

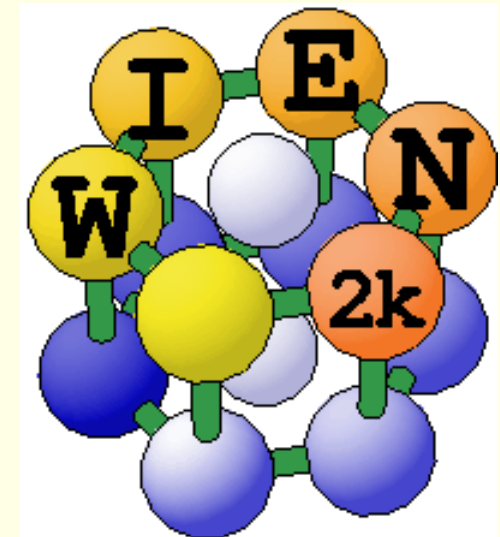


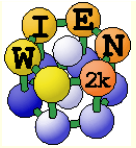
# The FP-LAPW and APW+lo methods

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**Peter Blaha**

Institute of Materials Chemistry  
TU Wien

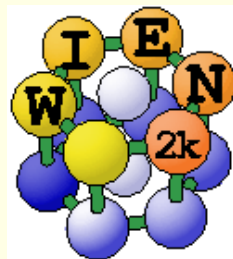




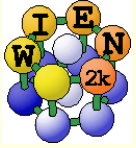
# APW based schemes



- **APW (J.C.Slater 1937)**
  - *Non-linear eigenvalue problem*
  - *Computationally very demanding*
- **LAPW (O.K.Andersen 1975)**
  - *Generalized eigenvalue problem*
  - *Full-potential (A. Freeman et al.)*
- **Local orbitals (D.J.Singh 1991)**
  - *treatment of semi-core states (avoids ghostbands)*
- **APW+lo (E.Sjöstedt, L.Nordström, D.J.Singh 2000)**
  - *Efficiency of APW + convenience of LAPW*
  - *Basis for*



K.Schwarz, P.Blaho, G.K.H.Madsen,  
Comp.Phys.Commun.**147**, 71-76 (2002)

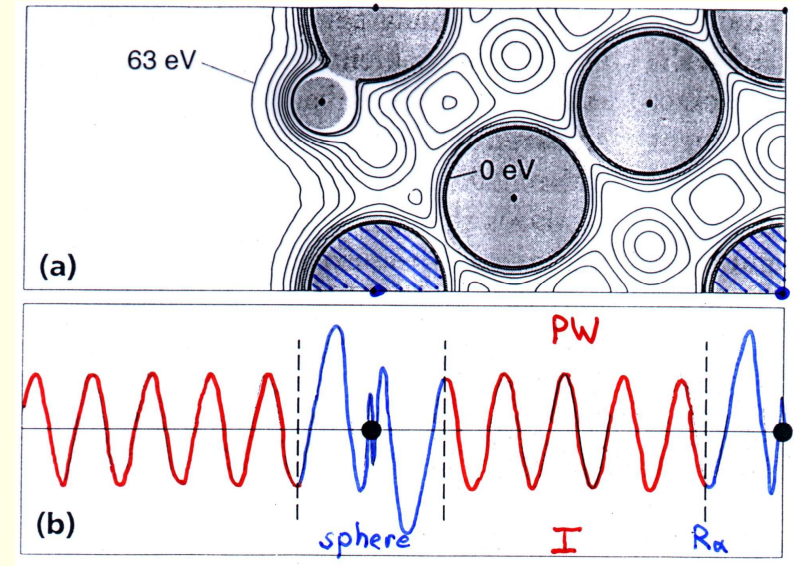
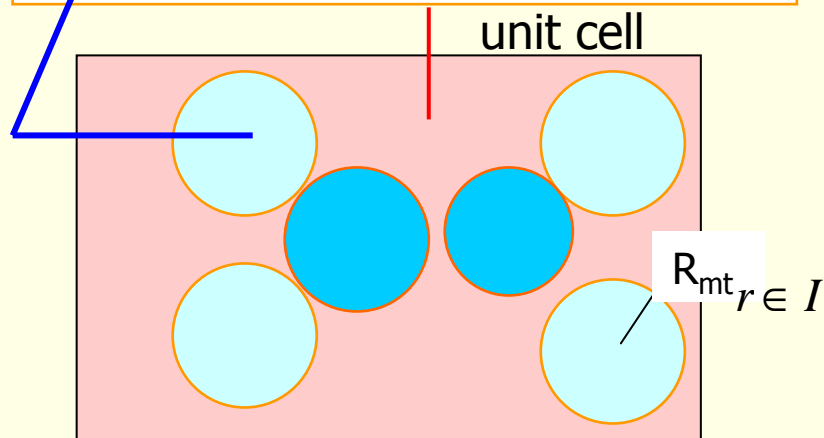


# APW Augmented Plane Wave method

The unit cell is partitioned into:

atomic spheres

Interstitial region



Basisset:

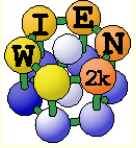
**PW:**  $e^{i(\vec{k} + \vec{K}) \cdot \vec{r}}$

Atomic partial waves

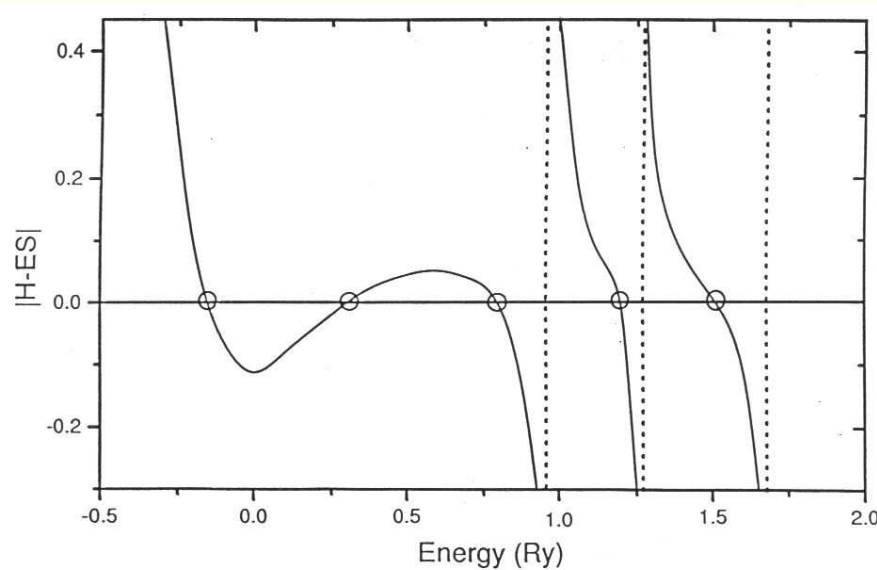
$$\sum_{\ell m} A_{\ell m}^K u_{\ell}(r', \epsilon) Y_{\ell m}(\hat{r}')$$

join

$u_{\ell}(r, \epsilon)$  are the numerical solutions of the radial Schrödinger equation in a given spherical potential for a particular energy  $\epsilon$   
 $A_{\ell m}^K$  coefficients for matching the PW



# Slater's APW (1937)



H Hamiltonian  
S overlap matrix

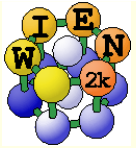
Atomic partial waves

$$\sum_{\ell m} A_{\ell m}^K u_{\ell}(r', \epsilon) Y_{\ell m}(\hat{r}')$$

Energy dependent basis  
functions lead to →

**Non-linear eigenvalue problem**

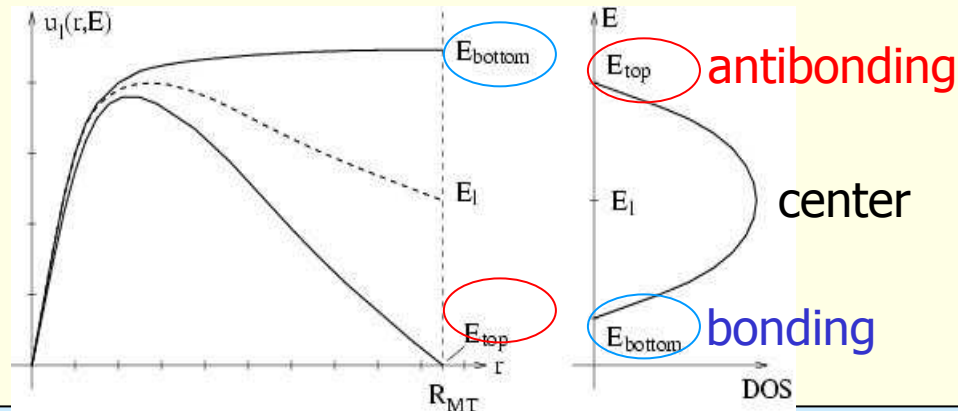
One had to numerically search for the energy, for which the  $\det|H-ES|$  vanishes. **Computationally very demanding.**  
"Exact" solution for given (spherical) potential!



# Linearization of energy dependence

**LAPW** suggested by

O.K.Andersen,  
Phys.Rev. B 12, 3060  
(1975)



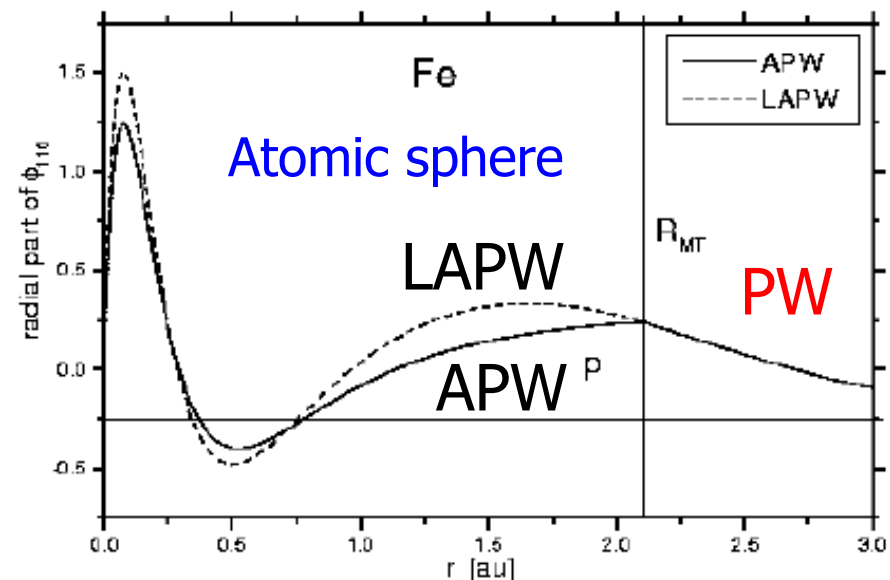
$$\Phi_{k_n} = \sum_{\ell m} [ \underline{A_{\ell m}}(k_n) u_{\ell}(E_{\ell}, r) + \underline{B_{\ell m}}(k_n) \dot{u}_{\ell}(E_{\ell}, r) ] Y_{\ell m}(\hat{r})$$

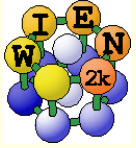
expand  $u_l$  at **fixed energy  $E_l$**  and  
add  $\dot{u}_l = \partial u_l / \partial \epsilon$

$A_{lm}^k, B_{lm}^k$ : join **PWs** in  
value and slope

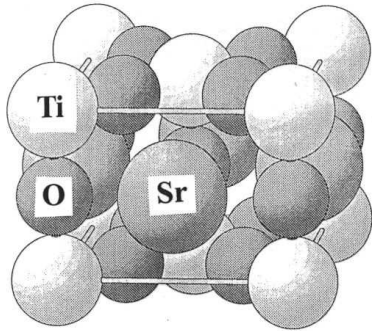
→ General eigenvalue problem  
(diagonalization)

→ additional constraint requires  
more **PWs** than APW

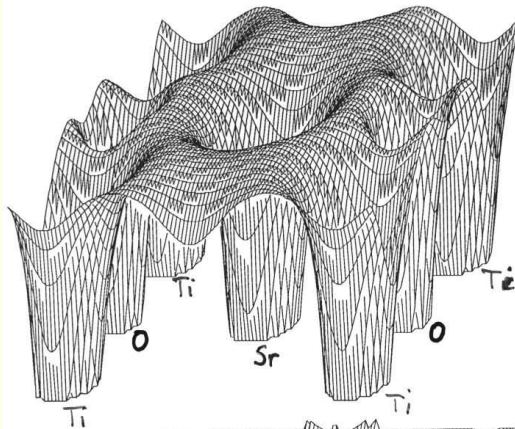




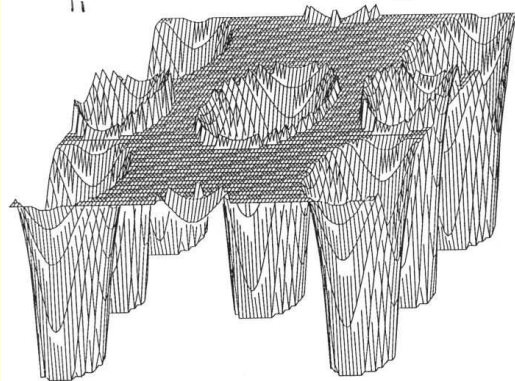
# Full-potential in LAPW (A.Freeman et al.)



