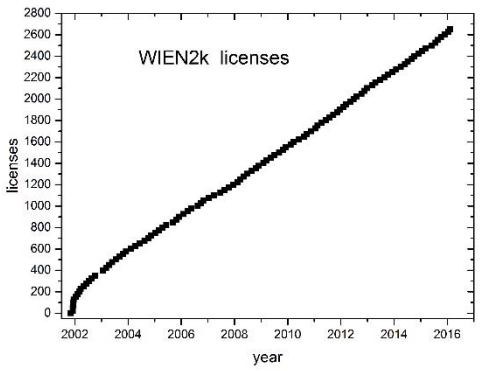
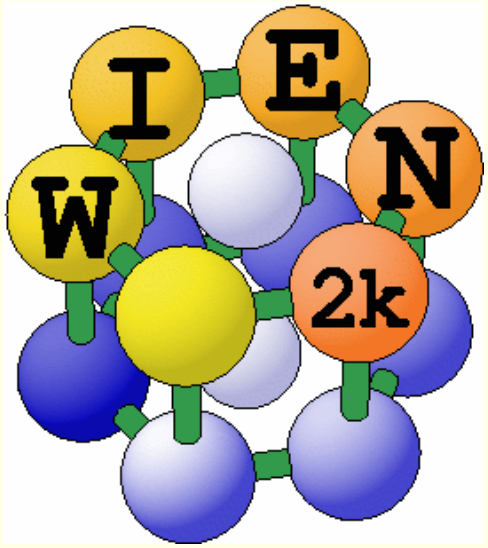


WIEN2k software package



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

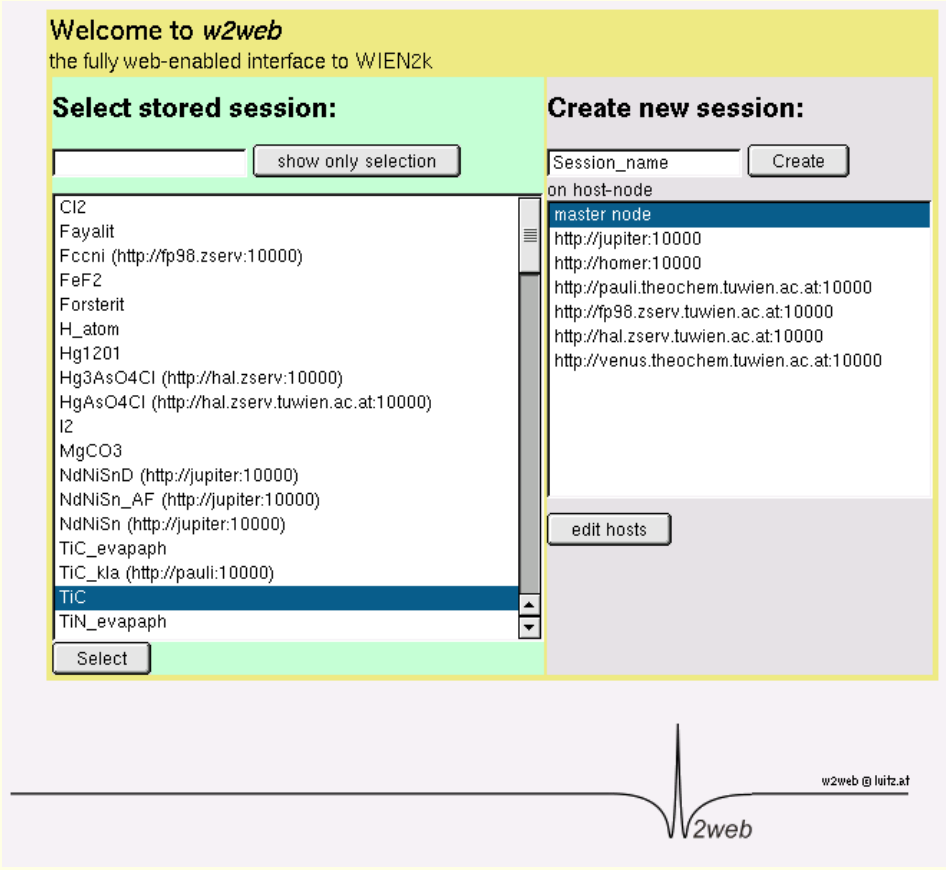
http://www.wien2k.at

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*