side of the page, there is a sidebar with various links under categories like Execution, Utilities, Tasks, Files, Session Management, and Configuration. At the bottom left, there is 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 "http://localhost:7890/index.pl?SID=139899". The session is identified as "Session: [TiC] /home/username/wiendata/TiC". A "Sign in" button is visible in the top right. The main content area displays a molecular model of TiC (Titanium Carbide) with atoms labeled T, C, W, N, and E. Below the model, a sidebar lists various execution and management options. The central panel contains sections for selecting the Exchange Correlation Potential (PBE-GGA) and specifying energy for core separation (-6.0 Ry). An "Execute!" button is highlighted with a cursor. The bottom right corner features a logo for "w2web © luitz.at".

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

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

Execution Options:

- [<< Execution]
 - [StructGen™]
 - [view structure]
 - [initialize calc.]
 - [run SCF]
 - [single prog.]
 - [optimize(V,c/a)]
 - [mini_positions]
 - [command line]
 - [frozen phonons]
- [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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48. Click the “initlapw” button:

TiC@localhost

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

16:11:13 idle
[\[refresh\]](#) || [\[no refresh\]](#)

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 0.004s 0:00.06 83.3% 0+0k 1176+968io 1pf+0w

Continue with

initlapw

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

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

The screenshot shows a web-based graphical user interface for a molecular simulation program. The title bar reads "TiC@localhost". The main content area displays a 3D ball-and-stick model of a TiC unit cell, featuring large yellow spheres labeled "Ti" and smaller orange spheres labeled "C". The URL in the address bar is "http://localhost:7890/index.pl?SID=139899".

The session information is shown as "Session: [TiC] /home/username/wiendata/TiC". The status bar at the top right indicates "16:11:13 idle" and provides links for "refresh" and "no refresh".

A file browser window is open, showing the path "/home/username/wiendata/TiC/TiC.outputst". It contains the following output text:

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

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

- [<< Execution]
- [StructGen™]
- [view structure]
- [initialize calc.]
- [run SCF]
- [single prog.]
- [optimize(V,c/a)]
- [mini_positions]
- [command line]
- [frozen phonons]

Utils. >>

Tasks >>

Files >>

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

Session Mgmt. >>

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

Configuration

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

In the bottom right corner, there is a stylized logo with the text "w2web" and "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:

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

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

initlapw without saving Save and initlapw Download this file:

```

WFFIL EF= 0.50000      (WFFIL, WFPRI, ENFIL, SUPWF)
 7.00   10   4   ELPA ppxq BL 64 (R-MT*K-MAX,MAX L IN WF,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

```

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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 recprlist
  
```

Execution

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

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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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" with the URL "http://localhost:7890/index.pl?SID=139899". The session name is "TiC" and the path is "/home/username/wiidata/TiC". The status bar indicates "16:12:43 idle [refresh] || [no refresh]".

The main content area displays various configuration options for a calculation, including:

- 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)

A red box highlights the message "Your input seems to be ok and you can start the initialization" and the "RUN BATCH INITIALISATION" button.

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.

The "Individual mode" section contains several buttons:

- 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 outputsgroup
- Perform spin-polarized calc.?
- x symmetry
- check TiC.in2_st set Fermi-method and GMAX
- copy struct_st and view outputs
- in0, in1, in2, inc and inm files generated
- x instgen_lapw TiC.inst exists, run instgen_lapw only for non-default spin-configuration
- x lstart
- x kgen
- x view klist
- x dstart interactively
- x view outputs

A red box highlights the "x kgen" button. A tooltip for "x kgen" says "view TiC.outputn and cp TiC.in0_std TiC.in0". A mouse cursor is hovering over the "Perform spin-polarized calc.?" button.

At the bottom right, there is a logo for "w2web" and the text "w2web © luitz.at".

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57. Click the “x kgen” button

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

The screenshot shows a web browser window titled "TiC@localhost" with the URL "http://localhost:7890/index.pl?SID=139899". The session name is "TiC" and the path is "/home/username/wiendata/TiC". The status bar indicates "16:13:13 idle" and provides links for "[refresh]" and "[no refresh]".

The main content area displays a molecular model of TiC with atoms labeled T, C, W, N, E, and 2k. Below the model, there are several execution-related buttons:

- Execution**: Includes links for "StructGen™", "view structure", "initialize calc.", "run SCF", "single prog.", "optimize(V,c/a)", "mini_positions", "command line", and "frozen phonons".
- Utils. >>**
- Tasks >>**
- Files >>**: Includes links for "struct file(s.)", "input files", "output files", and "SCF files".
- Session Mgmt. >>**: Includes links for "change session", "change dir", and "change info".
- Configuration**
- Usersguide**: Includes links for "html-Version" and "pdf-Version".

In the center, there is a form field labeled "Number of k-points" containing the value "1000". Below it is a dropdown menu "Shift k-mesh (if applicable)" set to "Yes". 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. A large "Execute!" button is prominently displayed.

On the right side of the interface, there is a watermark-like logo for "w2web" with the URL "w2web @ luitz.at".

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

59. Click the “initlapw” button:

The screenshot shows a web browser window titled "TiC@localhost". The URL is "http://localhost:7890/index.pl?SID=139899". The session name is "TiC" and the path is "/home/username/wiendata/TiC". The status bar indicates "16:13:13 idle" and "[refresh] || [no refresh]".

Molecular Structure: On the left, there is a 3D ball-and-stick model of a molecule with atoms labeled T, E, N, W, and 2k.

Commandline: The commandline is "x kgen" and the program input is "1000 1".

Output:

```
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
0.007u 0.003s 0:00.01 0.0% 0+0k 0+200io 0pf+0w
```

Buttons: A "Continue with" section contains a button labeled "initlapw" which is highlighted with a mouse cursor.

Navigation: The left sidebar lists various menu items such as "Execution", "StructGen™", "view structure", "initialize calc.", etc. Other sections include "Files >>", "Session Mgmt. >>", and "Configuration".

Footer: The footer includes a copyright notice: "Idea and realization by [luitz.at](#) © 2001-2006".

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, div:	(10	10								
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															

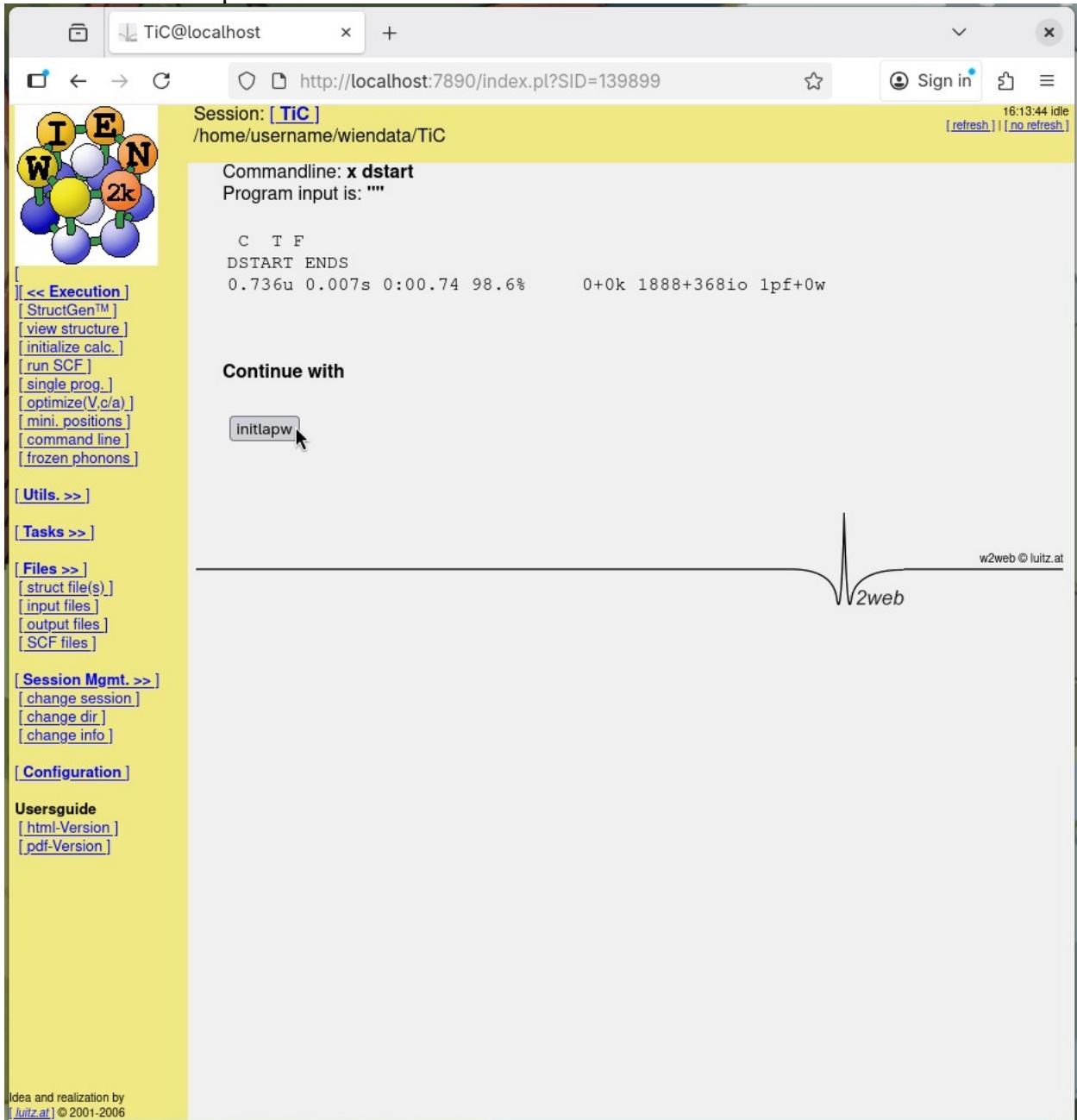
16:13:44 idle
[\[refresh\]](#) || [\[no refresh\]](#)

File menu options: initlapw without saving, Save and initlapw, Download this file.

Left sidebar links: Execution, Structure, View, Initialize calc., Run SCF, Single prog., Optimize, Mini positions, Command line, Frozen phonons, Utils, Tasks, Files, Session Mgmt., Configuration, Usersguide (html, pdf), and Luitz.at info.

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



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

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

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

File:
/home/username/wien2k/TiC/TiC.outputd

initlapw without saving Save and initlapw Download this file:

```
rmt(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, nmeig = 251
:NT0001: CHARGE SPHERE 1 = 19.823810
```

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Execution

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

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

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

Perform spin-polarized calc.?

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

TiC@localhost

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

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.outputnn and cp TIC.in0_std TIC.in0
view outputnn		check if gmax>gmin
x sgroup	check TIC.in2_st set Fermi-method and GMAX	
view outputsgroup		Prepare input files
x symmetry		
copy struct_st and view outputs		
instgen_lapw	TiC.inst exists, run instgen_lapw only for non-default spin-configuration	
	x kgen	
	view klist	
x lstart	x dstart	✓ interactively
view outputst		

Initialization done

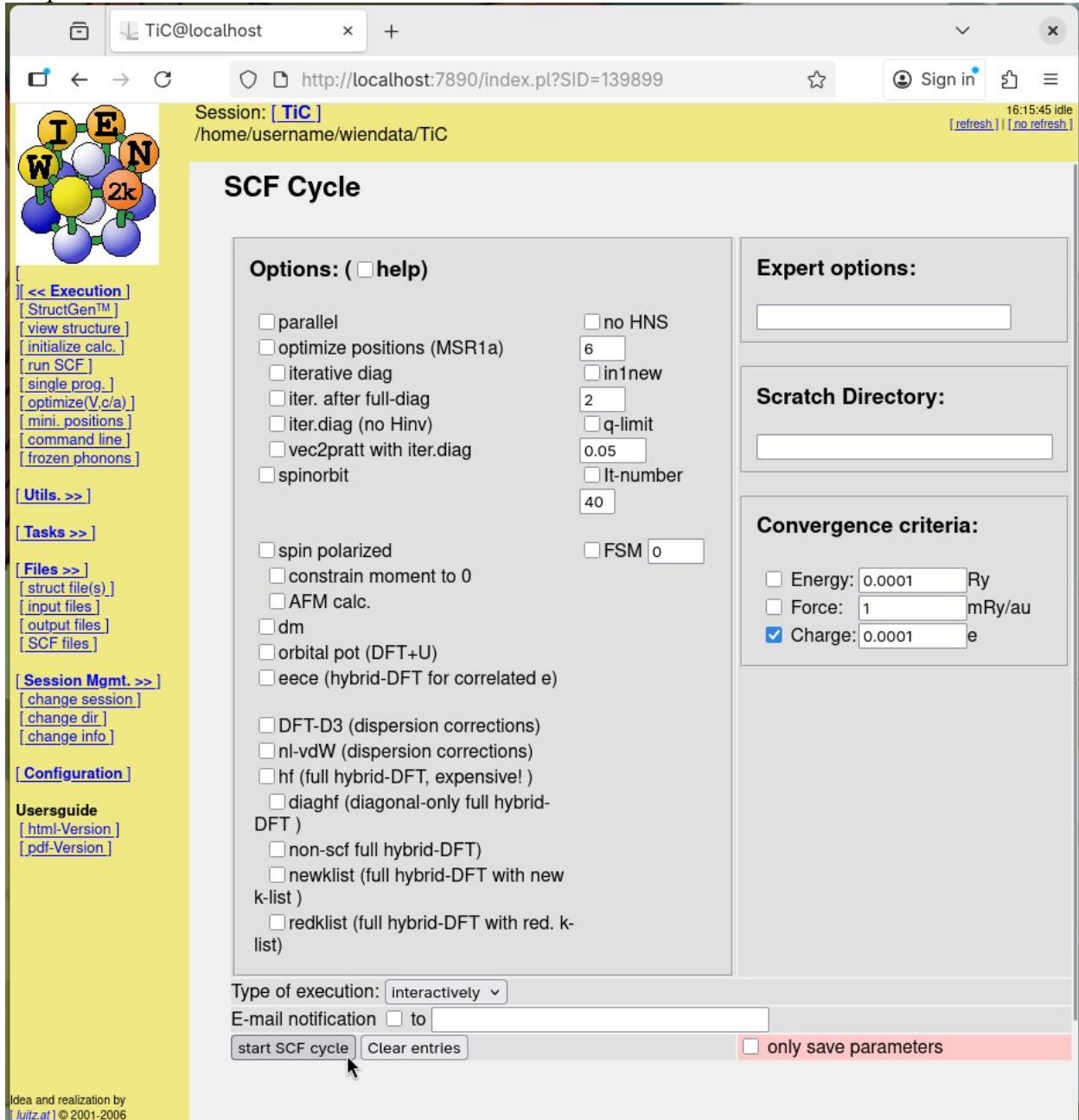
[Continue with run SCF]

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http://localhost:7890/exec/scf.pl?SID=139899

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
16:16:16 [running] (lapw0)
[refresh] || [no refresh]

LAPW1 END
LAPW2 END
CORE END
MIXER END
ec cc fc and str_conv 1 0 1 1
in cycle 8      ETEST: .0004534950000000    CTEST: .1361612    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: .0396236    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: .0002063600000000    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:

The screenshot shows the TiC@localhost web interface. On the left, there's a sidebar with a molecular model icon and a list of tasks: Execution >>, StructGen™, view structure, initialize calc., run SCF, single prog., optimize(V,c/a), mini_positions, Utils. >>, << Tasks, El. Dens. (which is selected), DOS, XSPEC, TELNES3, OPTIC, Bandstructure, 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). At the bottom of the sidebar, it says "Idea and realization by [luitz.at](#) © 2001-2006".

The main content area has a yellow header bar with "Session: [TiC]" and "http://localhost:7890/index.pl?SID=139899". It also shows the current time "16:16:47 idle" and refresh/no refresh buttons.

The main content starts with "Electron density plots". A message box says: "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, a note says: "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".

There are two buttons: "view TiC.scf1" and "view TiC.scf2". Below them is a form with a button labeled "x lapw2" which is being clicked. The form says: "Calculate clmval with Emin [-1.0] and Emax [] so".

Below the form, there's a note: "For difference densities only !". It has two sections: "default valence states:" and "non-default valence states:". Under "default valence states:", there's a button "edit TiC.inst" followed by "put P for all your states". Under "non-default valence states:", there's a button "edit TiC.in5" followed by "put P for all your states".

Further down, there are buttons for "x lstart -sigma" (Calculate atomic valence densities) and "x lstart" (Calculate atomic valence densities as defined above). There's also a button "Calculate density with XCrysDen" (or create TiC.in5 / execute lapw5 below).

Below that, there's a button "edit TiC.in5" followed by "Edit input-file and select the appropriate option for lapw5 below".

At the bottom, there's a button "x lapw5 -val" followed by "Calculate density with: -diff -val/-tot -pot/-coulomb/-exchange(2)/-halfR2v/-tau -sub/-add/-none". There's also a button "View density with XCrysDen" and a button "rhoplot" followed by "Plot Density or download [\[TiC.rho\]](#) for plotting with your own plotting program".

In the bottom right corner, it says "w2web © luitz.at".

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

The screenshot shows a web browser window for 'TiC@localhost' at the URL <http://localhost:7890/index.pl?SID=139899>. The session is labeled 'Session: [TiC] /home/username/wiendata/TiC'. The commandline used was `x lapw2 -emin -1.0` and the program input was empty. The LAPW2 calculation has ended with a total time of 0.226u, 0.117s, and 97.0% completion. The output includes statistics like 0+0k, 0+552io, 0pf+0w.

The main area displays a molecular structure diagram with atoms labeled T, E, N, W, and 2k. Below the diagram is a 'Continue with' section containing a button labeled 'continue with electron density'. A cursor arrow points to this button.

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]

At the bottom left, it says 'Idea and realization by [\[luitz.at\]](#) © 2001-2006'. On the right side, there is a small logo with the text 'w2web @ luitz.at' and '2web'.

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 <http://localhost:7890/index.pl?SID=139899>. The page displays the contents of the file 'TiC.in5' with several lines highlighted in red. The highlighted lines are:

```

-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
ORTHO             # optional: ORHO|NONORTHO plotting directions

```

The 'Save and continue with electron density' button is highlighted with a red box and a cursor is hovering over it. The page also includes a sidebar with various session management and configuration options.

77. Click the “x lapw5” button

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

The screenshot shows a web browser window titled "TiC@localhost". The URL is "http://localhost:7890/index.pl?SID=139899". The session name is "TiC" and the path is "/home/username/wiendata/TiC". The commandline is "x lapw5 -val" and the program input is empty. The output shows TOT changed to VAL in TiC.in5, DIFF changed to RHO in TiC.in5, and execution statistics: 0.086u 0.008s 0:00.09 88.8% 0+0k 920+880io 1pf+0w.

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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Session: **x lapw5 -val**
Program input is: ""

TOT changed to VAL in TiC.in5
DIFF changed to RHO in TiC.in5
0.086u 0.008s 0:00.09 88.8% 0+0k 920+880io 1pf+0w

Continue with

continue with electron density

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2web

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”

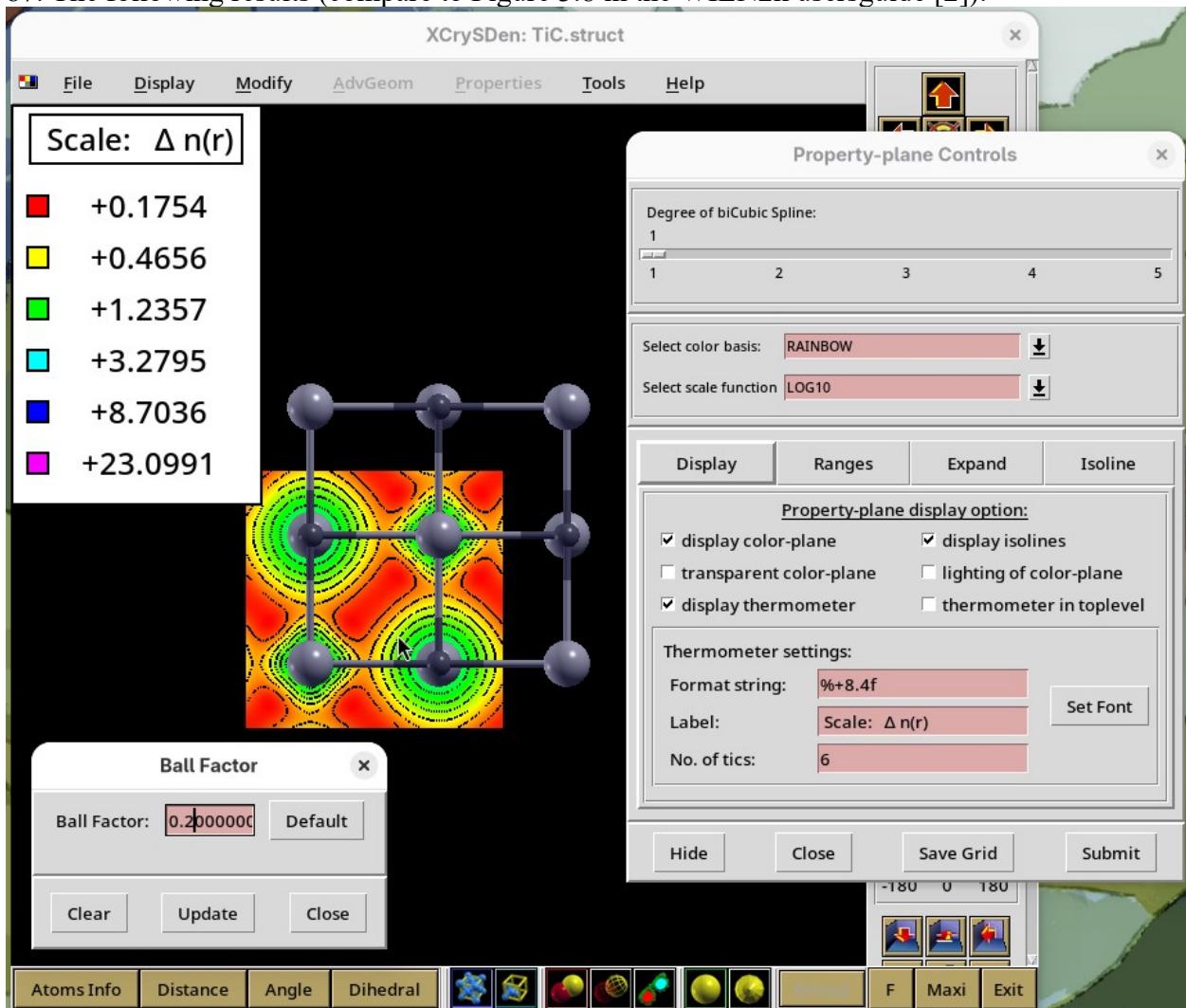
83. Click the “Submit” button

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

16:21:17 idle
[refresh] | [no refresh]

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.

[Show full menu]

We are in rhoplot mode

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

Min Max Delta

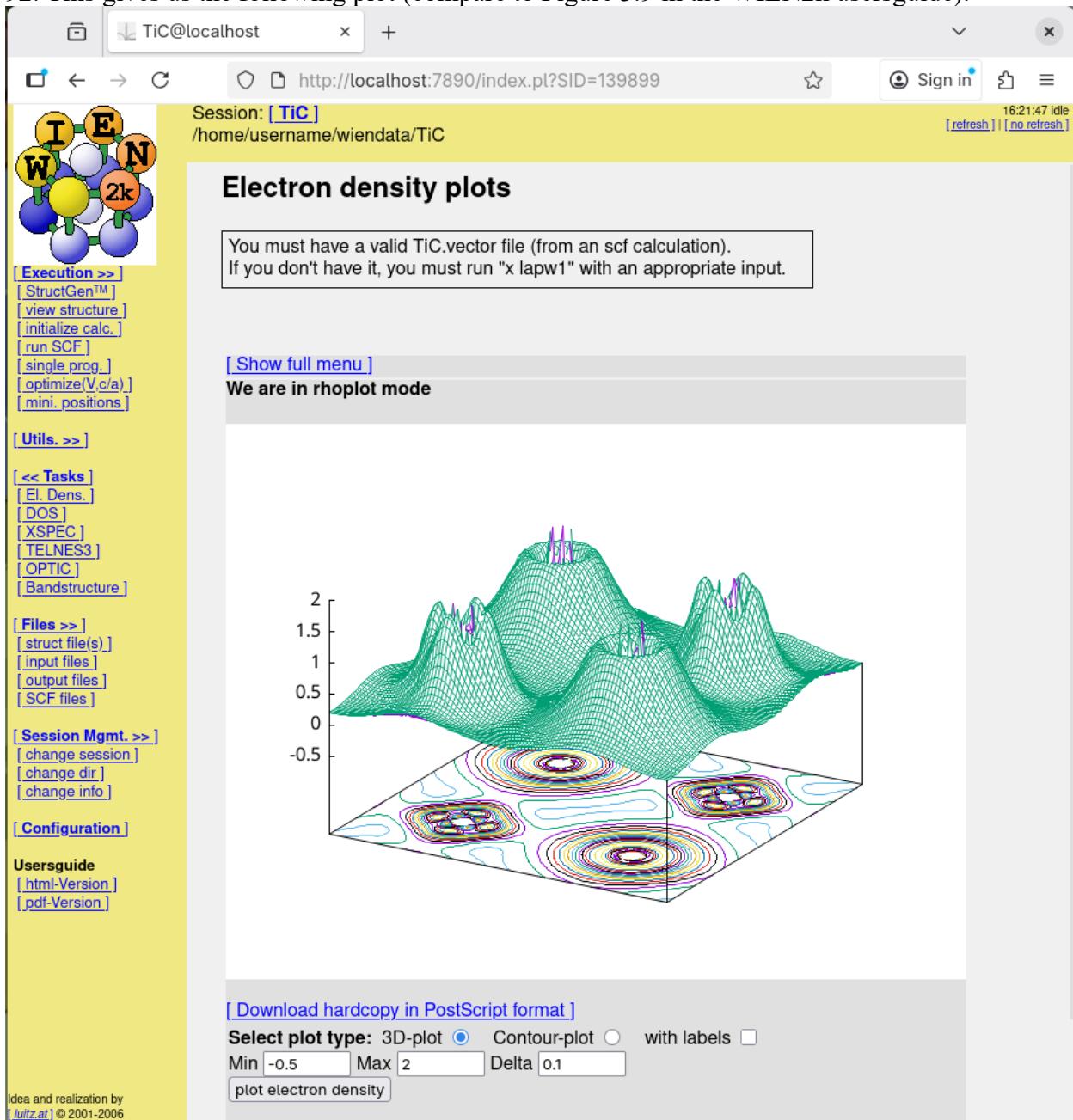
plot electron density

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V2web

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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.int` 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

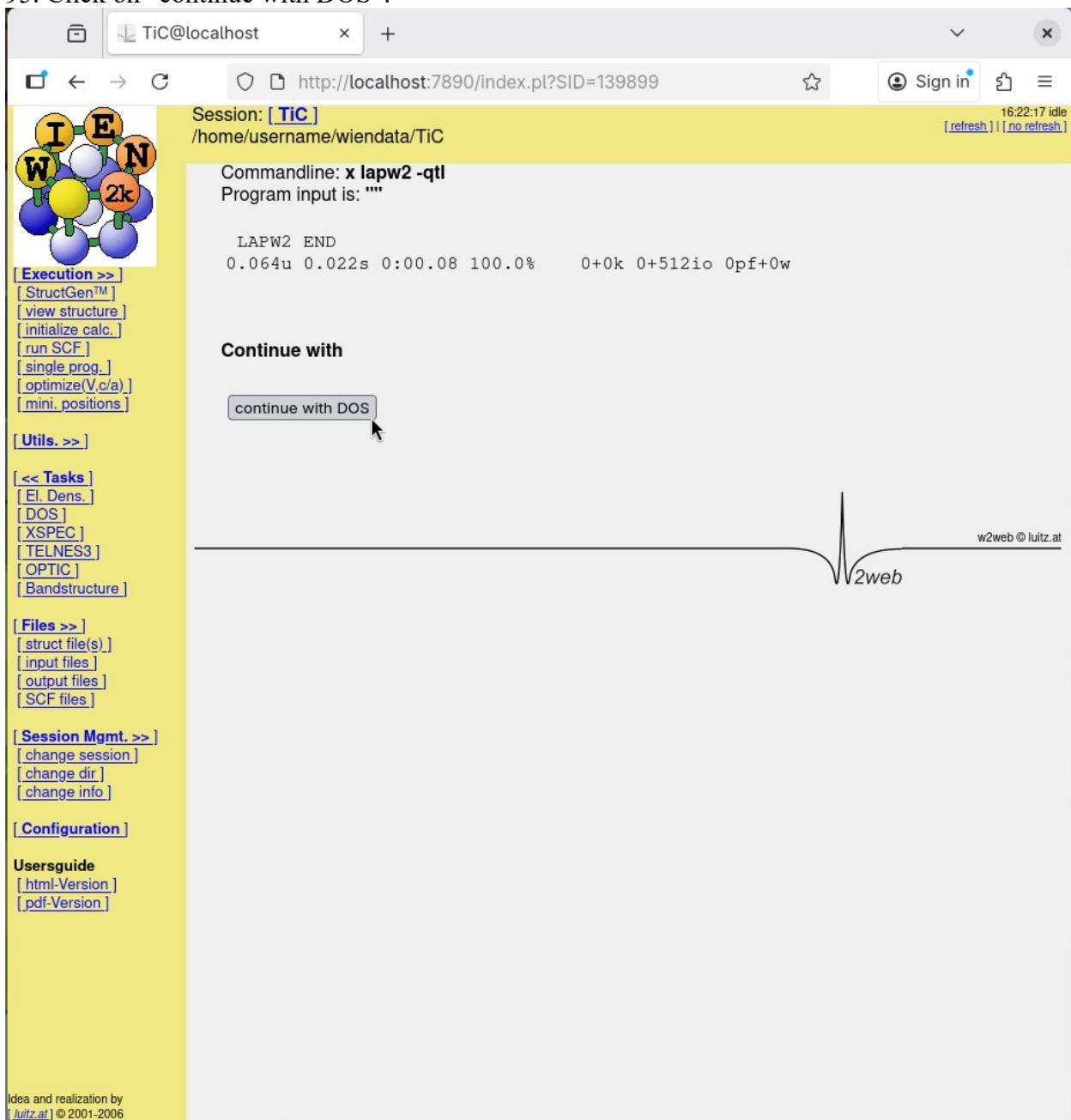
`dosplot` Plot DOS using renormalized DOS or download DOS-data for plotting with your plotting program:

`save_lapw -dos` with name:

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95. Click on “continue with DOS”:



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
```