SrTiO<sub>3</sub>



Full  
potential



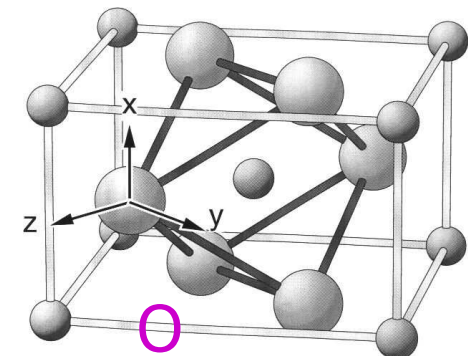
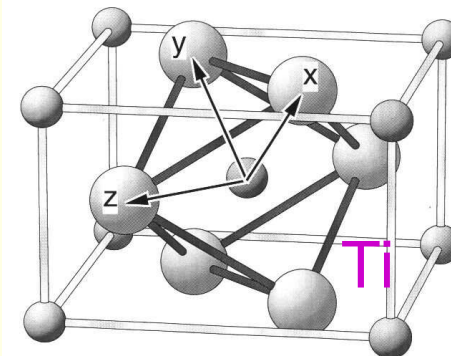
Muffin tin  
approximation

TiO<sub>2</sub> rutile

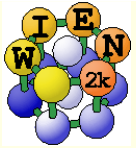
- The potential (and charge density) can be of general form (no shape approximation)

$$V(r) = \begin{cases} \sum_{LM} V_{LM}(r) Y_{LM}(\hat{r}) & r < R_\alpha \\ \sum_K V_K e^{i\vec{K} \cdot \vec{r}} & r \in I \end{cases}$$

- Inside each atomic sphere a local coordinate system is used (defining LM)



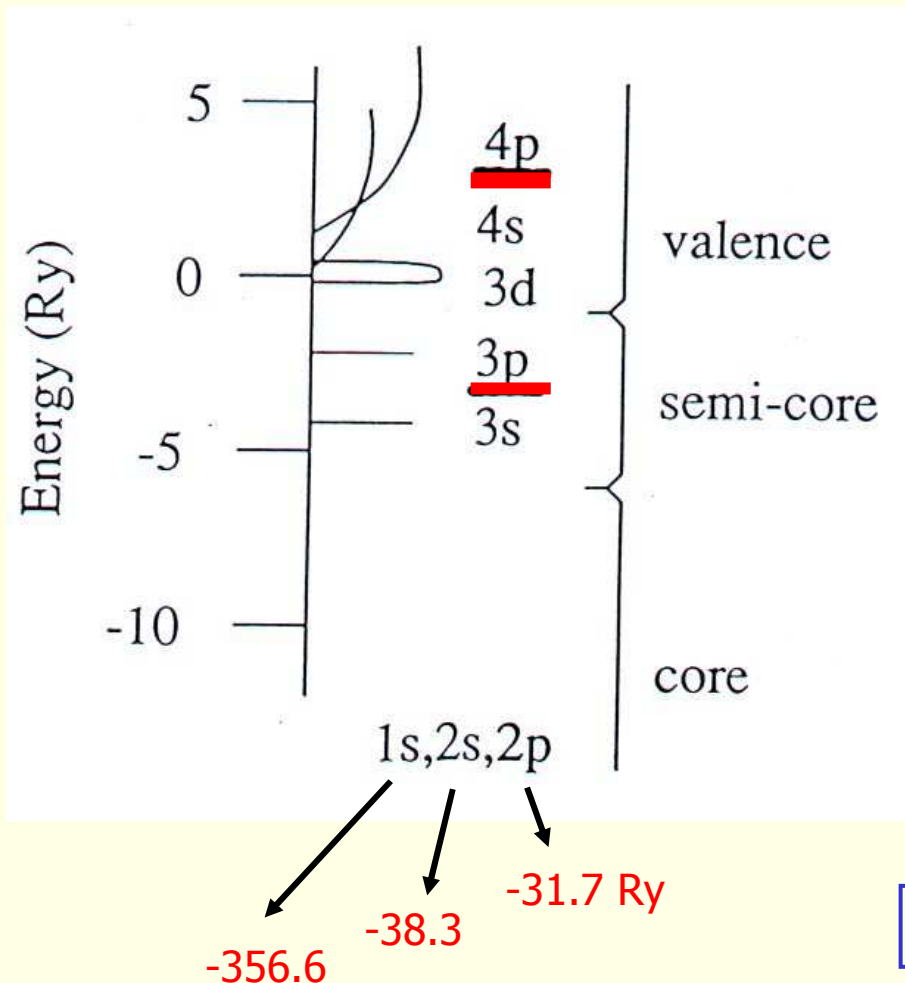




# Core, semi-core and valence states

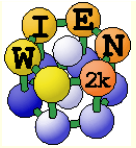


For example: **Ti**



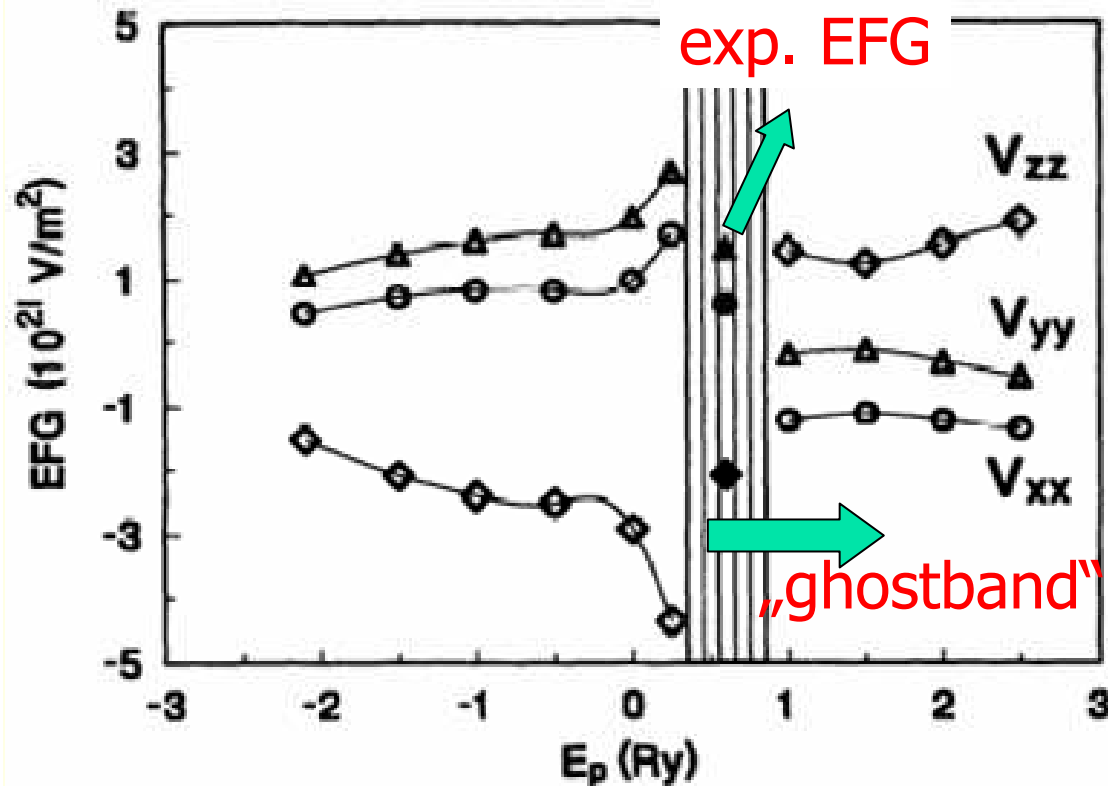
- **Valence states**
  - **High** in energy
  - **Delocalized** wavefunctions
- **Semi-core states**
  - **Medium** energy
  - Principal **QN** one less than valence (e.g. in Ti **3p** and **4p**)
  - **not completely confined** inside sphere
- **Core states**
  - **Low** in energy
  - Reside **inside sphere**

$$1 \text{ Ry} = 13.605 \text{ eV}$$



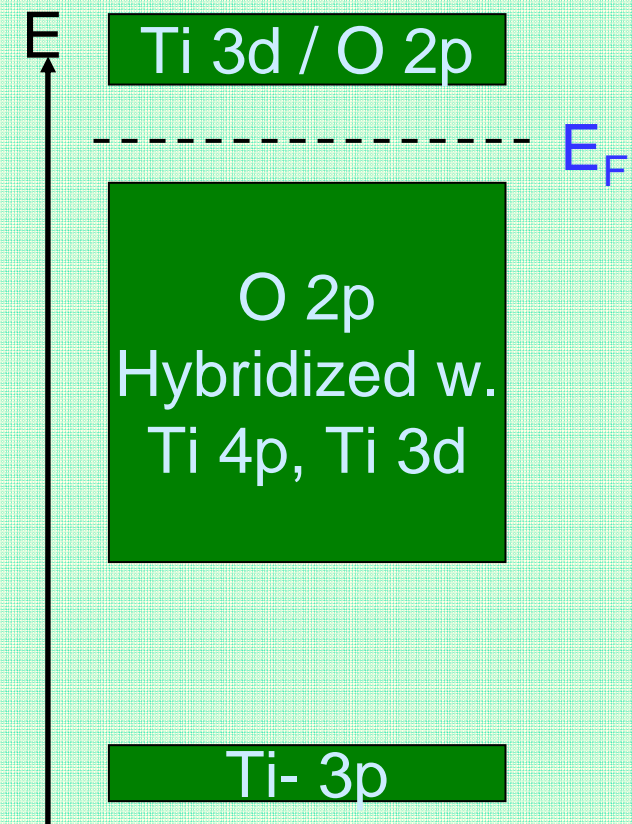
## Problems of the LAPW method:

EFG Calculation for Rutile  $\text{TiO}_2$  as a function of the Ti- $p$  linearization energy  $E_p$

