

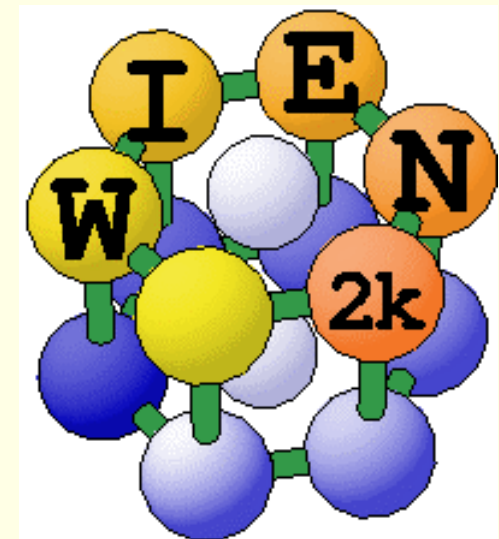


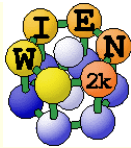
The FP-LAPW and APW+lo methods

Peter Blaha

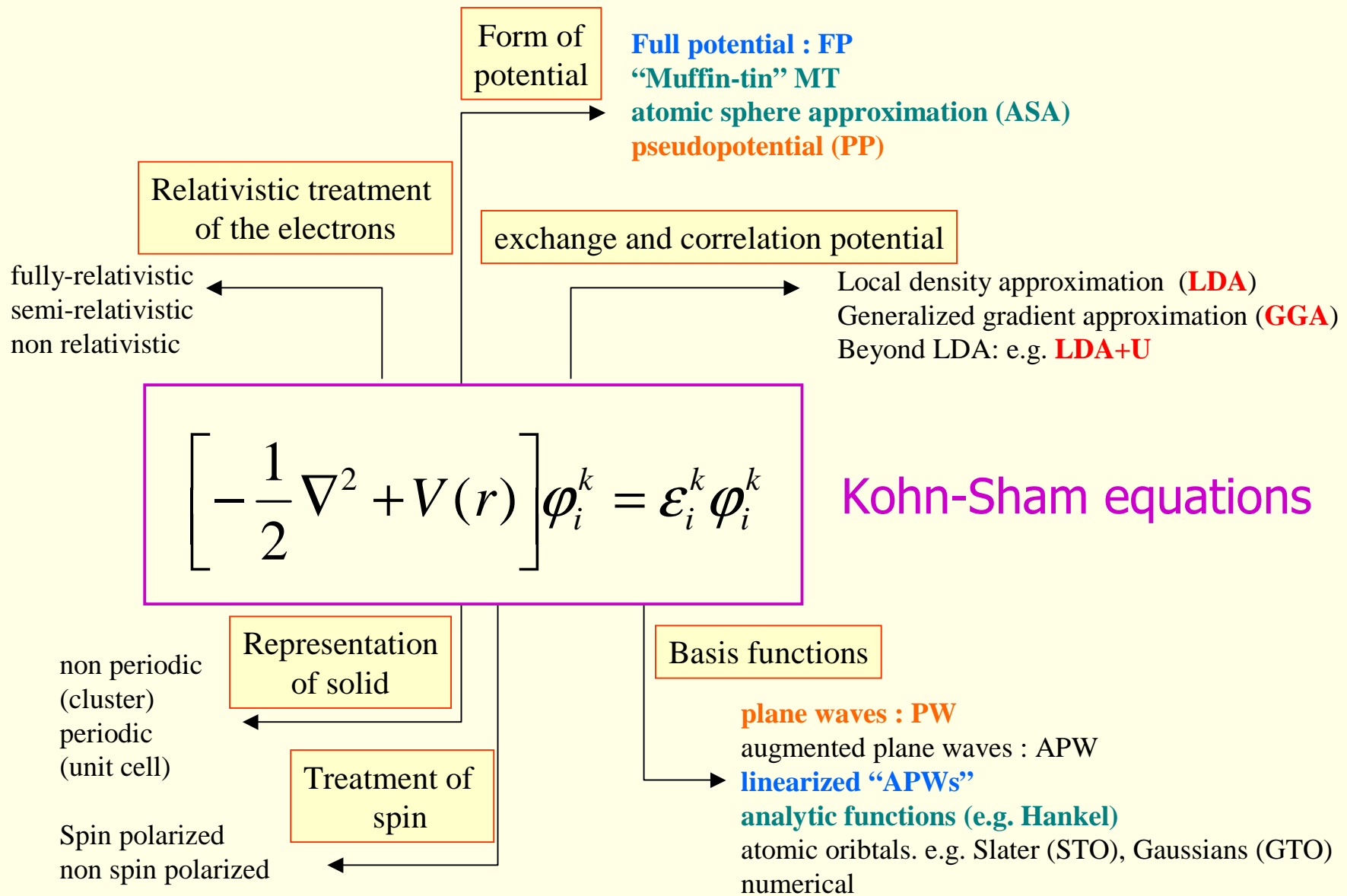
Institute of Materials Chemistry

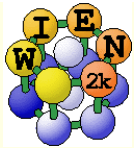
TU Wien





Overview of DFT concepts

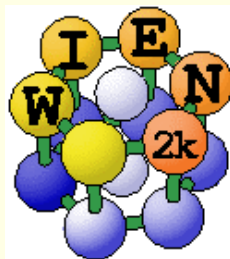




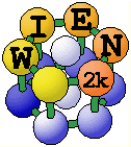
APW based schemes



- **APW (J.C.Slater 1937)**
 - *Non-linear eigenvalue problem*
 - *Computationally very demanding*
- **LAPW (O.K.Anderssen 1975)**
 - *Generalized eigenvalue problem*
 - *Full-potential*
- **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)