TiC@localhost

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

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

[continue with DOS without saving](#) [Save and continue with DOS](#) [Download this file:](#)

Header from TiC.qtl:

```

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

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),KSELect=XX
    0    1  total          # 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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2web

98. Click “Save and continue with DOS”

99. Click “x tetra”

100. Click “continue with DOS”:

The screenshot shows a web browser window for 'TiC@localhost' at 'http://localhost:7890/index.pl?SID=139899'. The session is named 'TiC' and is located at '/home/username/wiendata/TiC'. The commandline used is 'x tetra' and the program input is empty. The DOS plot shows a sharp peak at the bottom right labeled '2web'. The interface includes a sidebar with various menu items 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 >>', 'Session Mgmt. >>', and 'Configuration'. A 'Usersguide' section links to 'html-Version' and 'pdf-Version'. At the bottom left, it says 'Idea and realization by luitz.at © 2001-2006'. A watermark 'w2web © luitz.at' is visible on the right.

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

16:24:19 idle
 [refresh] || [no refresh]

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

DOS for tetrahedra around K= -1
 covered volume (%) 100.000000000000
 LEGAL END TETRA
 0.011u 0.004s 0:00.01 100.0% 0+0k 864+624io 1pf+0w

Continue with

continue with DOS

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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”:

TiC@localhost

Session: [TiC] /home/username/wiendata/TiC 16:55:00 idle
[refresh] | [no refresh]

Density of states

We are in Dosplot mode:

Set ranges (optional):
xmin= -13 xmax= 9 ymin= ymax= 4 PLOT

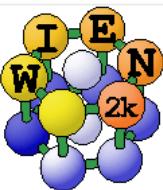
You can select from 6 DOS in TiC.int . Please select up to 4 lines to plot.

no line	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
line:1 (total DOS) of TiC	<input checked="" type="radio"/>	<input type="radio"/>	<input type="radio"/>
line:2 (d) of atom Ti	<input type="radio"/>	<input checked="" type="radio"/>	<input type="radio"/>
line:3 (d-eg) of atom Ti	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
line:4 (d-t2g) of atom Ti	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
line:5 (s) of atom C	<input type="radio"/>	<input checked="" type="radio"/>	<input type="radio"/>
line:6 (p) of atom C	<input type="radio"/>	<input type="radio"/>	<input checked="" type="radio"/>

Define for first line: Label= Linetype(0-9)=1 Linewidth=1
 Define for second line: Label= Linetype(0-9)=2 Linewidth=2
 Define for third line: Label= Linetype(0-9)=3 Linewidth=2
 Define for fourth line: Label= Linetype(0-9)=4 Linewidth=2

Plot DOS in eV Color Labelszie= 24 pt

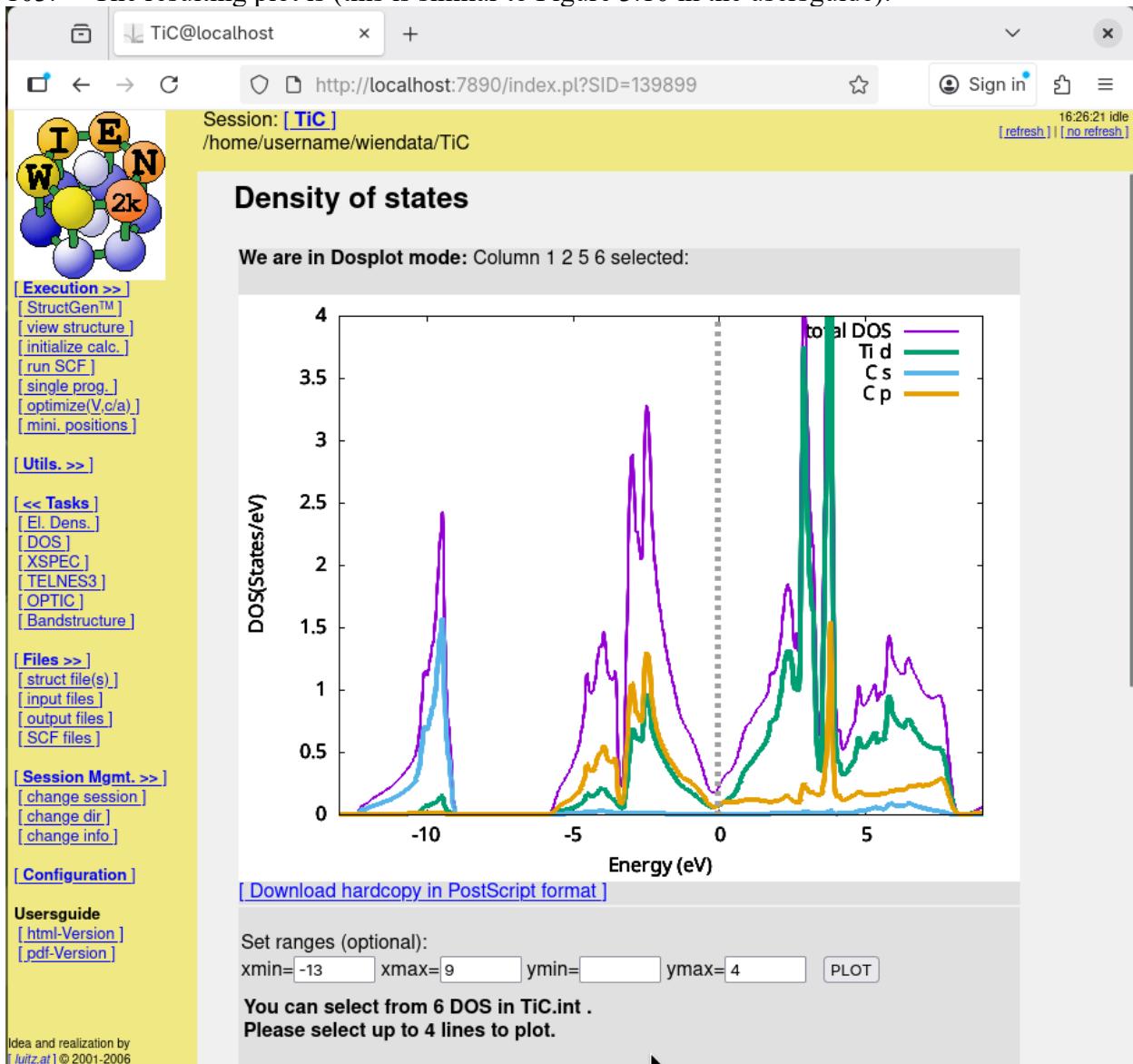
Show full menu save_lapw -dos with name:



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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 TiC@localhost web interface for a session named "TiC". The left sidebar has a yellow background with various links. The main area is titled "XSPEC" and contains several input fields with checkboxes. The "x lapw2 -qtl" field is highlighted with a mouse cursor. At the bottom, there is a plot of a partial charge distribution.

106. Click “continue with xspec”:

The screenshot shows a web browser window for 'TiC@localhost' at the URL <http://localhost:7890/index.pl?SID=139899>. The session is labeled 'Session: [TiC] /home/username/wiendata/TiC'. The commandline is 'x lapw2 -qtl' and the program input is ''. The output shows 'LAPW2 END' with various statistics. On the right, there is a small plot of a band structure with a peak labeled '2web'. 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 about the realization by 'luitz.at'.

Continue with

[continue with xspec](#)

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2web

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

107. Click “x xspec”

108. Click “continue with xspec”:

The screenshot shows a web browser window for 'TiC@localhost' at 'http://localhost:7890/index.pl?SID=139899'. The session is titled '[TiC]' and is located at '/home/username/wiendata/TiC'. The status bar indicates '16:27:21 idle [refresh] | [no refresh]'. On the left, there's a molecular model with atoms labeled T, E, N, W, and 2k. A sidebar contains links for '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', and 'Usersguide' (with links to 'html-Version' and 'pdf-Version'). The main content area displays a command-line log:

```

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

Commandline: x xspec
Program input is: ""

Start INITXSPEC
INIT_XSPEC - done
0.000u 0.002s 0:00.00 0.0%      0+0k 696+16io 1pf+0w
Start TETRA
covered volume (%)    100.000000000000
no broadening
no broadening
no broadening
LEGAL END TETRA
0.010u 0.002s 0:00.01 100.0%     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
0.029u 0.013s 0:00.04 75.0%     0+0k 928+360io 1pf+0w
Start LORENTZ
Lorentz done
0.006u 0.002s 0:00.01 0.0%     0+0k 808+56io 1pf+0w