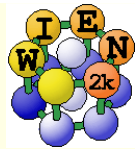


P. Blaha, D.J. Singh, P.I. Sorantin and K. Schwarz,  
Phys. Rev. B **46**, 1321 (1992).

### Electronic Structure







# Problems of the LAPW method



Atomic number

Symbol

Atomic weight

Metal

Semimetal

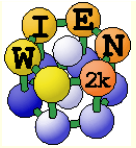
Nonmetal

1	2											13	14	15	16	17	18
1 <b>H</b> 1.008																	2 <b>He</b> 4.003
3 <b>Li</b> 6.941	4 <b>Be</b> 9.012											5 <b>B</b> 10.81	6 <b>C</b> 12.01	7 <b>N</b> 14.01	8 <b>O</b> 16.00	9 <b>F</b> 19.00	10 <b>Ne</b> 20.18
11 <b>Na</b> 22.99	12 <b>Mg</b> 24.31											13 <b>Al</b> 26.98	14 <b>Si</b> 28.09	15 <b>P</b> 30.97	16 <b>S</b> 32.07	17 <b>Cl</b> 35.45	18 <b>Ar</b> 39.95
19 <b>K</b> 39.10	20 <b>Ca</b> 40.08	21 <b>Sc</b> 44.96	22 <b>Ti</b> 47.88	23 <b>V</b> 50.94	24 <b>Cr</b> 52.00	25 <b>Mn</b> 54.94	26 <b>Fe</b> 55.85	27 <b>Co</b> 58.93	28 <b>Ni</b> 58.69	29 <b>Cu</b> 63.55	30 <b>Zn</b> 65.39	31 <b>Ga</b> 69.72	32 <b>Ge</b> 72.61	33 <b>As</b> 74.92	34 <b>Se</b> 78.96	35 <b>Br</b> 79.90	36 <b>Kr</b> 83.80
37 <b>Rb</b> 85.47	38 <b>Sr</b> 87.62	39 <b>Y</b> 88.91	40 <b>Zr</b> 91.22	41 <b>Nb</b> 92.91	42 <b>Mo</b> 95.94	43 <b>Tc</b> 98.91	44 <b>Ru</b> 101.1	45 <b>Rh</b> 102.9	46 <b>Pd</b> 106.4	47 <b>Ag</b> 107.9	48 <b>Cd</b> 112.4	49 <b>In</b> 114.8	50 <b>Sn</b> 118.7	51 <b>Sb</b> 121.8	52 <b>Te</b> 127.6	53 <b>I</b> 126.9	54 <b>Xe</b> 131.3
55 <b>Cs</b> 132.9	56 <b>Ba</b> 137.3	71 <b>Lu</b> 175.0	72 <b>Hf</b> 178.5	73 <b>Ta</b> 180.9	74 <b>W</b> 183.8	75 <b>Re</b> 186.2	76 <b>Os</b> 190.2	77 <b>Ir</b> 192.2	78 <b>Pt</b> 195.1	79 <b>Au</b> 197.0	80 <b>Hg</b> 200.6	81 <b>Tl</b> 204.4	82 <b>Pb</b> 207.2	83 <b>Bi</b> 209.0	84 <b>Po</b> 209.0	85 <b>At</b> 210.0	86 <b>Rn</b> 222.0
87 <b>Fr</b> 223.0	88 <b>Ra</b> 226.0	103 <b>Lr</b> 262.1	104 <b>Rf</b> 261.1	105 <b>Db</b> 262.1	106 <b>Sg</b> 263.1	107 <b>Bh</b> 264.1	108 <b>Hs</b> 265.1	109 <b>Mt</b> 268	110 <b>Uun</b> 269	111 <b>Uuu</b> 272	112 <b>Uub</b> 277	113 <b>Uut</b>	114 <b>Uuq</b> 289	115 <b>Uup</b>	116 <b>Uuh</b> 289	117 <b>Uus</b>	118 <b>Uuo</b> 293
		57 <b>La</b> 138.9	58 <b>Ce</b> 140.1	59 <b>Pr</b> 140.9	60 <b>Nd</b> 144.2	61 <b>Pm</b> 146.9	62 <b>Sm</b> 150.4	63 <b>Eu</b> 152.0	64 <b>Gd</b> 157.3	65 <b>Tb</b> 158.9	66 <b>Dy</b> 162.5	67 <b>Ho</b> 164.9	68 <b>Er</b> 167.3	69 <b>Tm</b> 168.9	70 <b>Yb</b> 173.0		
		89 <b>Ac</b> 227.0	90 <b>Th</b> 232.0	91 <b>Pa</b> 231.0	92 <b>U</b> 238.0	93 <b>Np</b> 237.0	94 <b>Pu</b> 244.1	95 <b>Am</b> 243.1	96 <b>Cm</b> 247.1	97 <b>Bk</b> 247.1	98 <b>Cf</b> 251.1	99 <b>Es</b> 252.0	100 <b>Fm</b> 257.1	101 <b>Md</b> 258.1	102 <b>No</b> 259.1		

(c)1998  
Kremer Paul



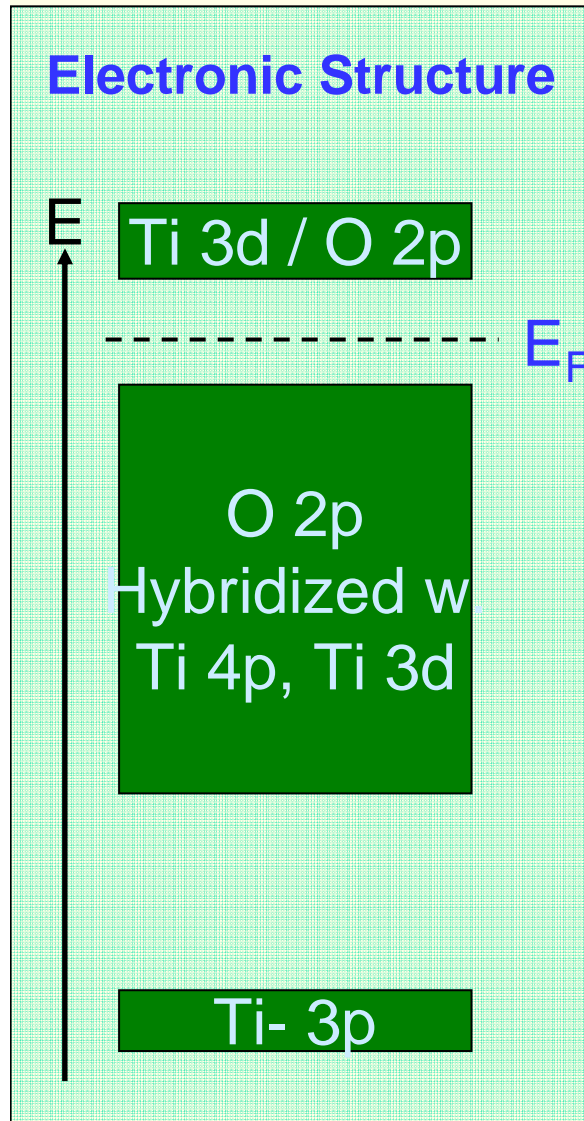
Problems with semi-core states



# ONE SOLUTION



## Electronic Structure

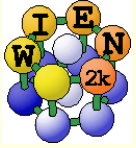


Treat all the states in a single energy window:

- Automatically orthogonal.
- Need to add variational freedom.
- Could invent quadratic or cubic APW methods.

$$\phi(\mathbf{r}) = \left\{ \begin{array}{l} \Omega^{-1/2} \sum_{\mathbf{K}} c_{\mathbf{K}} e^{i(\mathbf{K}+\mathbf{k})\cdot\mathbf{r}} \\ \sum_{lm} (A_{lm}u_l(r)+B_{lm}\dot{u}_l(r)+C_{lm}\ddot{u}_l(r)) Y_{lm}(\mathbf{r}) \end{array} \right.$$

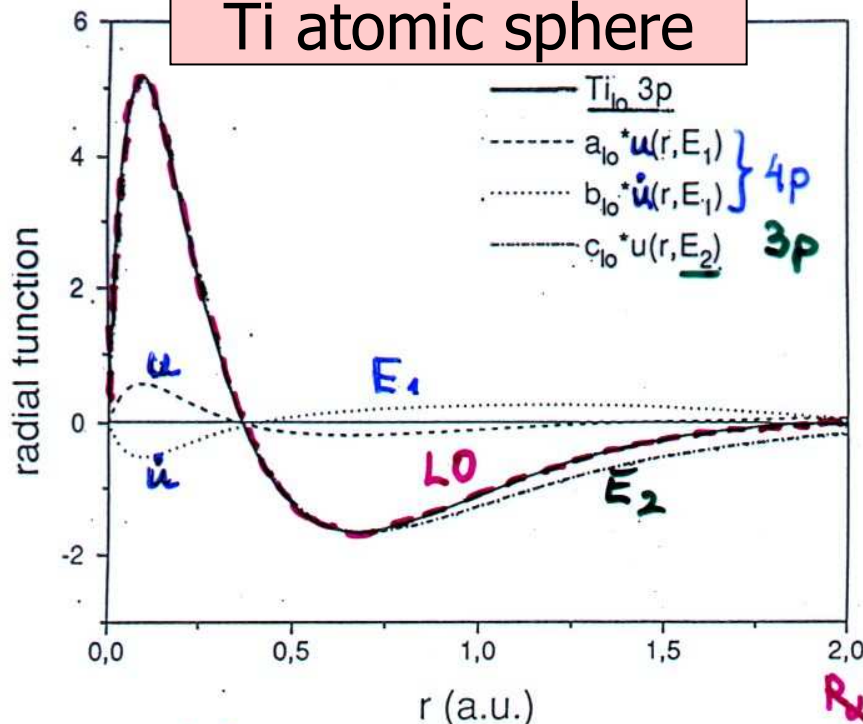
**Problem:** This requires an extra matching condition, e.g. second derivatives continuous  $\Rightarrow$  method will be impractical due to the high planewave cut-off needed.



# Extending the basis: Local orbitals (LO)



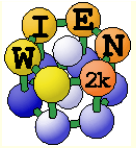
Ti atomic sphere



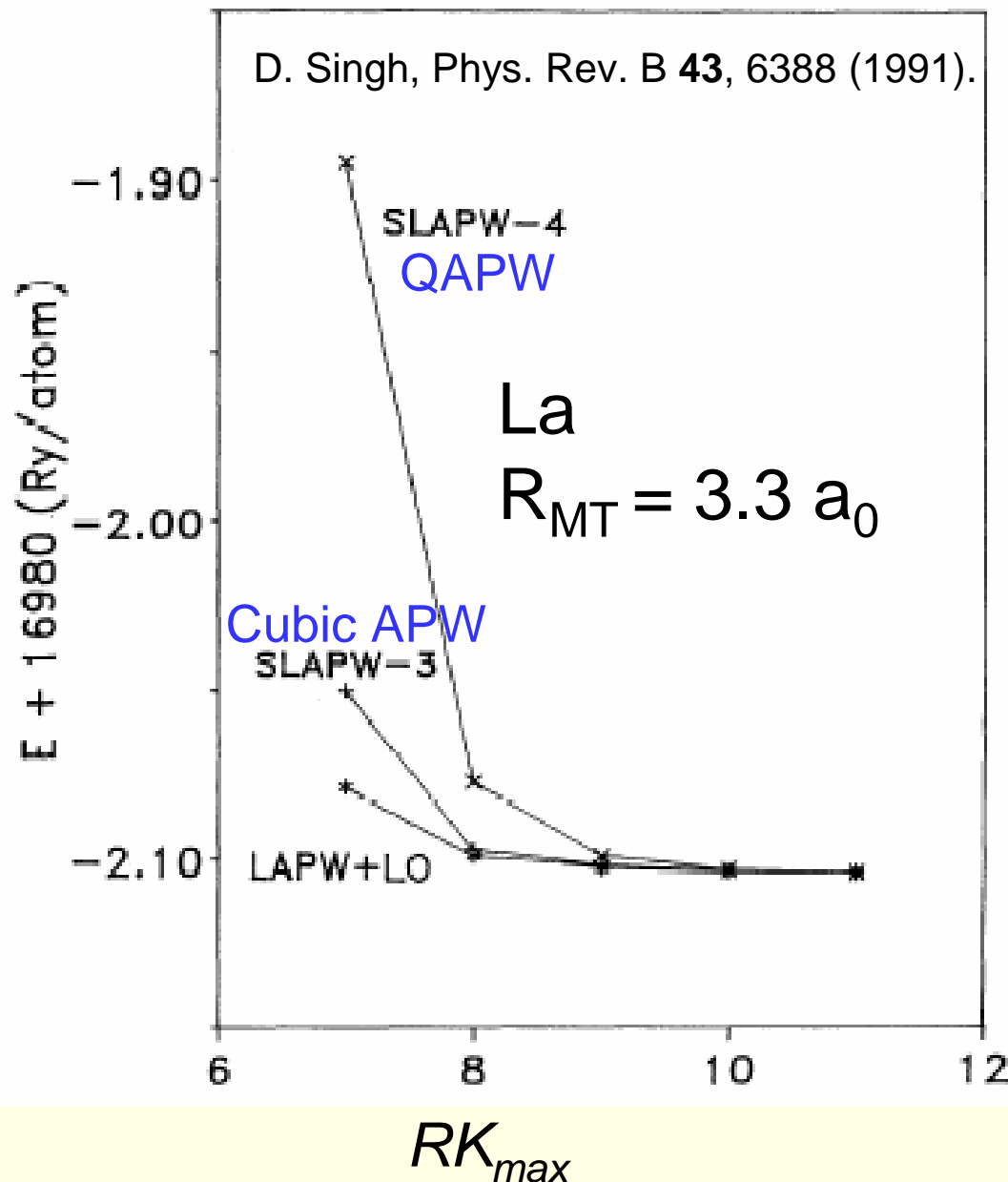
$$\Phi_{LO} = [A_{lm} u_l^{E_1} + B_{lm} \dot{u}_l^{E_1} + C_{lm} u_l^{E_2}] Y_{lm}(\hat{r})$$

- LO: contains a second  $u_l(E_2)$ 
  - is confined to an atomic sphere
  - has zero value and slope at  $R$
  - can treat two principal QN  $n$  for each azimuthal QN  $\ell$  (3p and 4p)
  - corresponding states are strictly orthogonal (no "ghostbands")
  - tail of semi-core states can be represented by plane waves
  - only slight increase of basis set (matrix size)

D.J.Singh,  
Phys.Rev. B 43 6388 (1991)



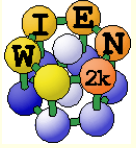
# The LAPW+LO Method



LAPW+LO **converges** like LAPW. The LO add a few basis functions (i.e. 3 per atom for p states). Can also use LO to relax linearization errors, e.g. for a narrow *d* or *f* band.