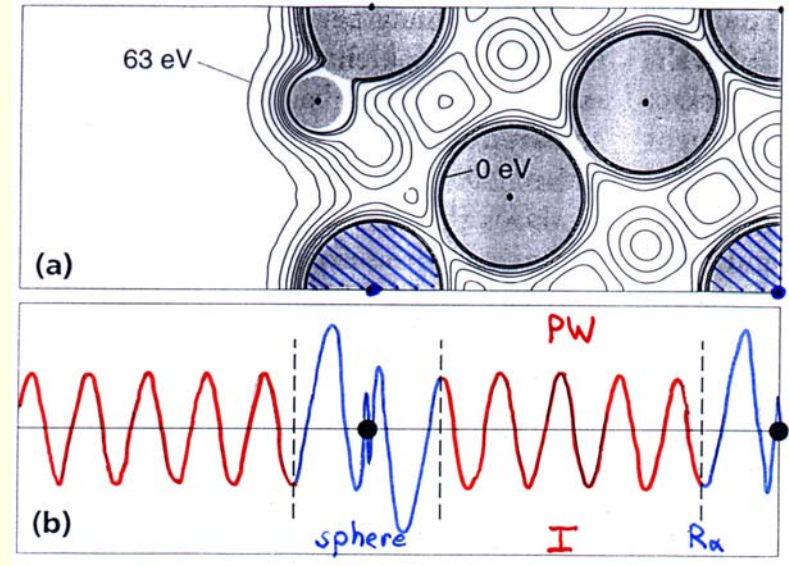
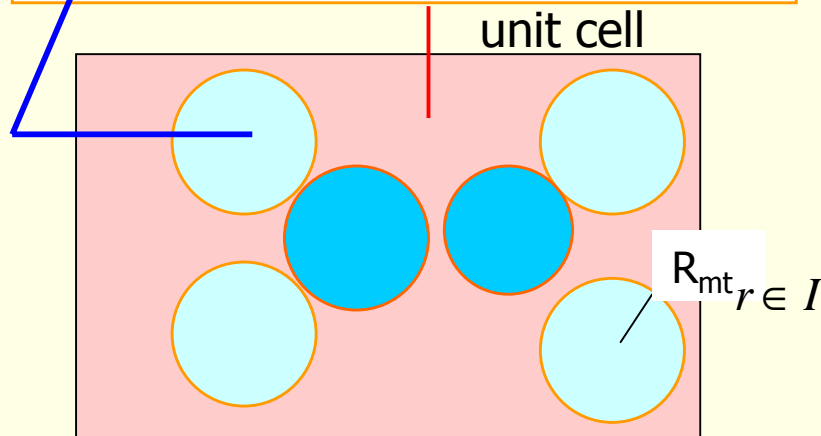
APW Augmented Plane Wave method



The unit cell is partitioned into:

atomic spheres

Interstitial region



Basisset:

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

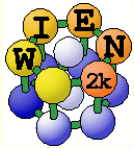
Atomic partial waves

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

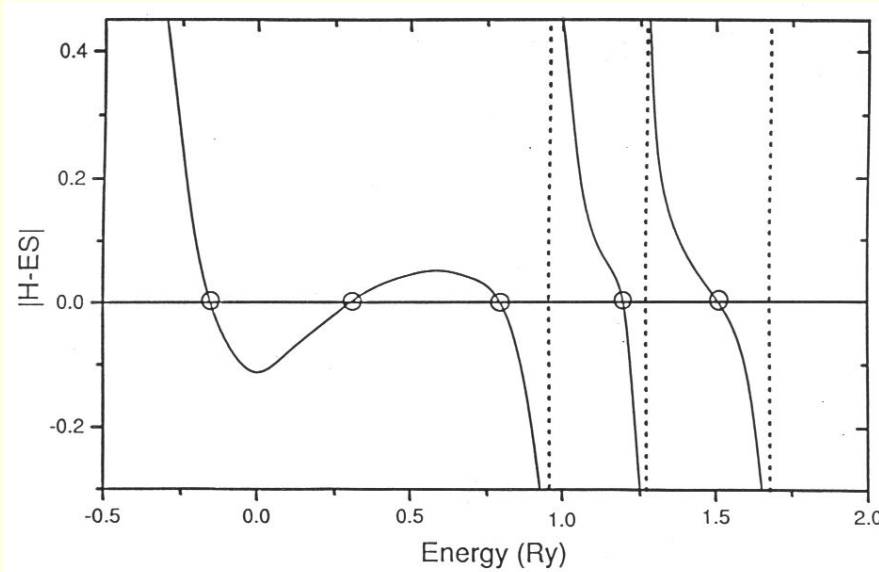
join

$u_{\ell}(r, \varepsilon)$ are the numerical solutions of the radial Schrödinger equation in a given spherical potential for a particular energy ε

