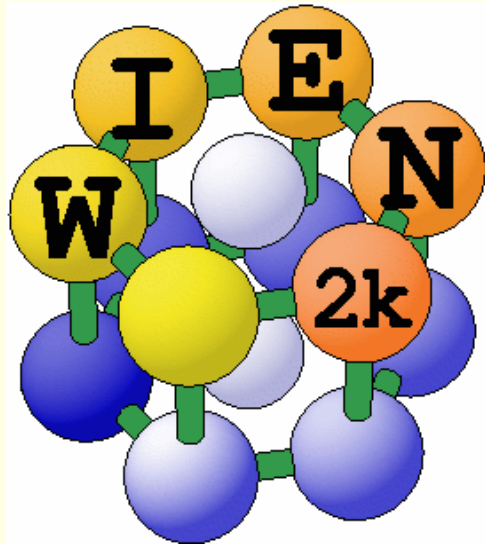
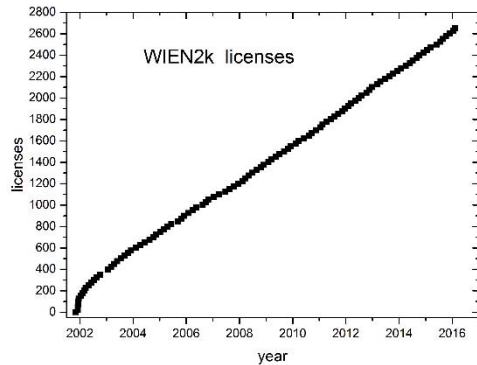


# WIEN2k software package



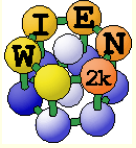
WIEN97: ~500 users  
WIEN2k: ~2750 users

## An Augmented Plane Wave Plus Local Orbital Program for Calculating Crystal Properties

**Peter Blaha**  
**Karlheinz Schwarz**  
**Georg Madsen**  
**Dieter Kvasnicka**  
**Joachim Luitz**

November 2001  
Vienna, AUSTRIA  
Vienna University of Technology

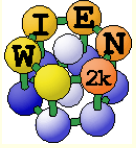
<http://www.wien2k.at>



## General remarks on WIEN2k



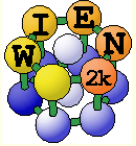
- WIEN2k consists of many independent F90 programs, which are linked together via C-shell scripts.
- Each „case“ runs in his own directory `./case`
- The „master input“ is called `case.struct`
- Initialize a calculation: `init_lapw`
- Run scf-cycle: `run_lapw (runsp_lapw)`
- You can run WIEN2k using any www-browser and the w2web interface, but also at the command line in an xterm.
- Input/output/scf files have endings as the corresponding programs:
  - *case.output1...lapw1; case.in2...lapw2; case.scf0...lapw0*
- Inputs are generated using STRUCTGEN(w2web) and `init_lapw`



# w2web: the web-based GUI of WIEN2k



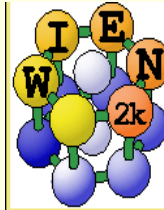
- Based on **www**
  - *WIEN2k can be managed remotely via w2web*
- Important steps:
  - *start w2web on all your hosts*
    - login to the desired host (ssh)
    - w2web (at first startup you will be asked for username/password, port-number, (master-)hostname. creates ~/.w2web directory)
  - *use your browser and connect to the (master) **host:portnumber***
    - firefox <http://fp98.zserv:10000>
  - *create a new session on the desired host (or select an old one)*



# w2web GUI (graphical user interface)



- **Structure generator**
  - *spacegroup selection*
  - *import cif or xyz file*
- **step by step initialization**
  - *symmetry detection*
  - *automatic input generation*
- **SCF calculations**
  - *Magnetism (spin-polarization)*
  - *Spin-orbit coupling*
  - *Forces (automatic geometry optimization)*
- **Guided Tasks**
  - *Energy band structure*
  - *DOS*
  - *Electron density*
  - *X-ray spectra*
  - *Optics*



#### Execution >>

StructGen™  
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

Session: TiC

/area51/pblaha/lapw/2005-june/TiC

## StructGen™

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

Save Structure

Title: TiC

Lattice:

Type: F

P  
F  
B  
CXY  
CYZ  
CXZ  
R  
H  
1\_P1

Spacegroups from  
Bilbao Cryst Server

Lattice parameters in Å

a=4.328000038 b=4.328000038 c=4.328000038

$\alpha$ =90.000000  $\beta$ =90.000000  $\gamma$ =90.000000

Inequivalent Atoms: 2

Atom 1: Ti Z=22.0 RMT=2.0000 remove atom

Pos 1: x=0.00000000 y=0.00000000 z=0.00000000 remove

add position

Atom 2: C Z=6.0 RMT=1.9000 remove atom

Pos 1: x=0.50000000 y=0.50000000 z=0.50000000 remove

add position