Suggested settings:

Two "energy" parameters, one for  $u$  and  $\bar{u}$  and the other for  $u^{(2)}$ . Choose one at the semi-core position and the other at the valence.



# New ideas from Uppsala and Washington



E.Sjöstedt, L.Nordström, D.J.Singh,  
*An alternative way of linearizing the augmented plane wave method,*  
Solid State Commun. 114, 15 (2000)

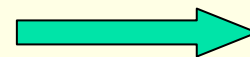
- Use **APW**, but at **fixed  $E_f$**  (superior PW convergence)
- **Linearize** with **additional lo** (add a few basis functions)

$$\Phi_{k_n} = \sum_{\ell m} A_{\ell m}(k_n) u_{\ell}(E_{\ell}, r) Y_{\ell m}(\hat{r})$$

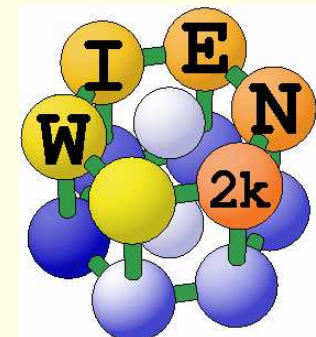
$$\Phi_{lo} = [A_{\ell m} u_{\ell}^{E_1} + B_{\ell m} \dot{u}_{\ell}^{E_1}] Y_{\ell m}(\hat{r})$$

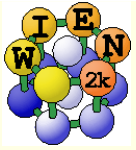
**optimal solution:** mixed basis

- use APW+lo for states which are difficult to converge:  
(f or d- states, atoms with small spheres)
- use LAPW+LO for all other atoms and  $\ell$



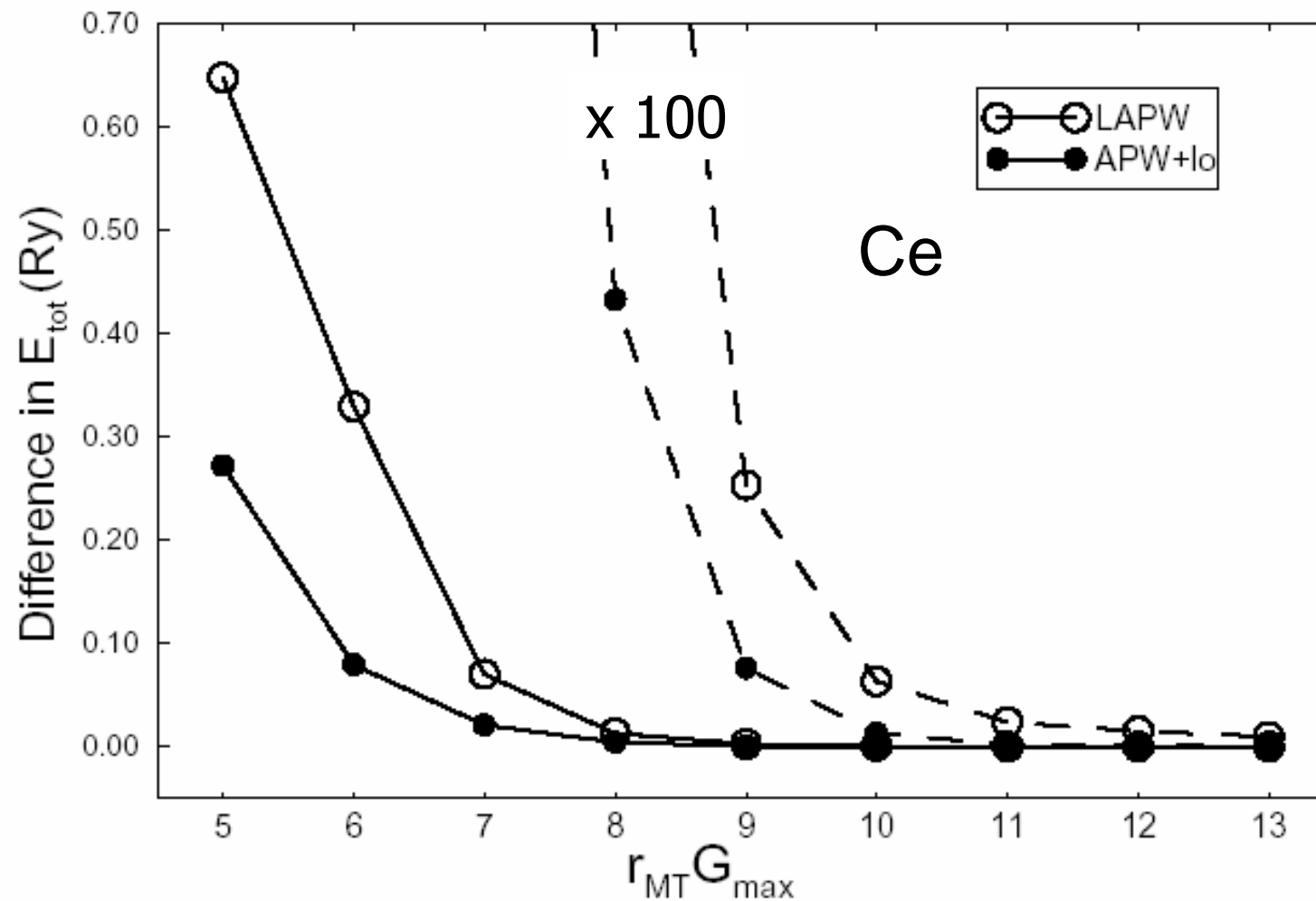
basis for

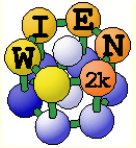




# Convergence of the APW+LO Method

E. Sjöstedt, L. Nordström and D.J. Singh, Solid State Commun. **114**, 15 (2000).





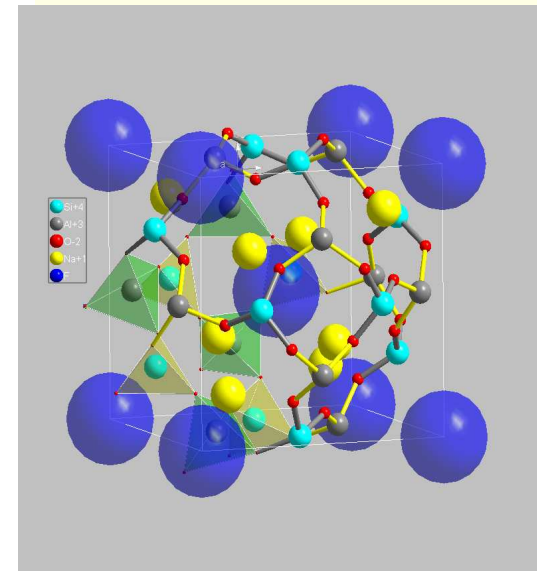
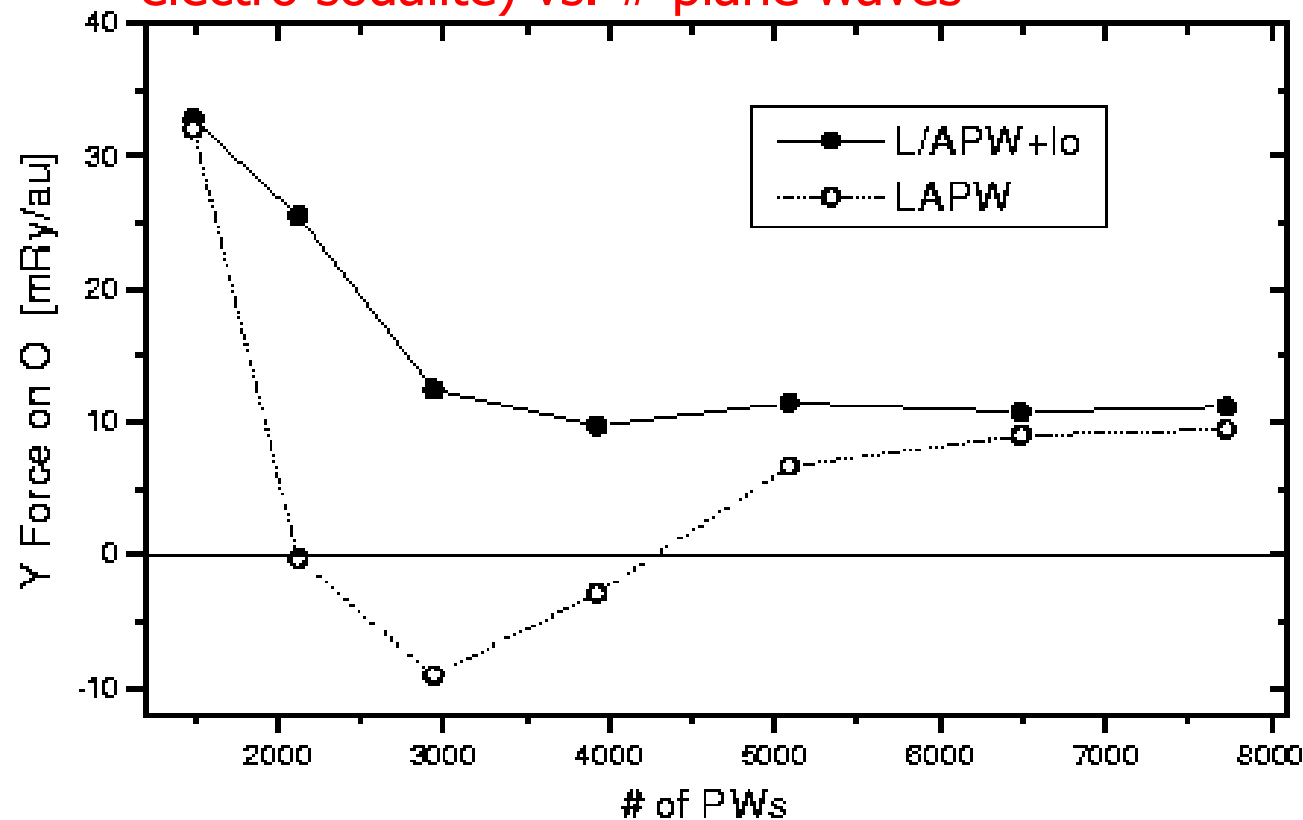
# Improved convergence of APW+lo



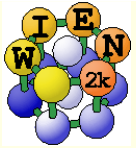
K.Schwarz, P.Blaha, G.K.H.Madsen,  
Comp.Phys.Commun.**147**, 71-76 (2002)

- changes sign and converges slowly in **LAPW**
- better convergence in **APW+lo**