$A_{\ell m}^K$ coefficients for matching the PW



Slater's APW (1937)



H Hamiltonian
S overlap matrix

Atomic partial waves

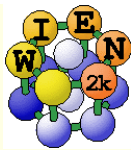
$$\sum_{\ell m} A_{\ell m}^K u_{\ell}(r', \varepsilon) Y_{\ell m}(\hat{r}')$$

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 MT potential!

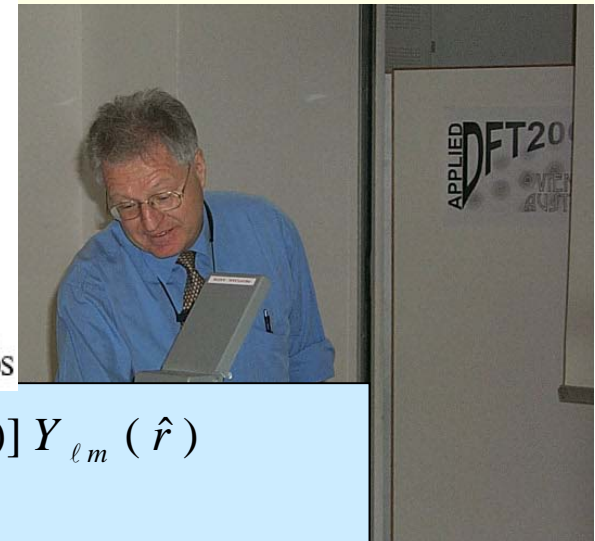
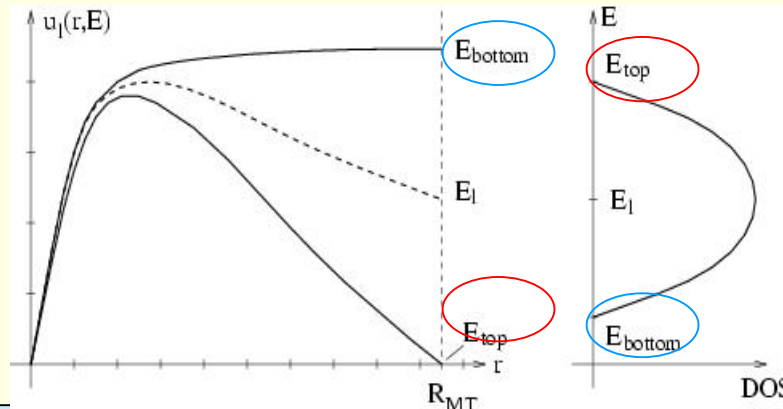


Linearization of energy dependence



LAPW suggested by

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



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

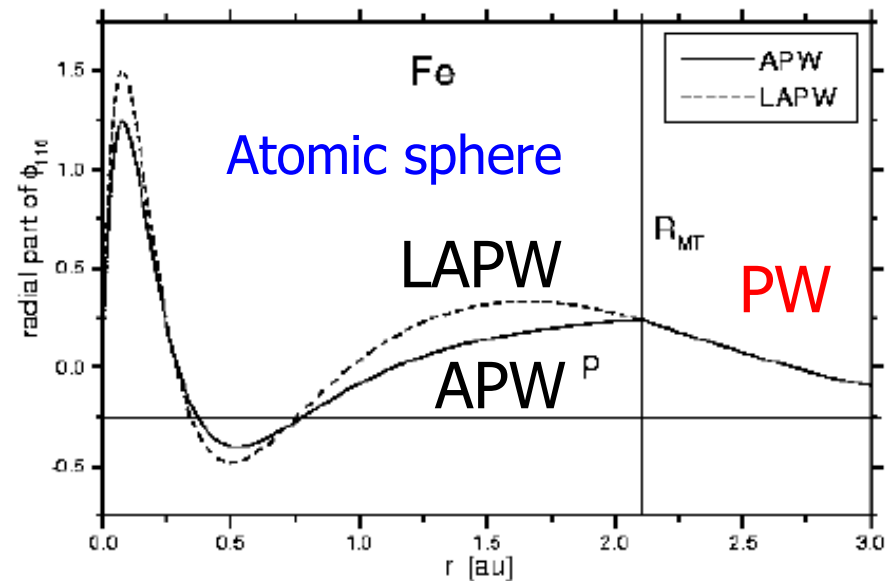
expand u_l at fixed energy E_l and
add $\dot{u}_l = \partial u_l / \partial \epsilon$

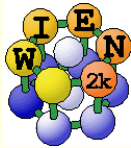
A_{lm}^k, B_{lm}^k : join PWs in value and
slope