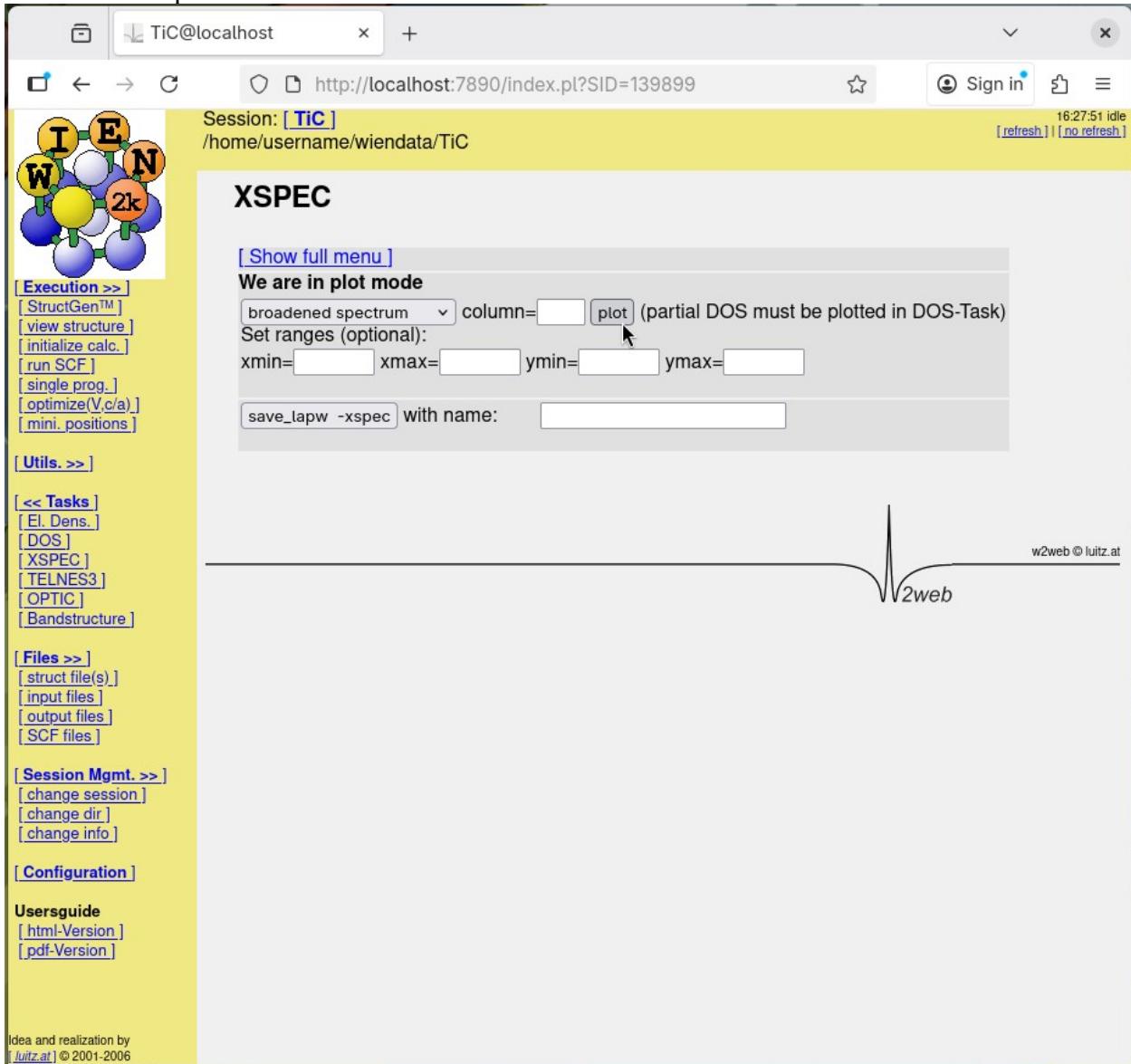
>   stop
>   xspec done
0.066u 0.038s 0:00.11 81.8%     0+0k 2432+792io 3pf+0w

```

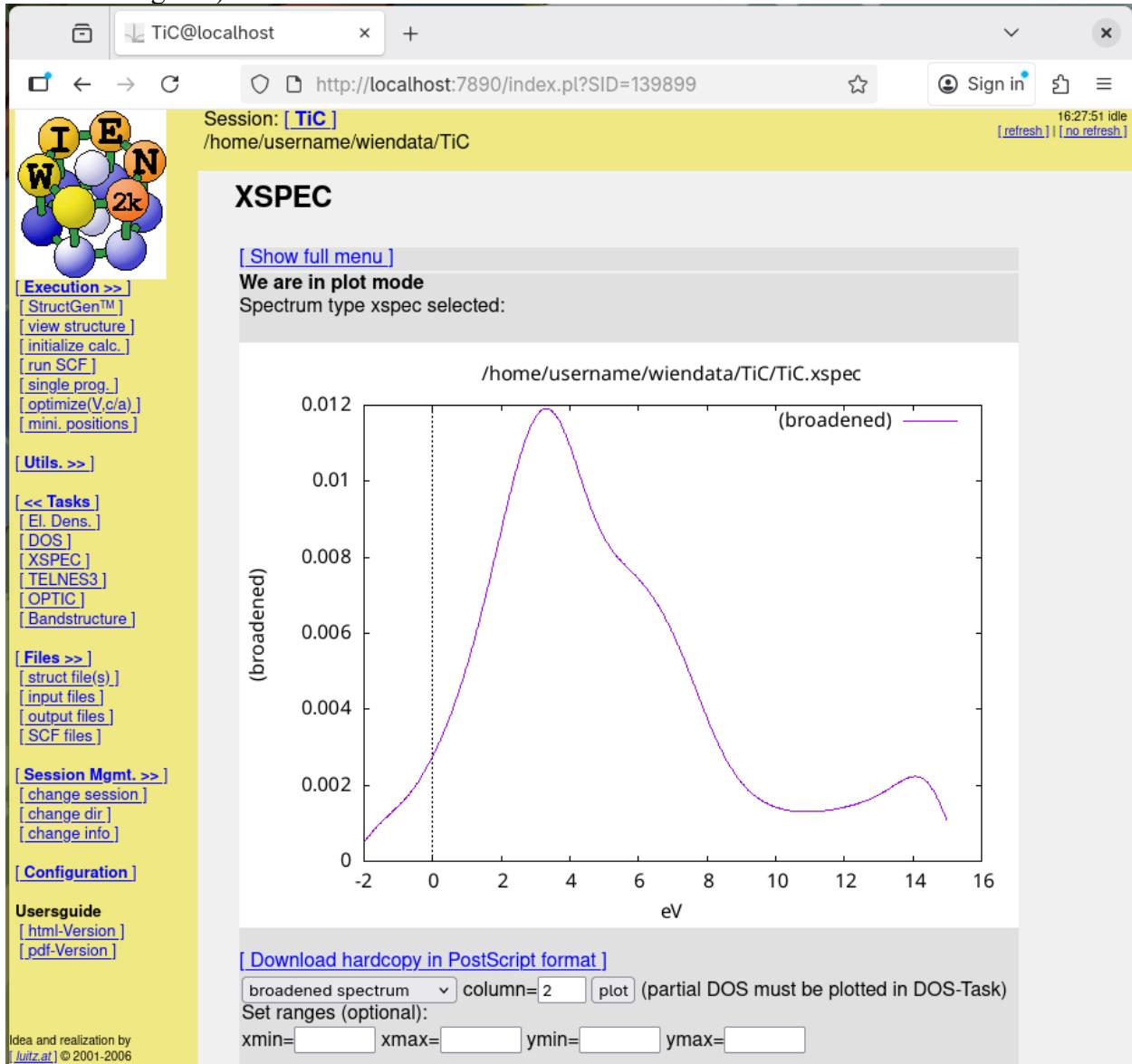
Below the log, a button labeled 'Continue with' has a mouse cursor hovering over it. At the bottom left, it says 'Idea and realization by [Jutz.at](#) © 2001-2006'.

109. Click “plot”

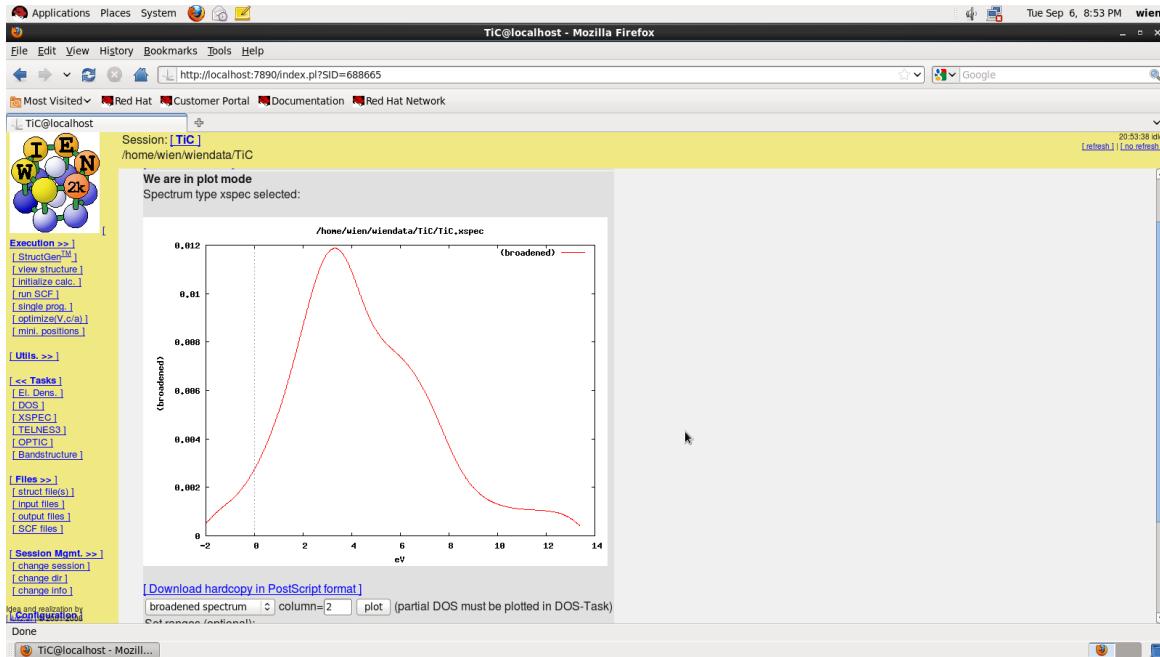
110. Click “plot”:



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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2web

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114. Click on “x lapw1 -band”

115. Click “continue with bandstructure”:

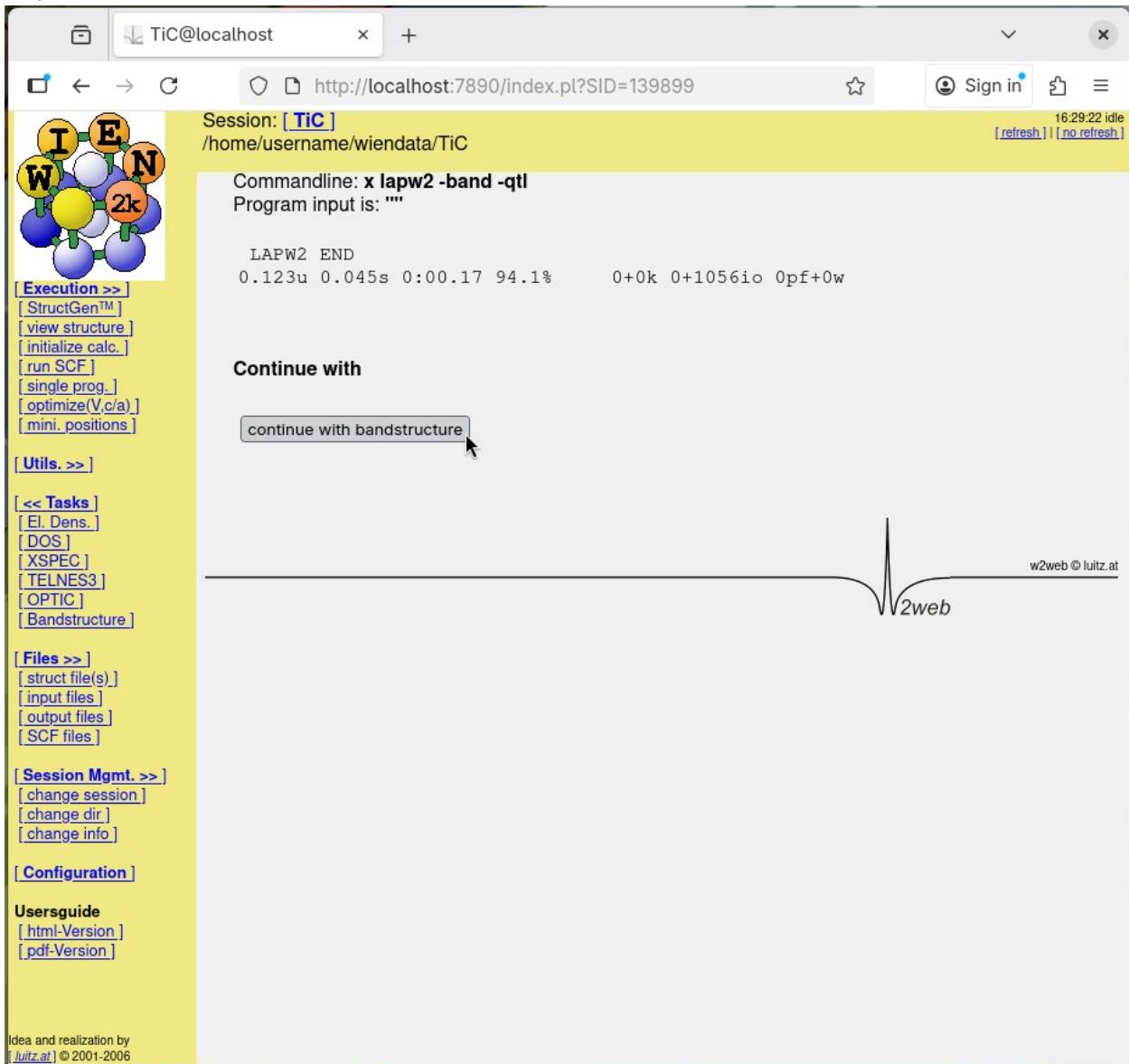
The screenshot shows a web browser window for 'TiC@localhost' at 'http://localhost:7890/index.pl?SID=139899'. The session is named 'TiC' and is located at '/home/username/wiendata/TiC'. The commandline used was 'x lapw1 -band' and the program input was empty. The LAPW1 END section shows statistics: 1.004u 0.286s 0:01.30 98.4% 0+0k 0+5976io 0pf+0w.

Continue with

continue with bandstructure

On the left sidebar, there is a molecular structure diagram with atoms labeled I, E, W, N, and 2k. Below the diagram are several menu options under 'Execution >>': StructGen™, view structure, initialize calc., run SCF, single prog., optimize(V,c/a), mini..positions, and Utils. >>. Under Utils. >>, there are links for El. Dens., DOS, XSPEC, TELNES3, OPTIC, and Bandstructure. Under Files >>, there are links for struct file(s.), input files, output files, and SCF files. Under Session Mgmt. >>, there are links for change session, change dir, and change info. Under Configuration, there is a link to the Usersguide (html-Version and pdf-Version). At the bottom, it says 'Idea and realization by luitz.at © 2001-2006'.

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



The screenshot shows a web browser window titled "TiC@localhost" with the URL "http://localhost:7890/index.pl?SID=139899". The session is named "TiC" and is located at "/home/username/wiendata/TiC". The status bar indicates "16:29:22 idle" and provides links for "[refresh]" and "[no refresh]".

The main content area displays a 3D molecular model of TiC with atoms labeled T, C, N, W, E, and 2k. Below the model is a commandline summary:

```
LAPW2 END
0.123u 0.045s 0:00.17 94.1%    0+0k 0+1056io 0pf+0w
```

Under the heading "Continue with", there is a button labeled "continue with bandstructure" which is being clicked by a mouse cursor.

In the bottom right corner, there is a small logo with the text "w2web @ luitz.at" and "2web".

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

At the bottom of the sidebar, it says "Idea and realization by [luitz.at] © 2001-2006".

118. Edit TiC.insp by clicking “edit TiC.insp”, change jatom to 1, jtype to 6, Fermi energy to 0.7425 (or could enter 0.7429563358 shown on the screen):

The screenshot shows the WiEN2k web interface for the session 'TiC@localhost'. The left sidebar contains various execution and configuration options. The main area shows the configuration file 'TiC.insp' with the following content:

```

## 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:

```

The 'Save and continue with bandstructure' button is highlighted with a red box. The status bar at the top right shows '16:30:22 idle [refresh] [no refresh]'.

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

The screenshot shows a web-based graphical user interface for a computational chemistry application. On the left, there is a sidebar with various menu items such as Execution, Utils., Files, Session Mgmt., Configuration, and Usersguide. The main area displays a molecular model with atoms labeled I, E, N, W, and 2k. Below the model, a command-line session is shown:

```

Session: [TiC]
/home/username/wiendata/TiC
16:30:52 idle
[refresh] | [no refresh]

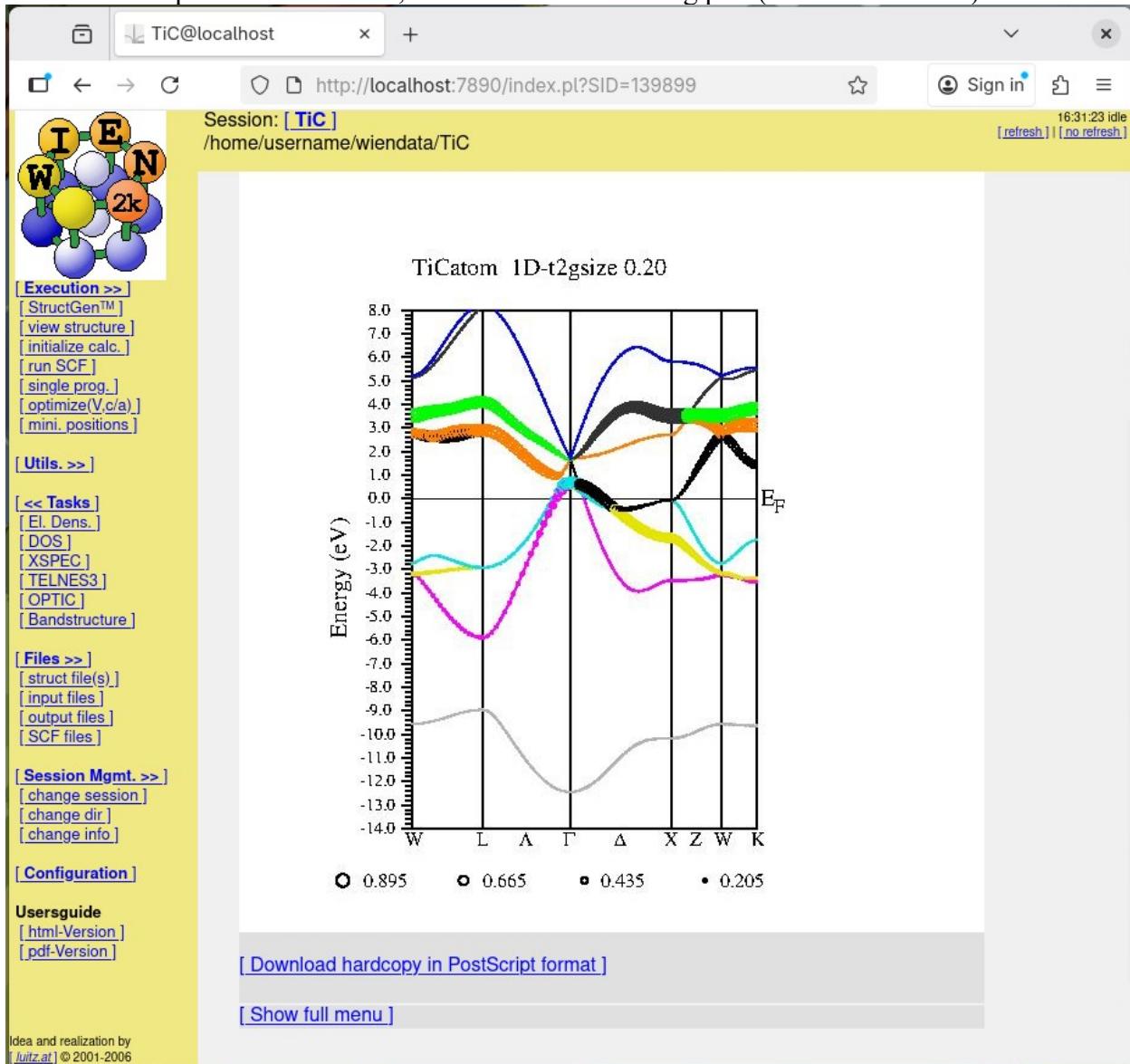
Commandline: x spaghetti
Program input is: ""