Force ( $F_y$ ) on oxygen in SES (sodium electro sodalite) vs. # plane waves

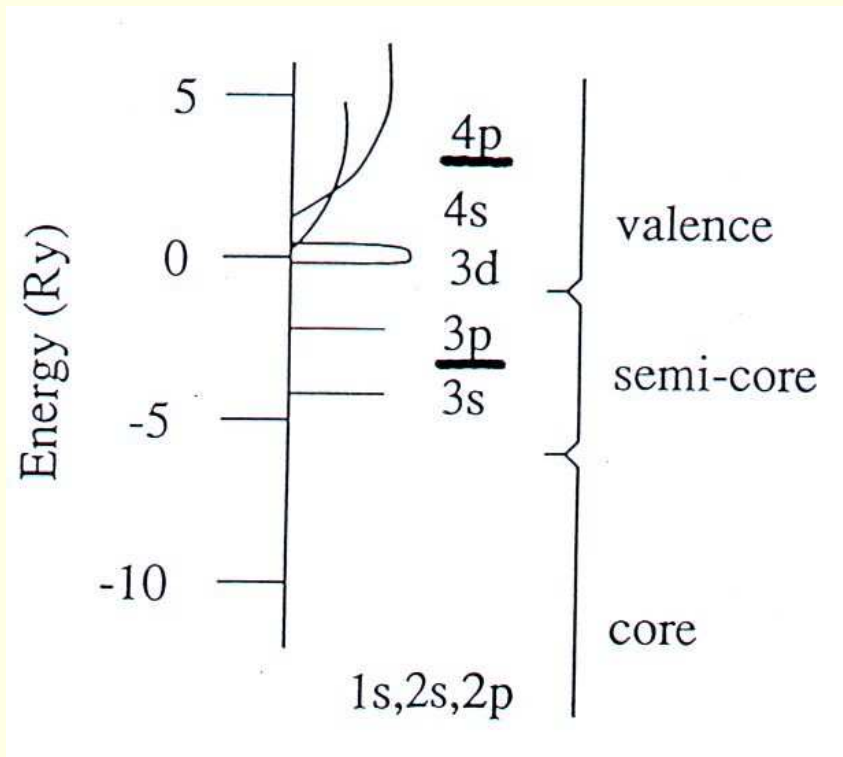






# Relativistic treatment

For example: Ti



## ■ Valence states

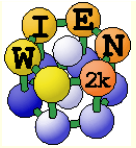
- *Scalar relativistic*
  - mass-velocity
  - Darwin s-shift
- *Spin orbit coupling **on demand** by second variational treatment*

## ■ Semi-core states

- *Scalar relativistic*
- *No spin orbit coupling*
- **on demand**
  - spin orbit coupling by second variational treatment
  - Additional local orbital (see Th-6p<sub>1/2</sub>)

## ■ Core states

- *Fully relativistic*
  - Dirac equation



# Relativistic semi-core states in fcc Th

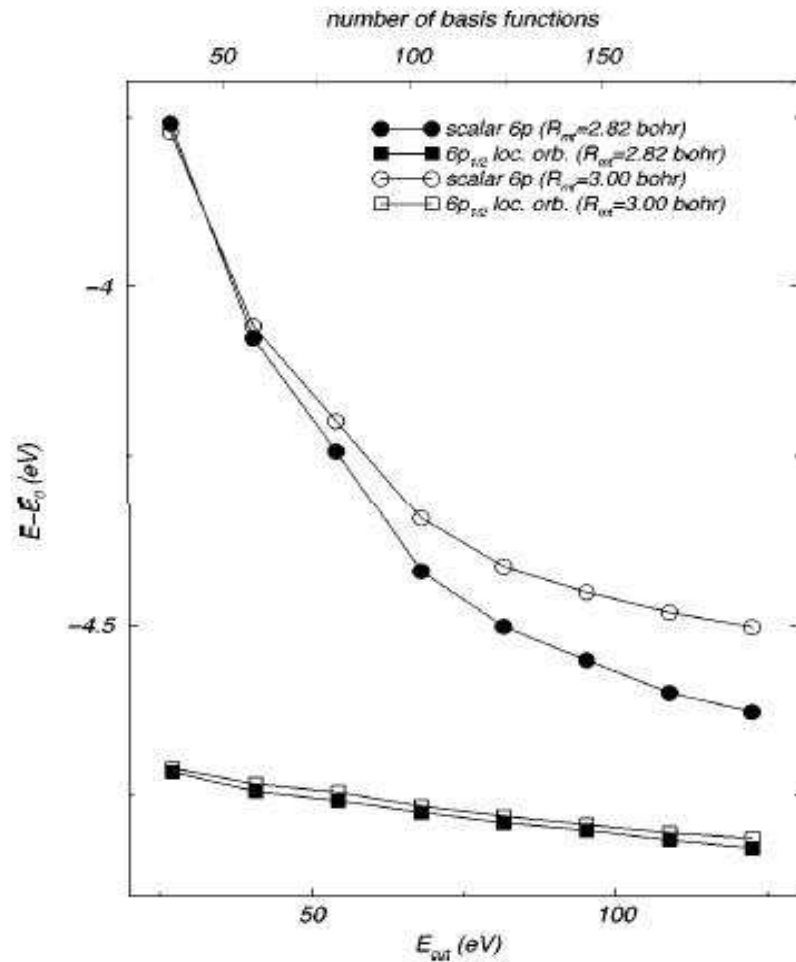


FIG. 1. The total energy  $E$  as a function of the second-variation cutoff energy  $E_{\text{cut}}$  (the approximate size of the second-variational-step basis, including spin, is marked on the top axis) for two different muffin-tin radii. The standard FLAPW results are marked with circles, the results obtained with the additional  $p_{1/2}$  local orbitals are marked with squares (the latter energies were increased by 3 eV in order to show the curves on the same plot).

- additional local orbitals for  $6p_{1/2}$  orbital in Th
- Spin-orbit (2<sup>nd</sup> variational method)

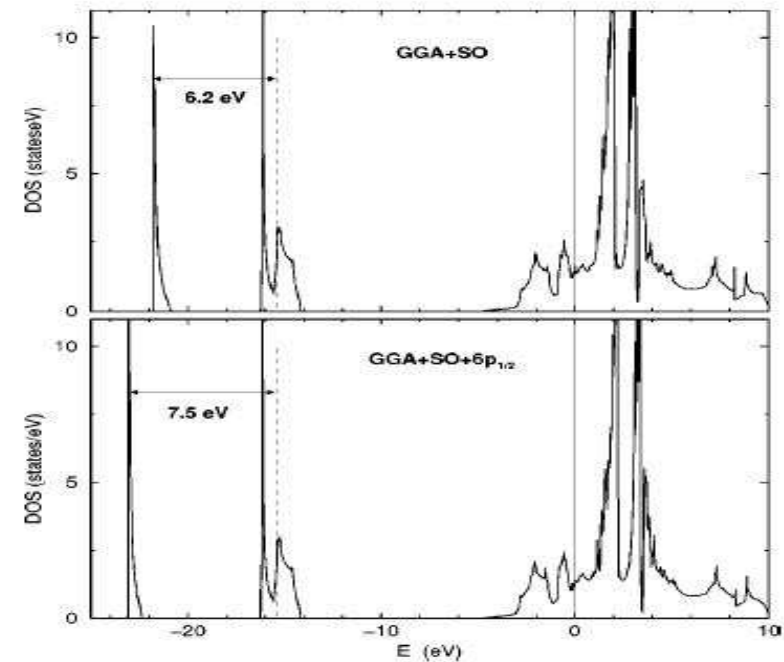
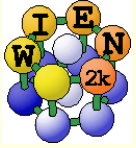


FIG. 2. Density of states calculated with the scalar relativistic basis (top panel) and with the  $p_{1/2}$  local orbitals extended basis (bottom panel). The splitting between the centers of  $6p_{1/2}$  and  $6p_{3/2}$  bands is shown.

J.Kuneš, P.Novak, R.Schmid, P.Blahá, K.Schwarz,  
Phys.Rev.B. 64, 153102 (2001)



# Atomic forces (Yu et al.; Kohler et al.)



## ■ Total Energy:

- *Electrostatic energy*
- *Kinetic energy*
- *XC-energy*

$$U[\rho] = \frac{1}{2} \int d^3\vec{r} \rho(\vec{r}) V_{es}(\vec{r}) + \frac{1}{2} \sum_{\alpha} Z_{\alpha} V_{es}^{\alpha}(\vec{r})$$

$$T[\rho] = \sum_i n_i \varepsilon_i - \int d^3\vec{r} \rho(\vec{r}) V_{eff}(\vec{r})$$

$$E_{xc}[\rho] = \int d^3\vec{r} \rho(\vec{r}) \varepsilon_{xc}(\vec{r})$$

## ■ Force on atom $\alpha$ :

$$\vec{F}^{\alpha} = \frac{-dE_{tot}}{d\vec{R}_{\alpha}} = F_{HF}^{\alpha} + F_{core}^{\alpha} + F_{val}^{\alpha}$$

- *Hellmann-Feynman-force*
- *Pulay corrections*

- Core
- Valence

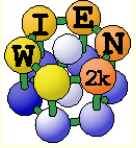
$$F_{HF}^{\alpha} = Z_{\alpha} \sum_{m=-1}^1 \lim_{r_{\alpha} \rightarrow 0} \frac{V_{1m}^{es}(r_{\alpha})}{r_{\alpha}} \nabla_{\alpha} [r_{\alpha} Y_{1m}(\hat{r})]$$

$$F_{core}^{\alpha} = - \int \rho_{core}(r) \nabla_{\alpha} V_{eff}(r) d\vec{r}$$

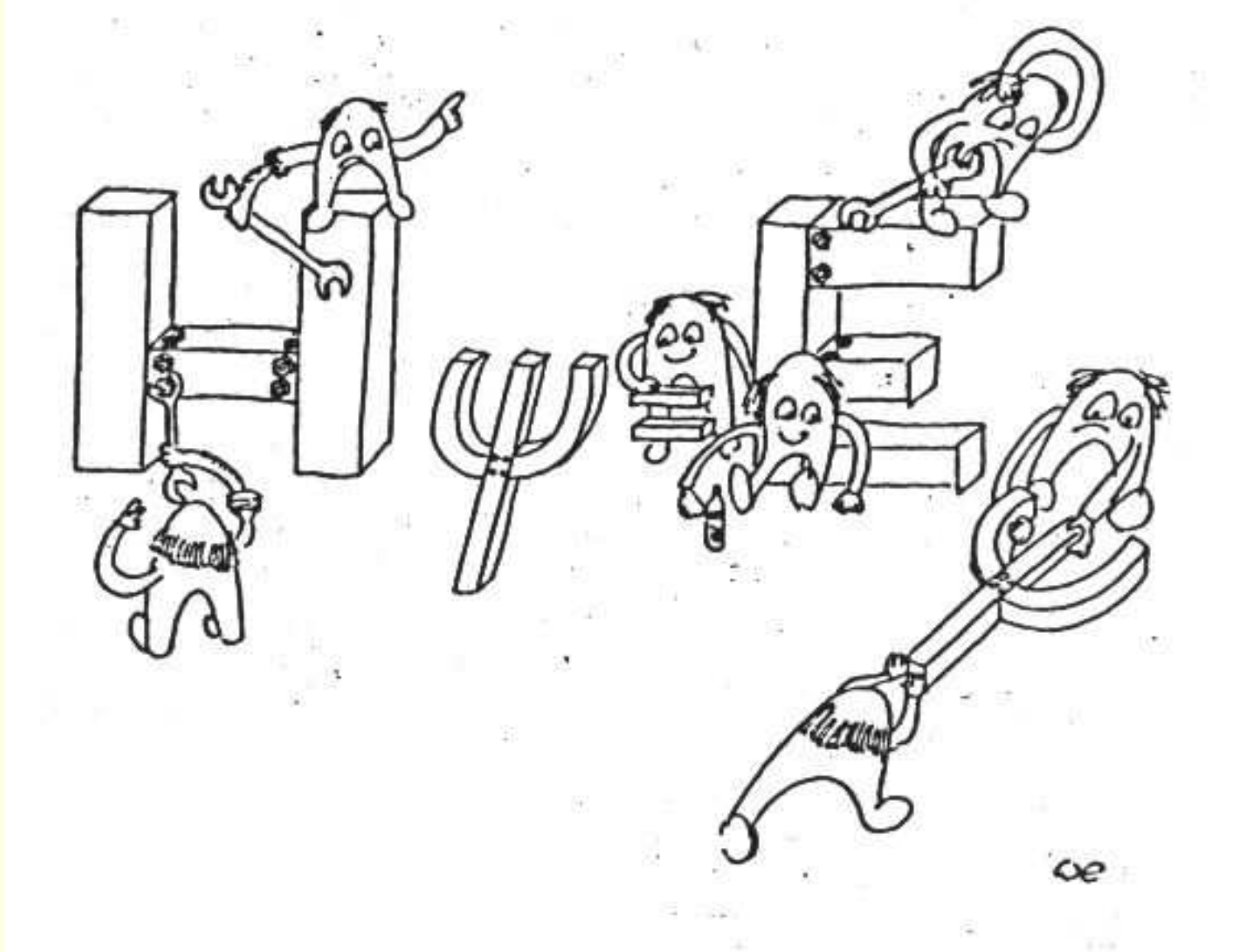
- expensive, contains a summation of matrix elements over all occupied states