→ additional constraint requires

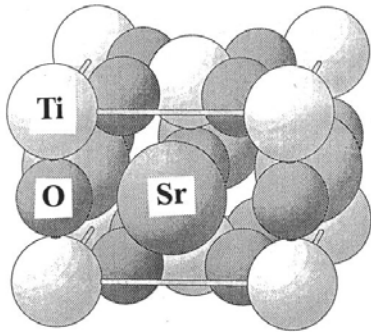
more PWs than APW

→ basis flexible enough for single
diagonalization

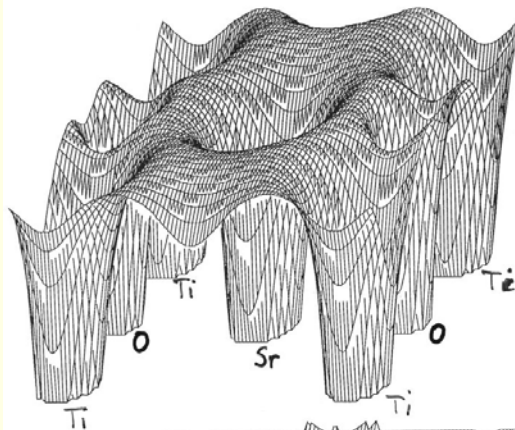




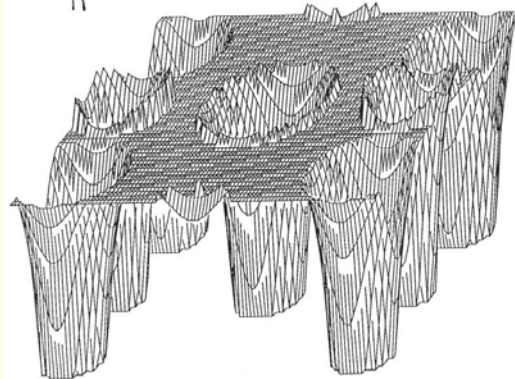
Full-potential in LAPW (A.Freeman et al.)



SrTiO₃



Full potential



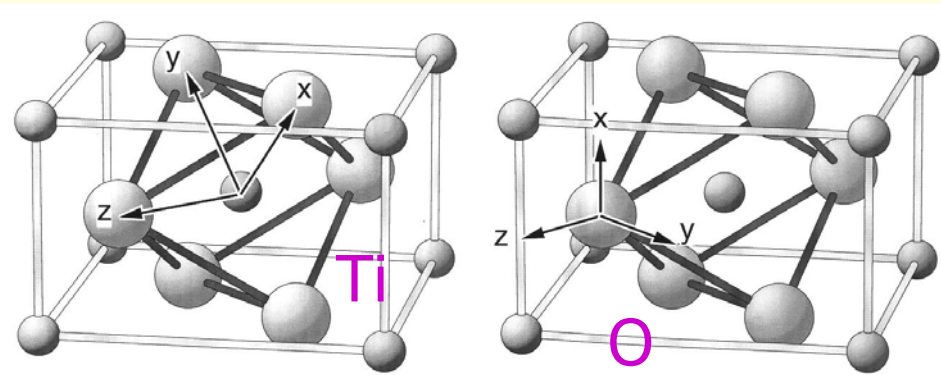
Muffin tin approximation

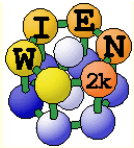
TiO₂ rutile

- 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)