SPAGH: Read band energy from case.output1
number of k-points read in case.vector= 111
SPAGH END
0.013u 0.003s 0:00.01 100.0% 0+0k 952+624io 1pf+0w

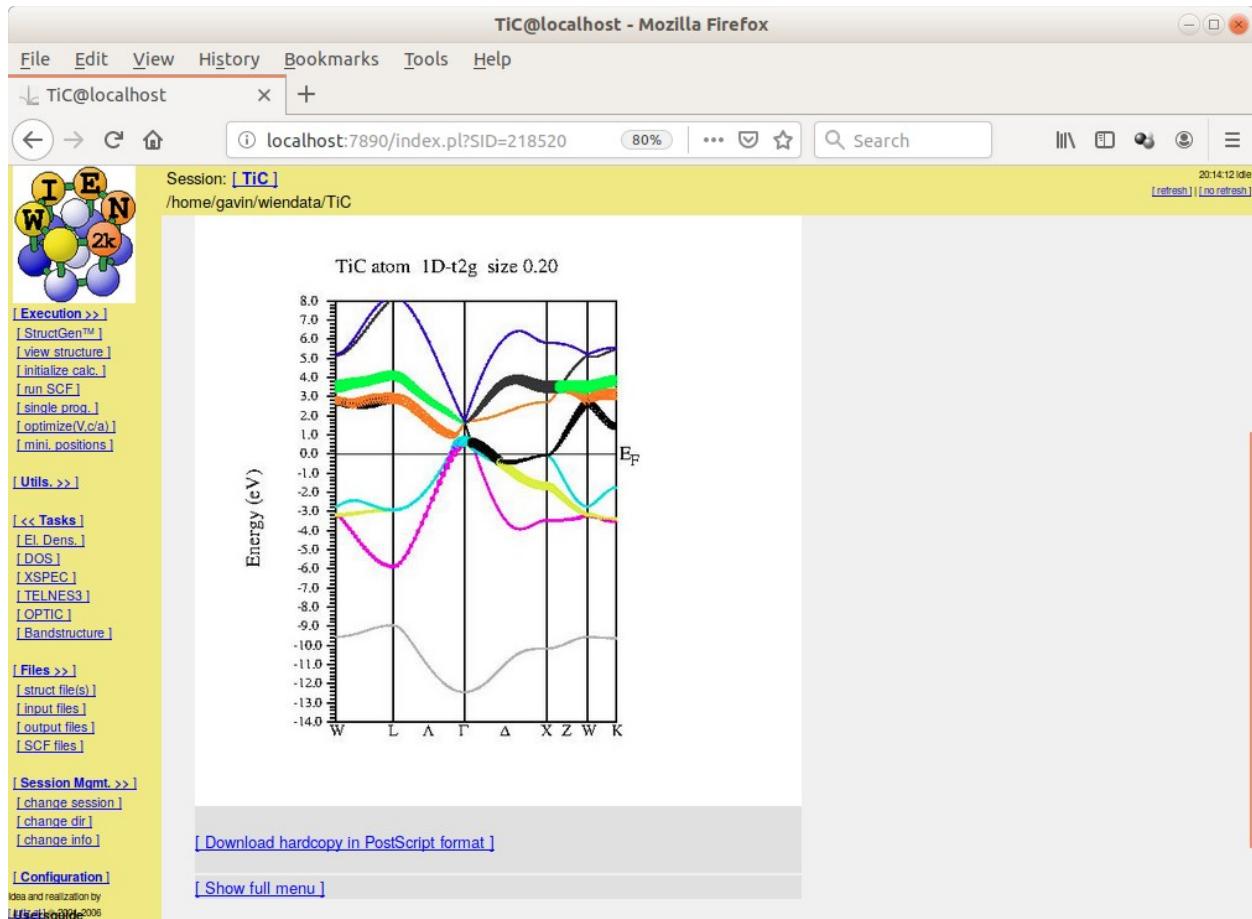
```

Below the command-line session, there is a "Continue with" section containing a button labeled "continue with bandstructure". A cursor arrow is pointing at this button. To the right of the button, there is a small plot of a band structure with a peak labeled "2web".

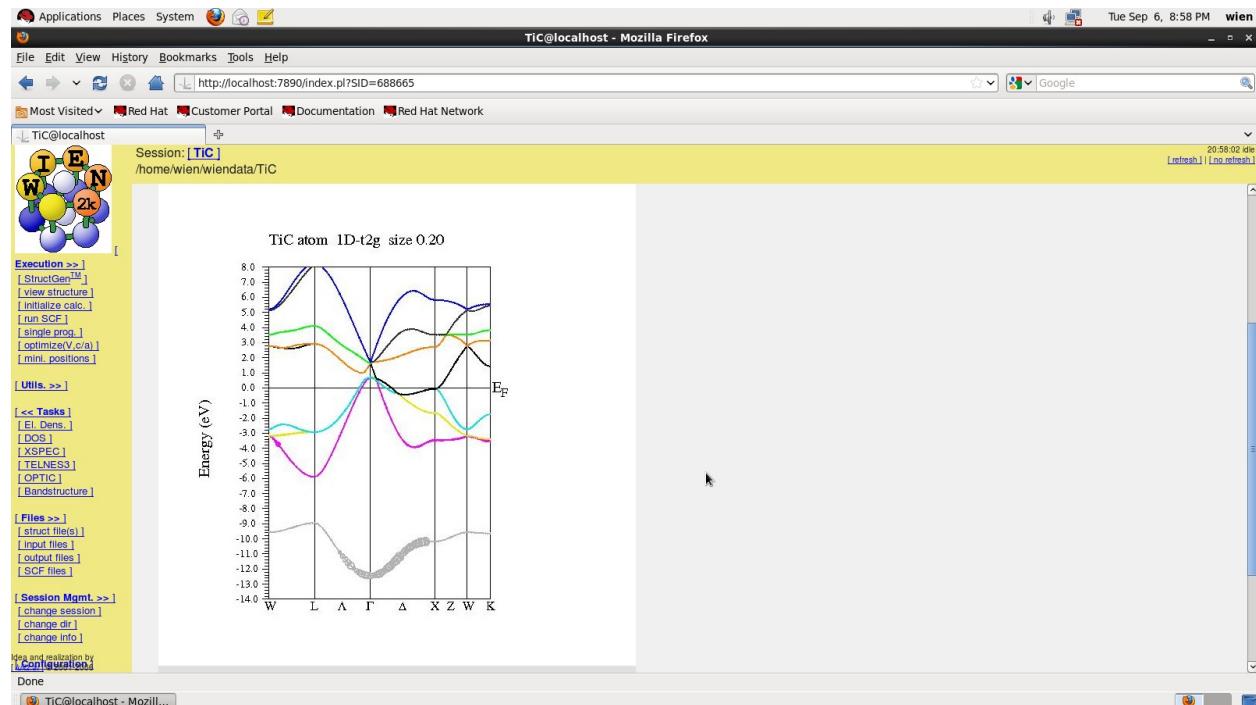
122. Click “plot bandstructure”, the creates the following plot (version 24.1-23.2):



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”:

The screenshot shows the TiC@localhost web interface. The left sidebar contains a molecular model of TiC and a list of execution and utility options. The main panel displays a plot titled "Optimize volume, c/a-ratio, ...". A tooltip for the "x optimize" button is shown, indicating it generates structure files from "TiC.struct". The plot shows a single sharp minimum, characteristic of a diamond cubic lattice. The bottom right corner of the plot area has the text "w2web @ luitz.at" and "w2web".

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

126. Click “Execute!”:

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

optimizer

1) vary VOLUME with constant a:b:c ratio

For option 1-4: specify structure changes in % (each value in separate line)

-10
-5
0
5
10

For option 5: specify number of structures: 6, 9 (3x3), 16 (4x4), 25 (5x5), 36

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

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

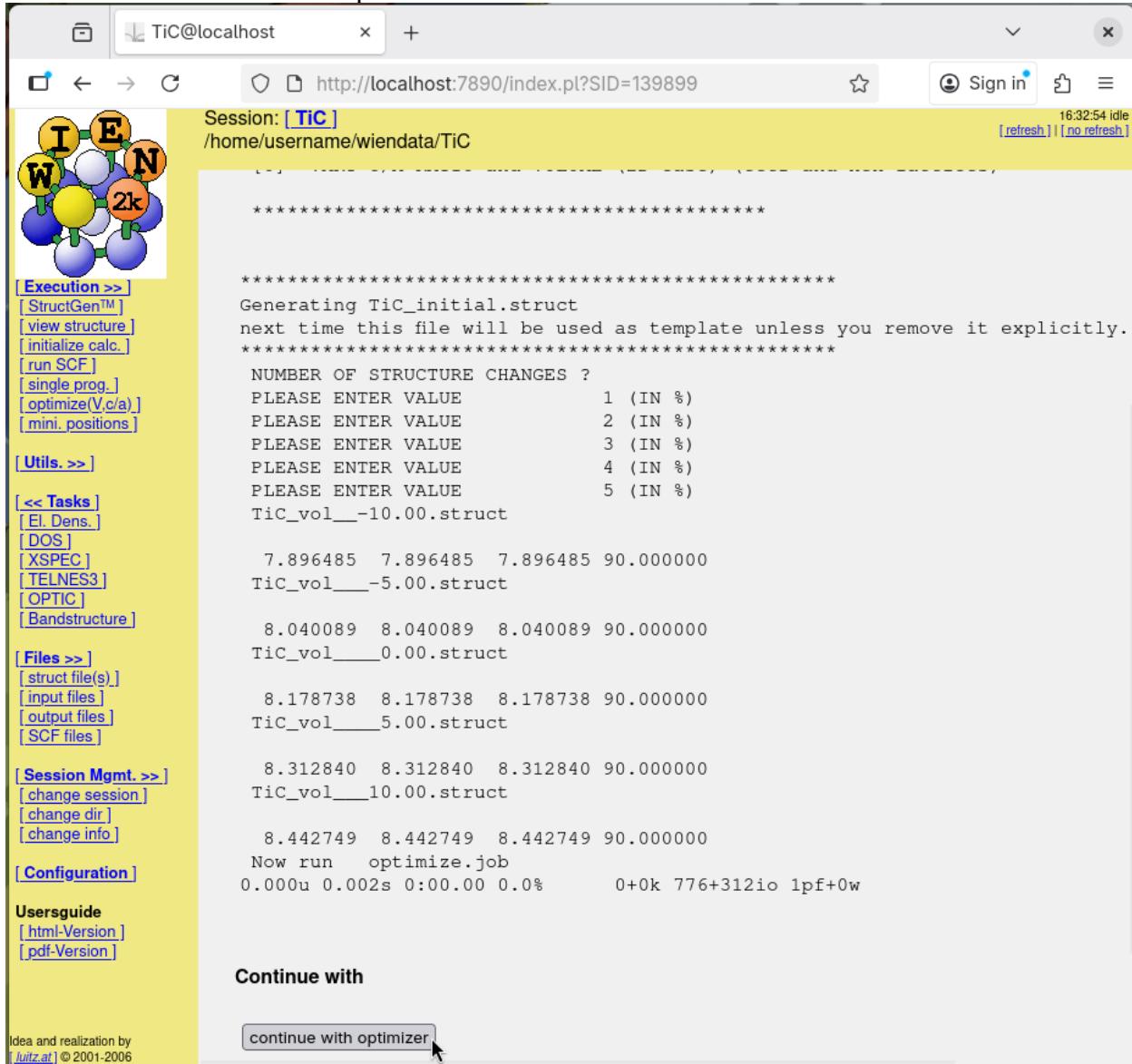
Execute!

w2web © luitz.at

2web

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

127. Click “continue with optimizer”:



The screenshot shows a web browser window for 'TiC@localhost' at 'http://localhost:7890/index.pl?SID=139899'. The session is named 'TiC'.

Molecular Structure: A ball-and-stick model of a molecule with atoms labeled T, E, N, W, and 2k.

Left Sidebar (Navigation):

- 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]

Log Output:

```
*****
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 776+312io 1pf+0w
```

Bottom Buttons:

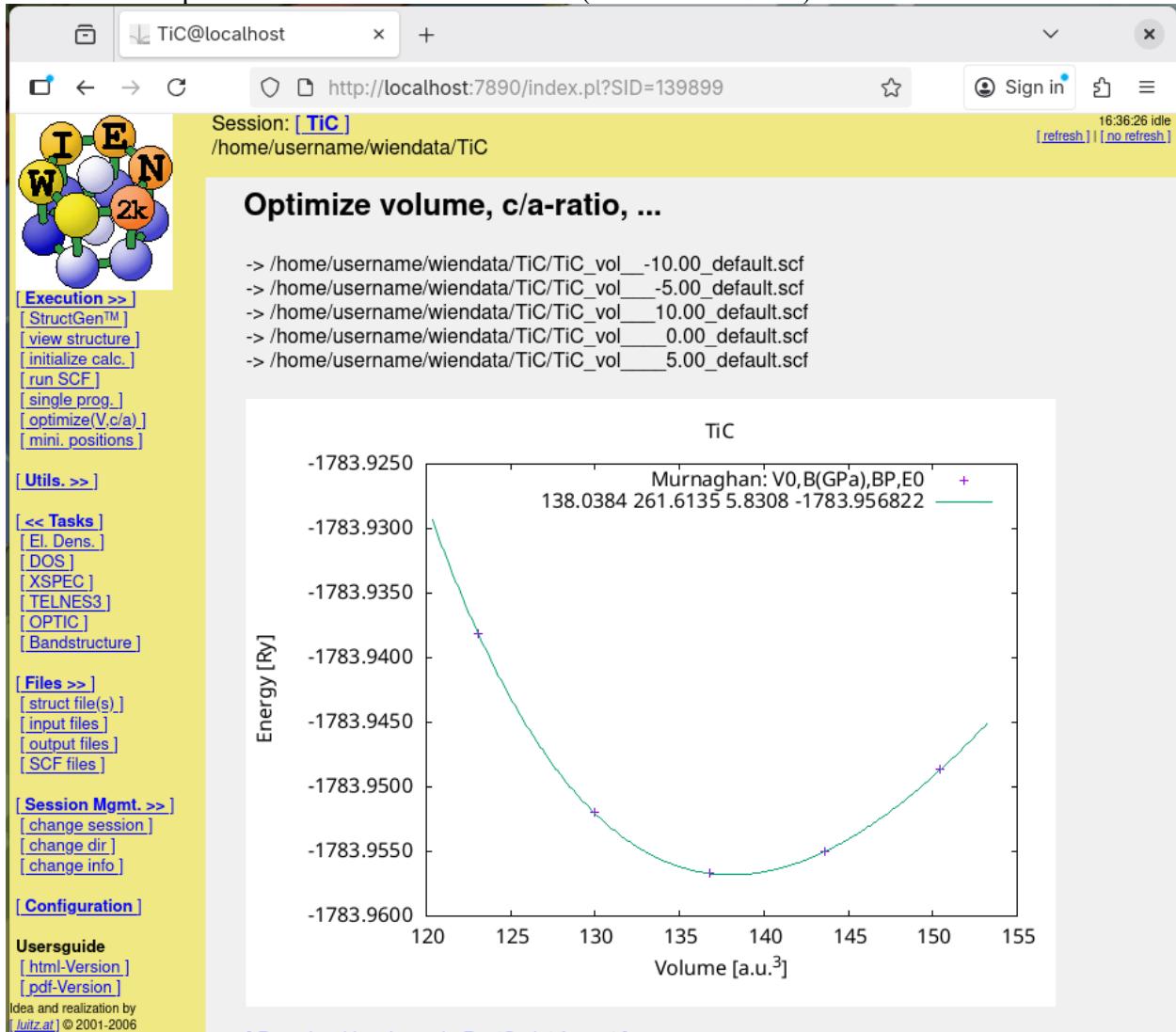
Continue with

128. Click “run optimize.job”

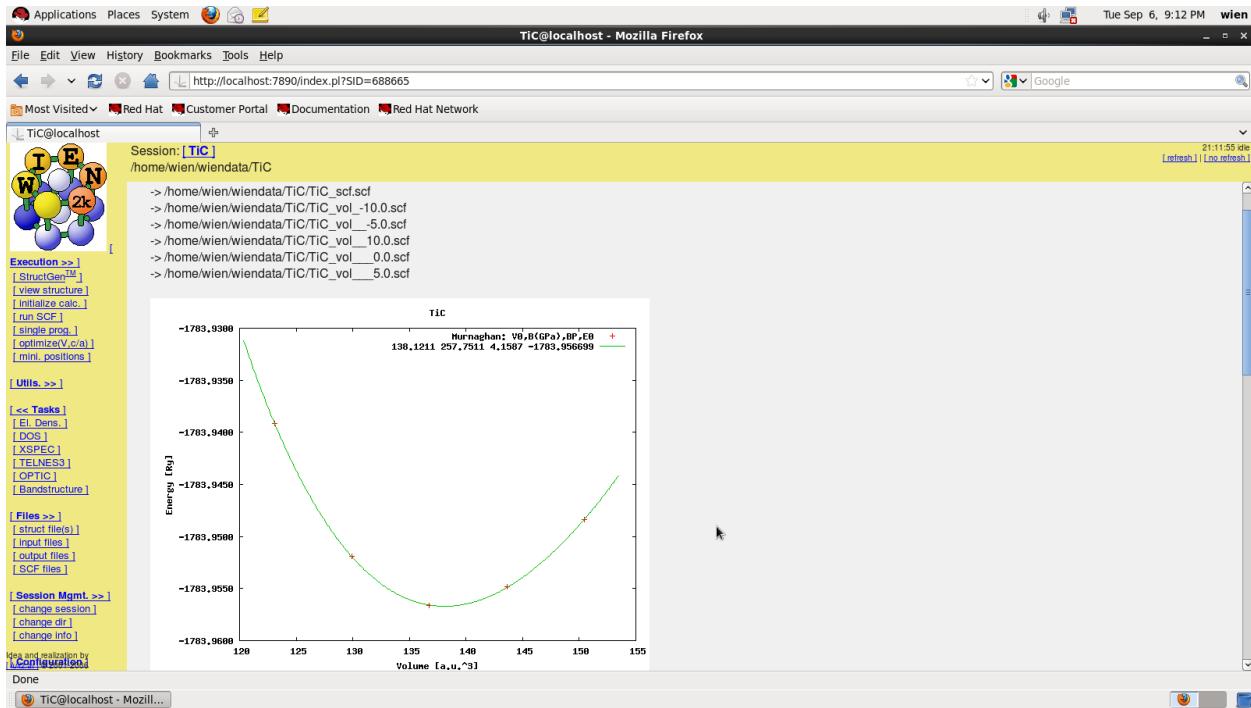
129. Click “continue with optimizer”:

The screenshot shows a web browser window titled "TiC@localhost" with the URL "http://localhost:7890/index.pl?SID=139899". The session is named "TiC" and the path is "/home/username/wiendata/TiC". The commandline is set to "./optimize.job" and the program input is empty. A note says "[View STDOUT] to monitor the progress of this command". Below it, there's a "Continue with" section containing a button labeled "continue with optimizer" which has a mouse cursor hovering over it. On the left side, there's a sidebar with various links for "Execution >>", "Utils. >>", "Tasks", "Files >>", "Session Mgmt. >>", "Configuration", and "Usersguide". At the bottom left, it says "Idea and realization by [luitz.at] © 2001-2006". On the right side, there's a watermark for "w2web" with the URL "w2web © luitz.at".

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.