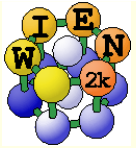
$$F_{val}^{\alpha} = \int_{\alpha} V_{eff}(r) \nabla_{\alpha} \rho_{val}(r) d\vec{r} + \sum_{k,i} n_i \sum_{K,K'} c_i^{*}(K') c_i(K) \times$$

$$\left[ (K^2 - \varepsilon_i) \oint \phi_{K'}^{*}(r) \phi_K(r) dS_{\alpha} - i(K - K') \langle \phi_{K'} | H - \varepsilon_i | \phi_K \rangle_{\alpha} \right]$$

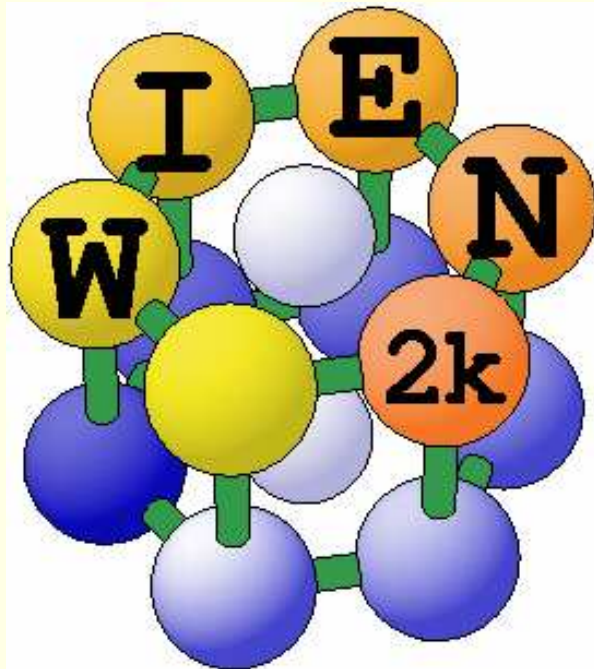


# Quantum mechanics at work





# WIEN2k software package



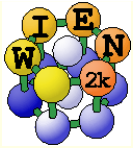
WIEN97: ~500 users  
WIEN2k: ~1100 users  
mailinglist: 1800 users

**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>



# Development of WIEN2k



## ■ Authors of WIEN2k

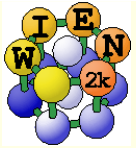
*P. Blaha, K. Schwarz, D. Kvasnicka, G. Madsen and J. Luitz*

## ■ Other contributions to WIEN2k

- **C. Ambrosch-Draxl** (Univ. Graz, Austria), optics
- *T. Charpin (Paris), elastic constants*
- *R. Dohmen und J. Pichlmeier (RZG, Garching), parallelization*
- **R. Laskowski (Vienna)**, non-collinear magnetism, parallelization
- *L. Marks (Northwestern, US) , various optimizations*
- **P. Novák** and *J. Kunes (Prague), LDA+U, SO*
- *B. Olejnik (Vienna), non-linear optics,*
- *C. Persson (Uppsala), irreducible representations*
- **M. Scheffler** (Fritz Haber Inst., Berlin), forces
- **D.J.Singh** (NRL, Washington D.C.), local orbitals (LO), APW+lo
- *E. Sjöstedt and L Nordström (Uppsala, Sweden), APW+lo*
- *J. Sofo and J. Fuhr (Barriloché), Bader analysis*
- *B. Yanchitsky and A. Timoshevskii (Kiev), spacegroup*

## ■ and many others ....





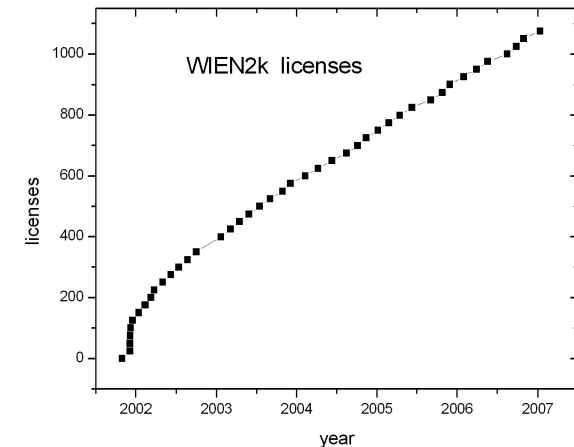
# International co-operations

## ■ More than 1000 user groups worldwide

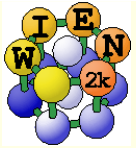
- *Industries* (Canon, Eastman, Exxon, Fuji, A.D.Little, Mitsubishi, Motorola, NEC, Norsk Hydro, Osram, Panasonic, Samsung, Sony).
- *Europe*: (EHT Zürich, MPI Stuttgart, Dresden, FHI Berlin, DESY, TH Aachen, ESRF, Prague, Paris, Chalmers, Cambridge, Oxford)
- *America*: ARG, BZ, CDN, MX, USA (MIT, NIST, Berkeley, Princeton, Harvard, Argonne NL, Los Alamos Nat.Lab., Penn State, Georgia Tech, Lehigh, Chicago, SUNY, UC St.Barbara, Toronto)
- *far east*: AUS, China, India, JPN, Korea, Pakistan, Singapore, Taiwan (Beijing, Tokyo, Osaka, Sendai, Tsukuba, Hong Kong)

## ■ Registration at [www.wien2k.at](http://www.wien2k.at)

- 400/4000 Euro for Universities/Industries
- code download via www (with password), updates, bug fixes, news
- usersguide, faq-page, mailing-list with help-requests



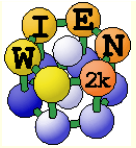




# WIEN2k - WORKSHOPS



- "WIEN-workshops" started in 1993 in Vienna and subsequent workshops were held not only in Vienna, but also in Trieste, Isfahan (Iran), twice at PennState (US), in Kyoto (Japan) and at UCLA (California,US).
- **WIEN2007: Hands on Workshop on the WIEN2k package**  
**Penn State University, USA, June 11-14, 2007**
- **14th WIEN2k – WORKSHOP, a satellite meeting to ICMAT'07 (Symposium O)**  
**IHPC, Singapore, July 6-9, 2007**



# General remarks on WIEN2k



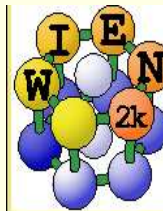
- WIEN2k consists of many independent F90 programs, which are linked together via C-shell scripts (needs Unix/Linux)
- real/complex version (inversion)
- 10 atom cells on 256Mb PC / 100 atom cells require 1-2 Gb RAM
- k-point parallel on clusters with common NFS (slow network)
- MPI/Scalapack parallelization for big cases (>100 atoms) and fast network (h-BN/Rh(111) nanomesh: 1100 atoms+vacuum on 64-100 cpus)
- You can run WIEN2k using any www-browser and the w2web interface, but also at the command line of an xterm.
- 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)`
- 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 GUI (graphical user interface)



- **Structure generator**
  - *spacegroup selection*
  - *import **cif** 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

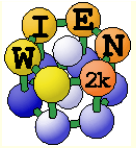
Inequivalent Atoms: 2

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



# Program structure of WIEN2k



## ■ **init\_lapw**

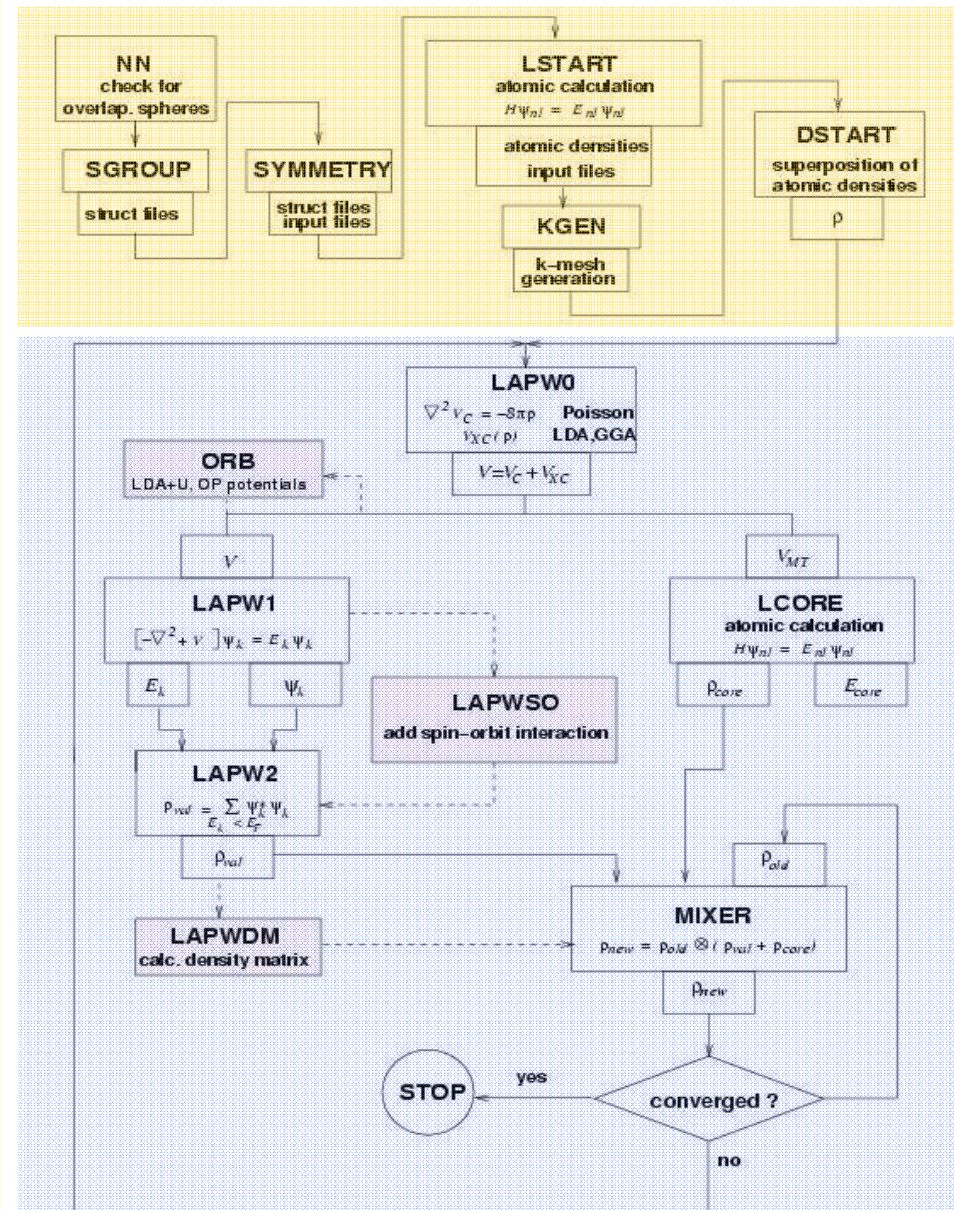
- *initialization*
- *symmetry detection (F, I, C-centering, inversion)*
- *input generation with recommended defaults*
- *quality (and computing time) depends on k-mesh and R.Kmax (determines #PW)*

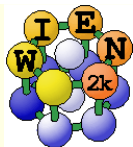
## ■ **run\_lapw**

- *scf-cycle*
- *optional with SO and/or LDA+U*
- *different convergence criteria (energy, charge, forces)*

## ■ **save\_lapw tic\_gga\_100k\_rk7\_vol0**

- *cp case.struct and clmsum files,*
- *mv case.scf file*
- *rm case.broyd\* files*





# Task for electron density plot



- A task consists of
  - a series of steps
  - that must be executed
  - to generate a plot
- For electron density plot
  - select states by E-window in case.in2 (e.g. valence  $e^-$ : Ti-3d,4s, C-2s,2p)
  - for difference densities make sure you calculate the same states for the free atoms
  - select plane for plot (do not put an atom at the corner or edges)
  - generate 3D or contour plot with gnuplot or Xcrysden (Tone.Kokalj@ijs.si)
  - reset EMIN in case.in2



## Execution >>

StructGen™  
initialize calc.  
run SCF  
single prog.  
optimize(V,c/a)  
mini. positions