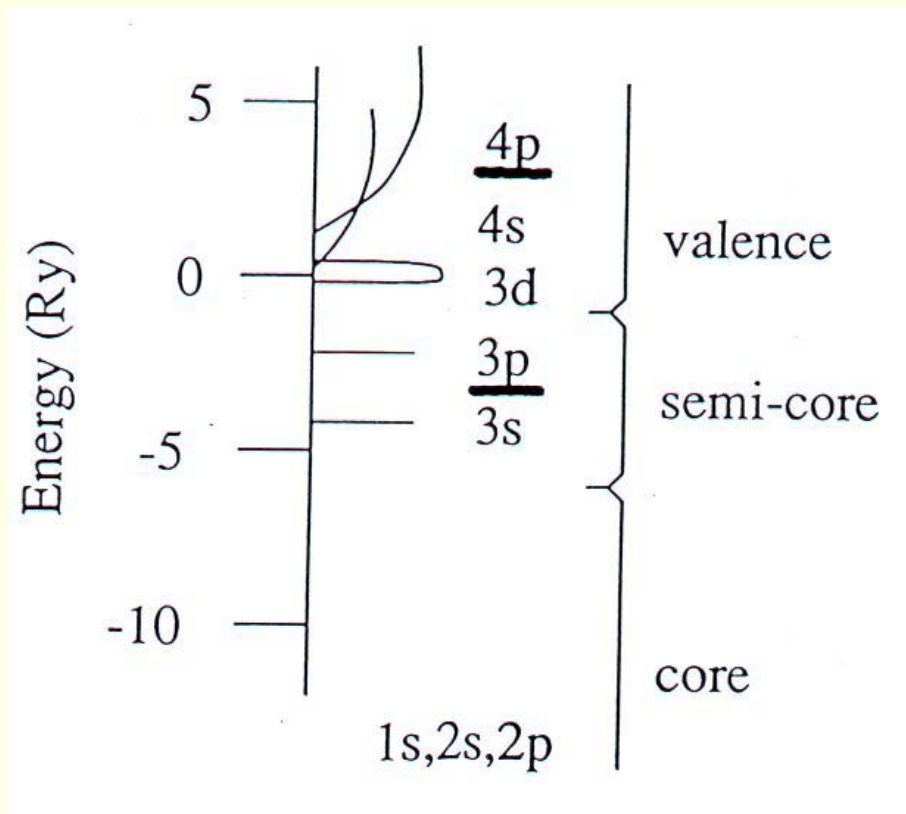




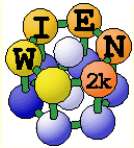
Core, semi-core and valence states



For example: **Ti**

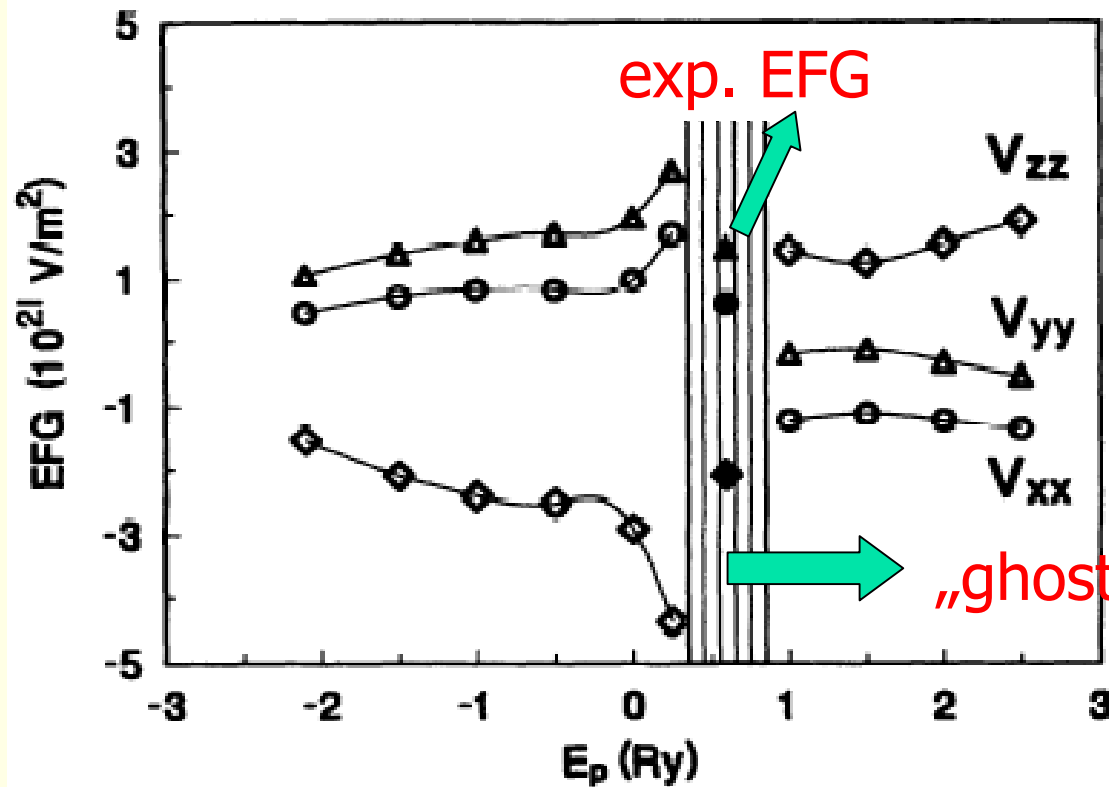


- **Valence states**
 - *High in energy*
 - *Delocalized wavefunctions*
- **Semi-core states**
 - *Medium energy*
 - *Principal QN one less than valence (e.g. in Ti 3p and 4p)*
 - *not completely confined inside sphere*
- **Core states**
 - *Low in energy*
 - *Reside inside sphere*

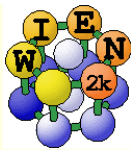


Problems of the LAPW method:

EFG Calculation for Rutile 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).



Problems of the LAPW method



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

Metal
 Semimetal
 Nonmetal

 Problems with semi-core states

(c) 1998
Kremer Paul



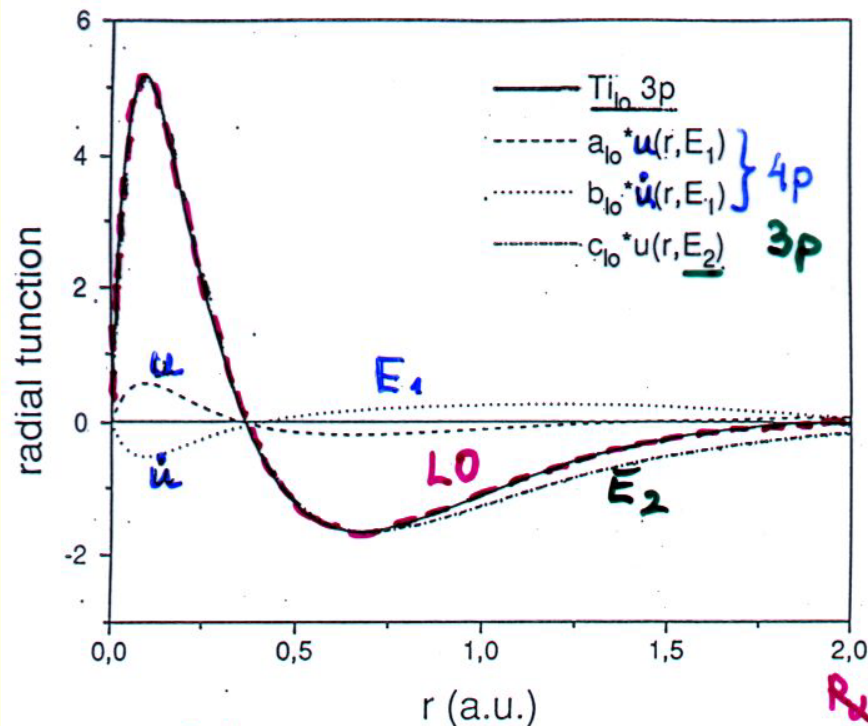
Problems with semi-core states



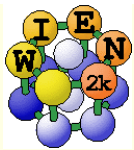
$$\Phi_{LO} = [A_{\ell m} u_{\ell}^{E_1} + B_{\ell m} \dot{u}_{\ell}^{E_1} + C_{\ell m} u_{\ell}^{E_2}] Y_{\ell m}(\hat{r})$$

■ LO

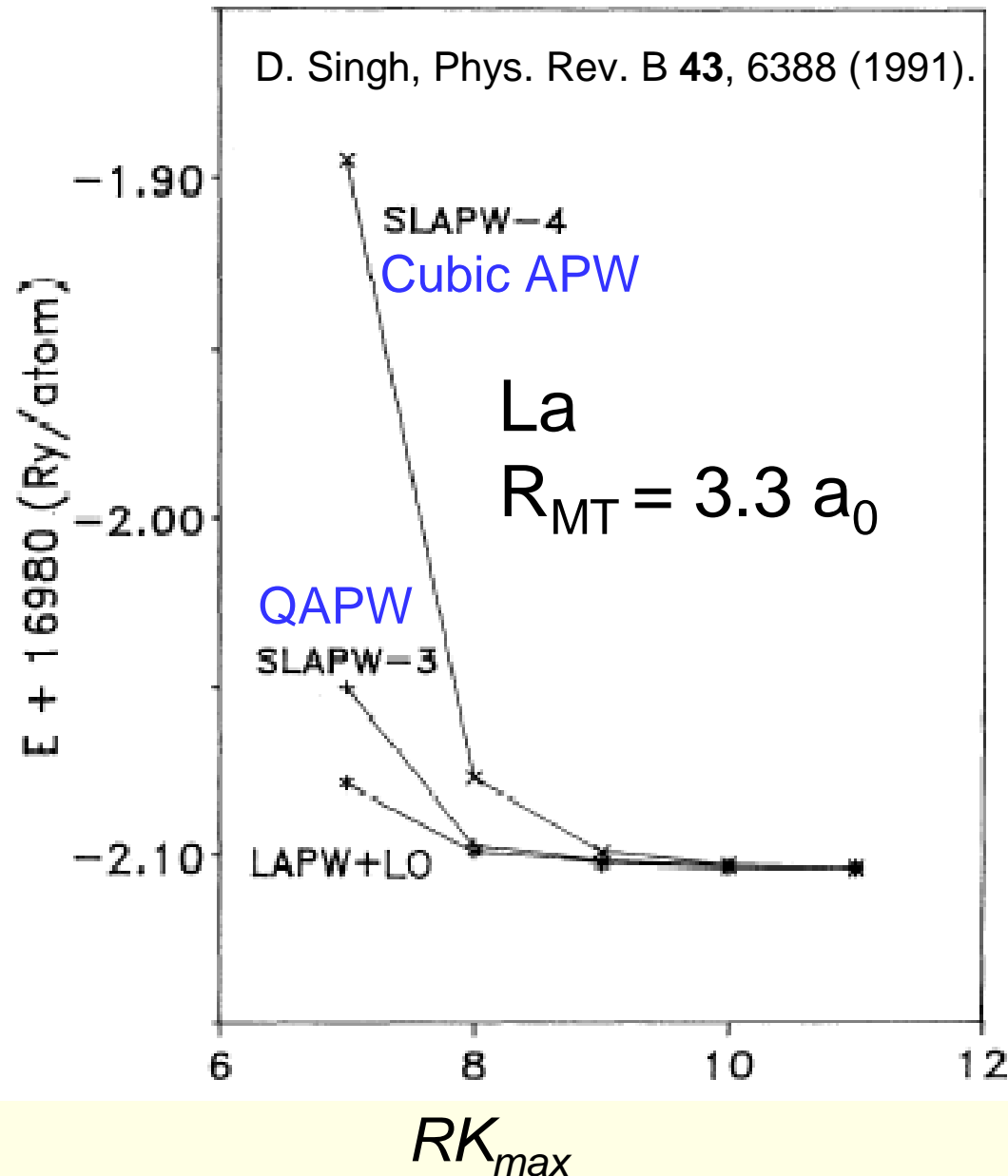
- *is confined to an atomic sphere*
- *has zero value and slope at R*
- *can treat two principal QN n for each azimuthal QN ℓ (3p and 4p)*
- *corresponding states are strictly orthogonal (no "ghostbands")*
- *tail of semi-core states can be represented by plane waves*
- *only slight increase of basis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