## Utils. >>

## << Tasks

El. Dens.  
DOS  
XSPEC  
TELNES.2  
OPTIC  
Bandstructure

## Files >>

struct file(s)  
input files  
output files  
SCF files

## Session Mgmt. >>

change session  
change dir  
change info

## Configuration

Usersguide  
html-Version

Session: TiC

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

23:05:35 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.

edit TiC.in2 change EMIN to truncate semicore

x lapw2 Calculate clmval

### For difference densities only !

#### default valence states:

#### non-default valence states:

edit TiC.inst put P for all your states

x lstart -sigma Calculate atomic  
valence densities

x lstart Calculate atomic valence densities  
as defined above

Calculate density with XCrysden

edit TiC.in5 Edit input-file

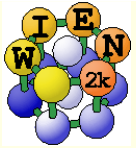
x lapw5 Calculate density

Preview density with XCrysden

rhoplot Plot Density

edit TiC.in2 reset EMIN

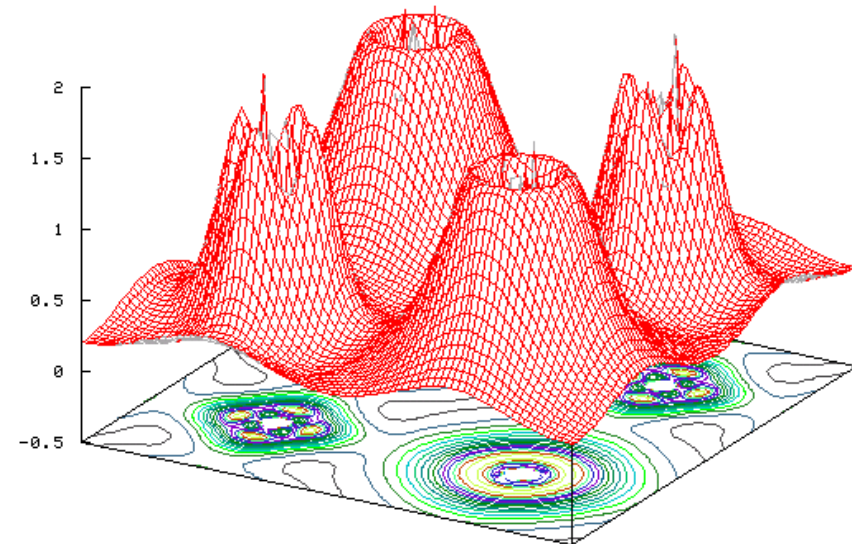
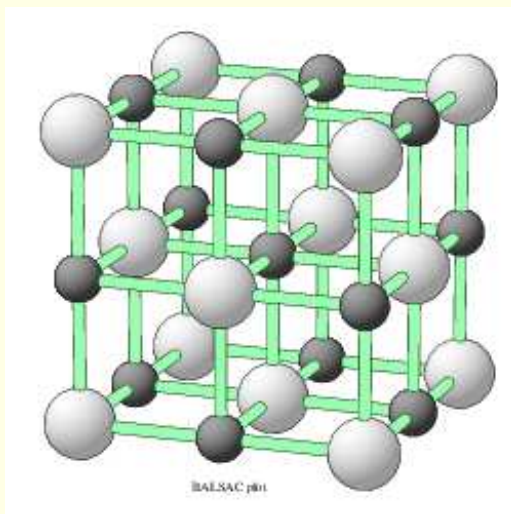




# TiC electron density



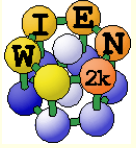
- NaCl structure (100) plane
- Valence electrons only
- plot in 2 dimensions
- Shows
  - *charge distribution*
  - *covalent bonding*
    - between the Ti-3d and C-2p electrons
  - $e_g/t_{2g}$  symmetry



[Download hardcopy in PostScript format](#)

Select plot type: 3D-plot ☒ Contur-plot ☐ with labels ☐

Min  Max  Delta

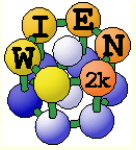


# Getting help



- `*_lapw -h` „help switch“ of all WIEN2k-scripts
- `help_lapw`:
  - opens *usersguide.pdf*; Use *^f keyword* to search for an item („index“)
- html-version of the UG: (`$WIENROOT/SRC_usersguide/usersguide.html`)
- [http://www.wien2k.at/reg\\_user](http://www.wien2k.at/reg_user)
  - *FAQ page with answers to common questions*
  - *Update information: When you think the program has an error, please check newest version*
  - *Textbook section: DFT and the family of LAPW methods by S.Cottenier*
  - *Mailing-list:*
    - **subscribe** to the list (always use the same email)
    - **full text search** of the „digest“ (your questions may have been answered before)
    - **posting questions:** **Provide sufficient information**, locate your problem (case.dayfile, \*.error, case.scf, case.outputX).
    - „**My calculation crashed. Please help.**“ This will most likely not be answered.



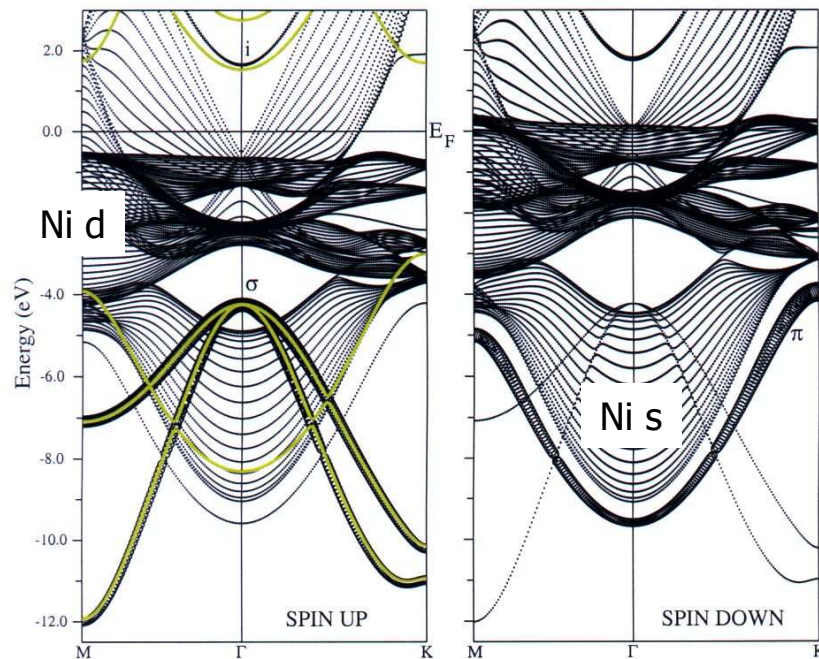


# Properties with WIEN2k - I

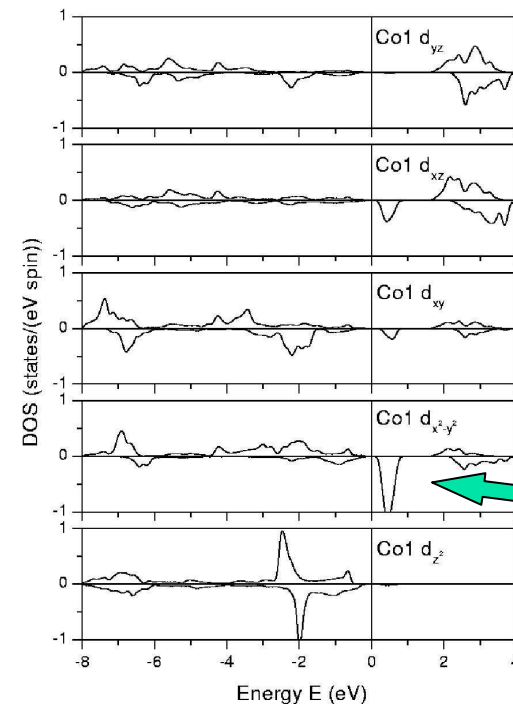


- **DFT:** LDA, various GGAs; meta-GGA, LDA+U; Hybrids for „correlated electrons“)
- **Energy bands**
  - *classification of irreducible representations*
  - *'character-plot' (emphasize a certain band-character)*
- **Density of states**
  - *including partial DOS with  $l$  and  $m$ - character (eg.  $p_x, p_y, p_z$ )*

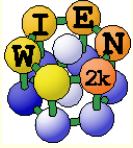
## h-BN/Ni(111): $\sigma$ and $\pi$ bands



## BaCoO<sub>3</sub>



**$d_{x^2-y^2}$**



# Properties with WIEN2k - II

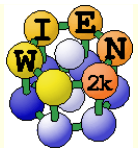


## ■ Electron density, potential

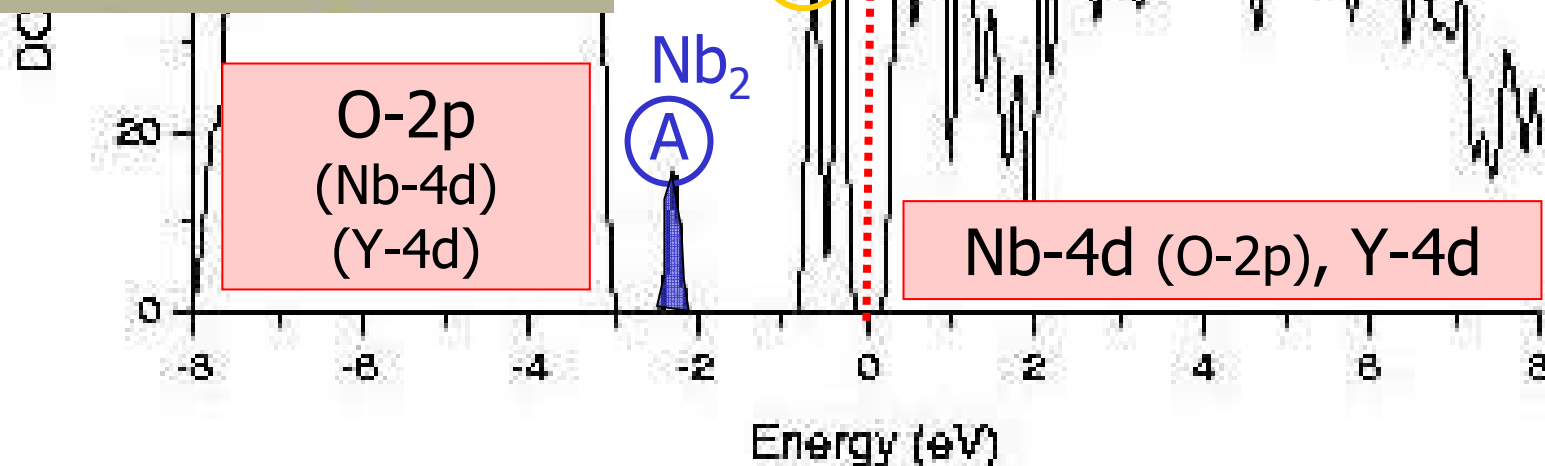
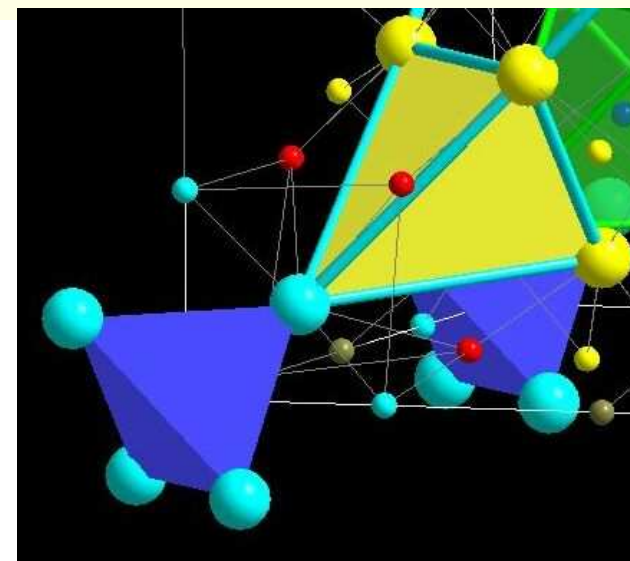
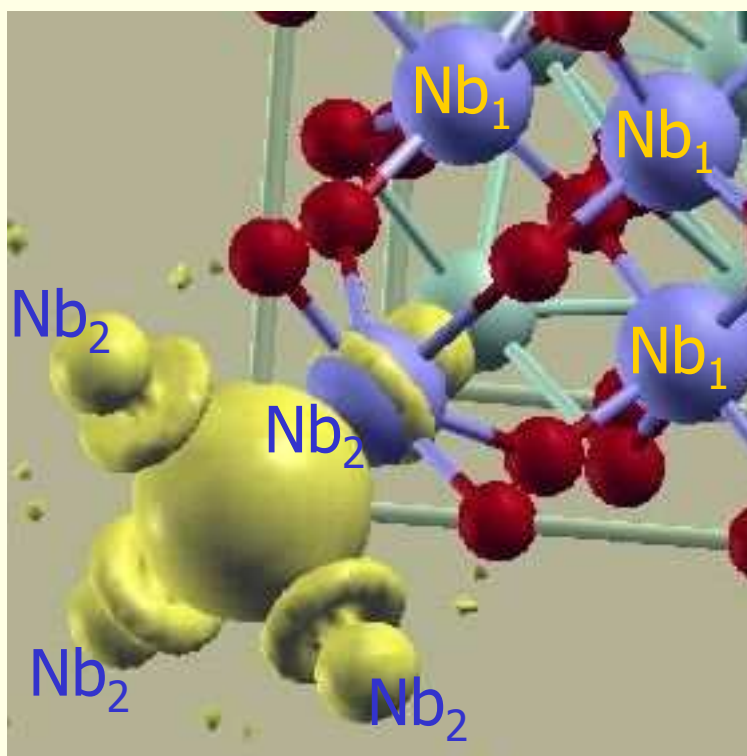
- *total-, valence-, difference-, spin-densities,  $\rho$  of selected states*
- *1-D, 2D- and 3D-plots (Xcrysden)*
- *X-ray structure factors*
- *Bader's atom-in-molecule analysis, critical-points, atomic basins and charges ( $\nabla \rho \cdot \vec{n} = 0$ )*
- *spin+orbital magnetic moments (+ spin-orbit )*