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



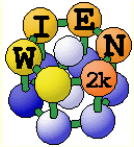
The LAPW+LO Method



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 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)

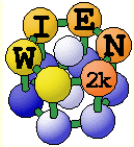
- Use **APW**, but at **fixed E_l** (superior PW convergence)
- **Linearize** with **additional lo** (add a few basis functions)

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

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

optimal solution: mixed basis

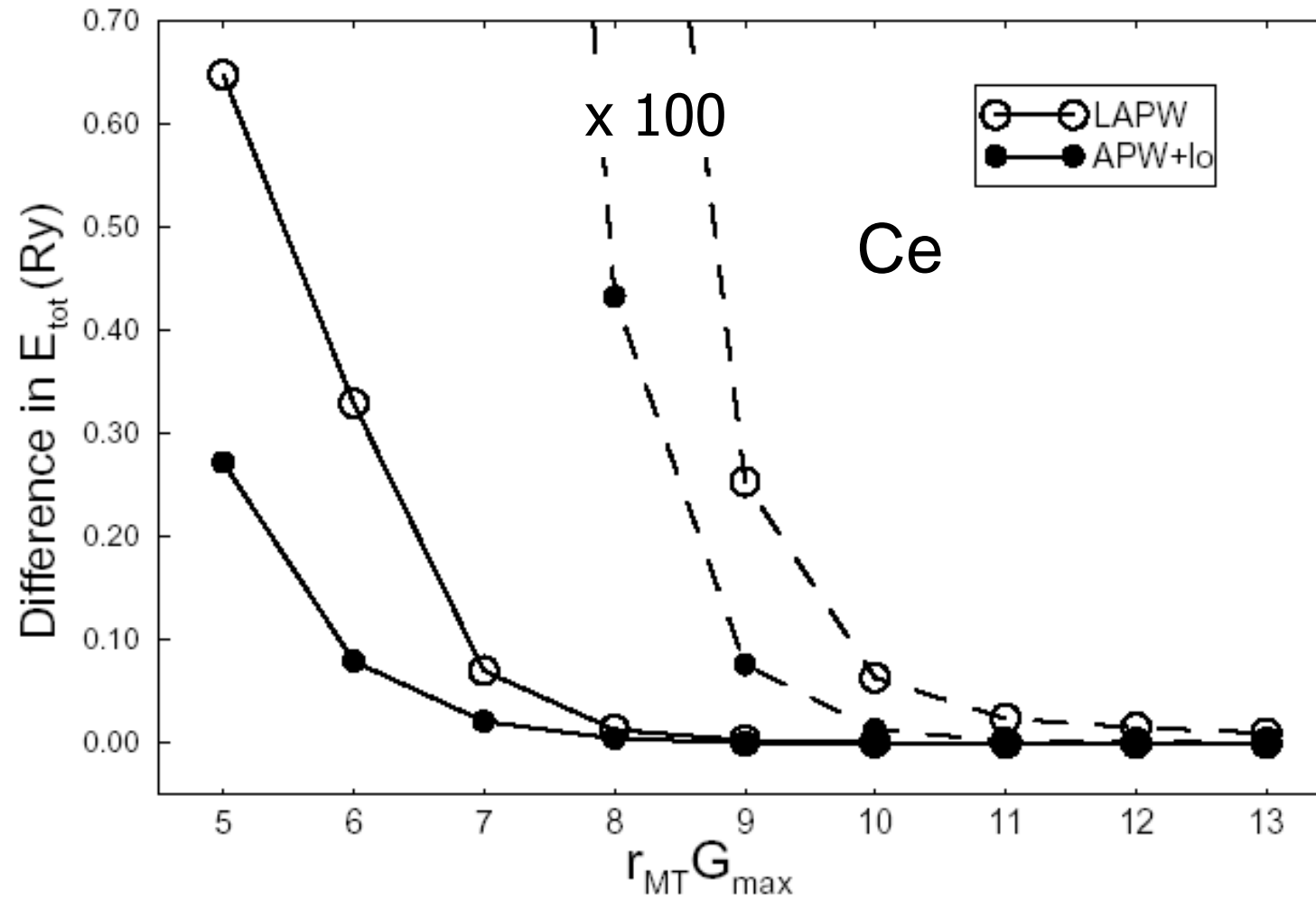
- use APW+lo for states which are difficult to converge:
(f or d- states, atoms with small spheres)
- use LAPW+LO for all other atoms and angular momenta