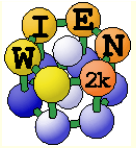
## ■ Hyperfine parameters

- *hyperfine fields (contact + dipolar + orbital contribution)*
- *Isomer shift*
- *Electric field gradients*



# $\text{Y}_2\text{Nb}_2\text{O}_7$ : Peak A ( $\text{Nb}_2$ ) 4-center bond ( $d\text{-}z^2$ )





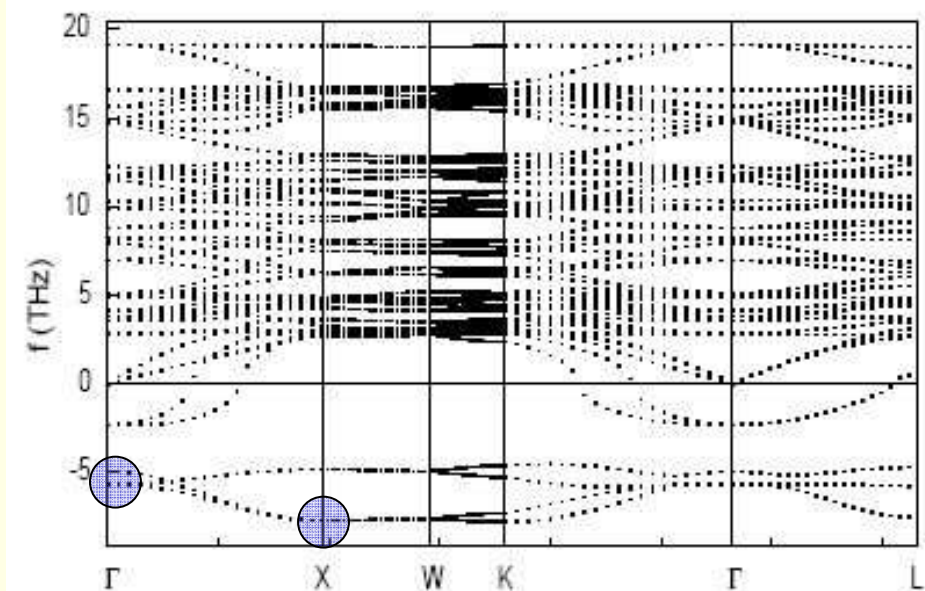
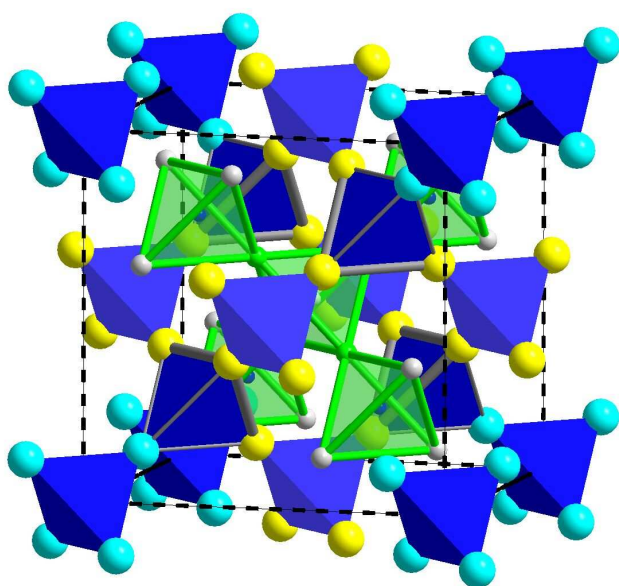
# Properties with WIEN2k - III

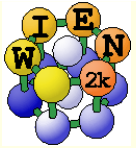


## ■ Total energy and forces

- *optimization of internal coordinates, (damped MD, BROYDEN)*
- *cell parameter only via  $E_{tot}$  (no stress tensor)*
- *elastic constants for cubic cells*
- *Phonons via a direct method (based on forces from supercells)*
  - interface to PHONON (K.Parlinski) – bands, DOS, thermodynamics, neutrons

Pyrochlore structure of  $\text{Y}_2\text{Nb}_2\text{O}_7$ : strong phonon instabilities  $\rightarrow$  phase transition



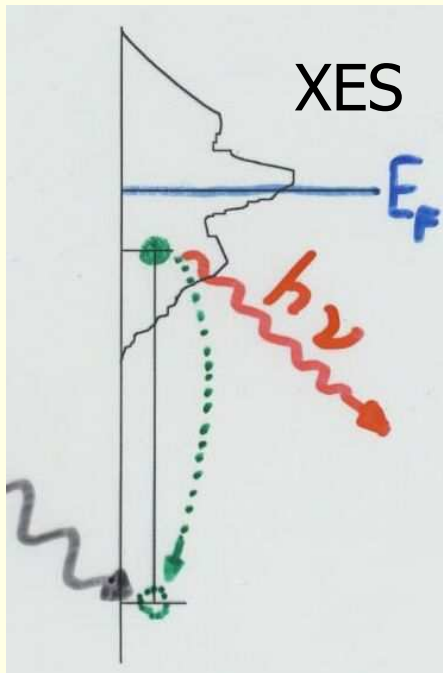


# Properties with WIEN2k - IV



## ■ Spectroscopy

- *core levels (with core holes)*
- *X-ray emission, absorption, electron-energy-loss*
  - (core - valence/conduction-band transitions including matrix elements and angular dep.)
  - EELS inclusion of possible non-dipol transistons (momentum transfer)
- *optical properties (dielectric function in RPA, JDOS including momentum matrix elements and Kramers-Kronig)*
- *fermi surface (2D, 3D)*

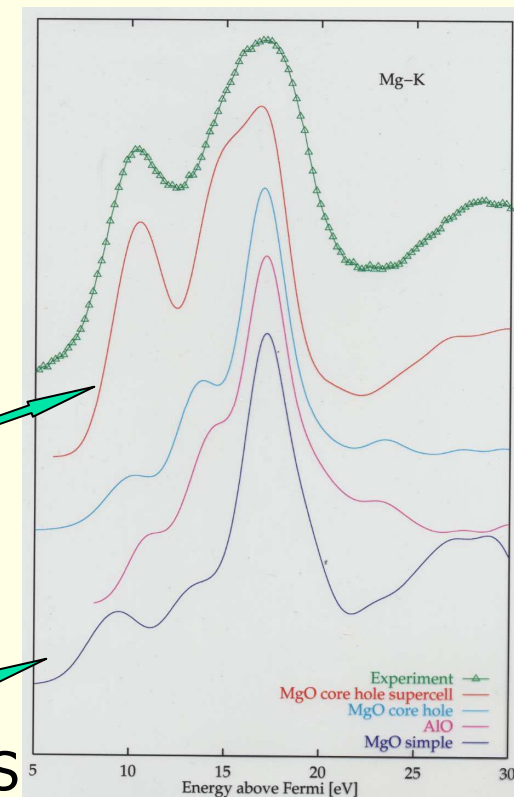


## Mg-K XAS

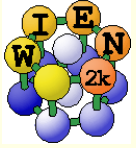
probes empty Mg-p

including a core-hole  
in supercell  
(Final state rule)

from ground-state DOS





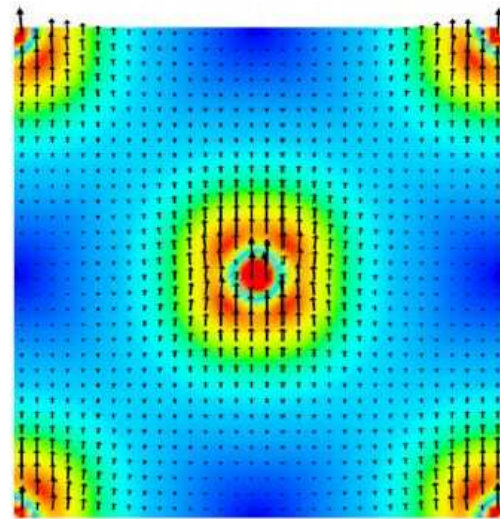


# Properties with WIEN2k - V

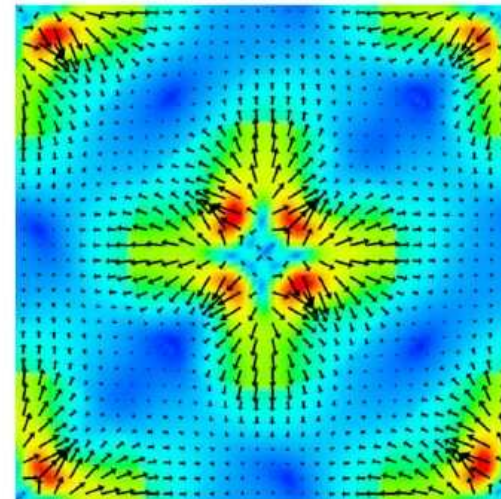


- **New developments (available)**
  - *non-linear optics (B.Olejník)*
  - *non-collinear magnetism (spin-spirals to fully-relativistic) (R.Laskowski)*
  - *transport properties (Fermi velocities, Seebeck, conductivity, thermoelectrics, ..) (G.Madsen)*

## Intra-atomic NCM, fcc $Pu$

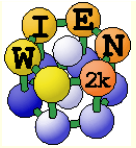


(a) plane  $x = 0$



(b) plane  $z = 1/10$

Spin density maps of **fcc Pu**. Calculation in FULL mode with SO. Average momenta point to  $\langle 001 \rangle$

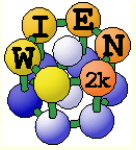


# Advantage/disadvantage of WIEN2k



- + robust all-electron full-potential method
- + unbiased basisset, one convergence parameter (LDA-limit)
- + all elements of periodic table (equal expensive), metals
- + LDA, GGA, meta-GGA, LDA+U, spin-orbit
- + many properties and tools (supercells, symmetry)
- + w2web (for novice users)
- ? speed + memory requirements
  - + *very efficient basis for large spheres (2 bohr) (Fe: 12Ry, O: 9Ry)*
  - *less efficient for small spheres (1 bohr) (O: 25 Ry)*
  - *large cells, many atoms ( $n^3$ , iterative diagonalization not perfect)*
  - *full H, S matrix stored  $\rightarrow$  large memory required*
  - + *many k-points do not require more memory*
- no stress tensor
- no linear response

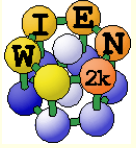




# Conclusion



- There are many ways to make efficient use of DFT calculations
- APW+lo method (as implemented in WIEN2k) is one of them
  - *all electron*
  - *full-potential*
  - *highly accurate - benchmark for other methods*
  - *many properties*
  - *user friendly*
  - *widely used*
    - development by several groups
    - large user community
    - used by many experimental groups



Thank you for  
your attention !