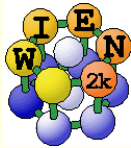


Convergence of the APW+LO Method



E. Sjostedt, L. Nordstrom and D.J. Singh, Solid State Commun. 114, 15 (2000).





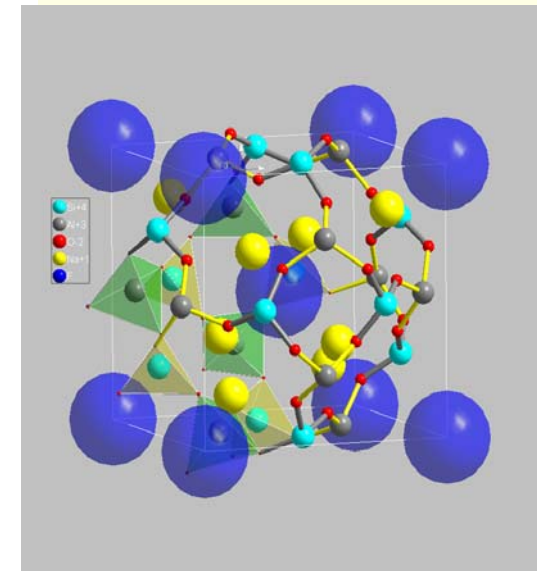
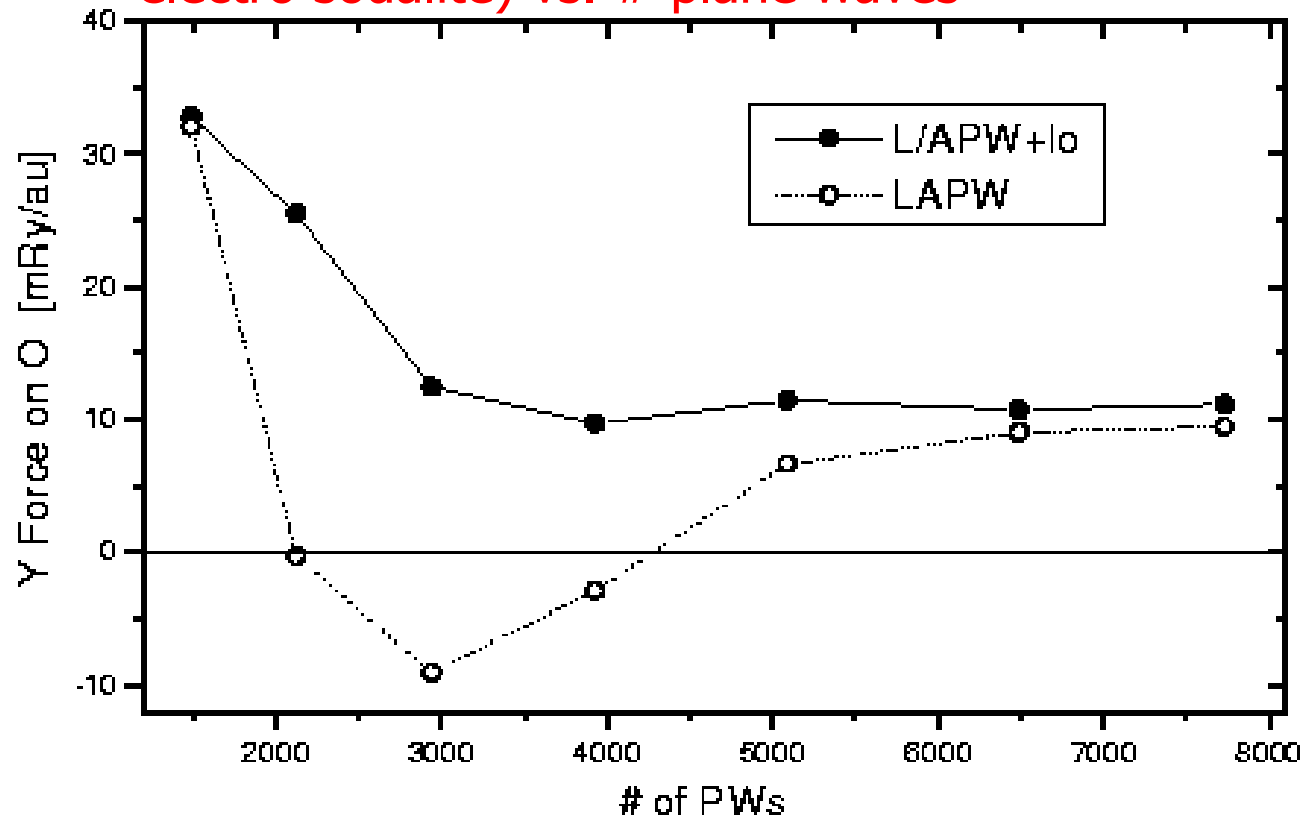
Improved convergence of APW+lo

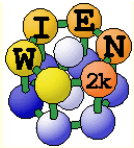


K.Schwarz, P.Blaha, G.K.H.Madsen,
Comp.Phys.Commun.147, 71-76 (2002)

- 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

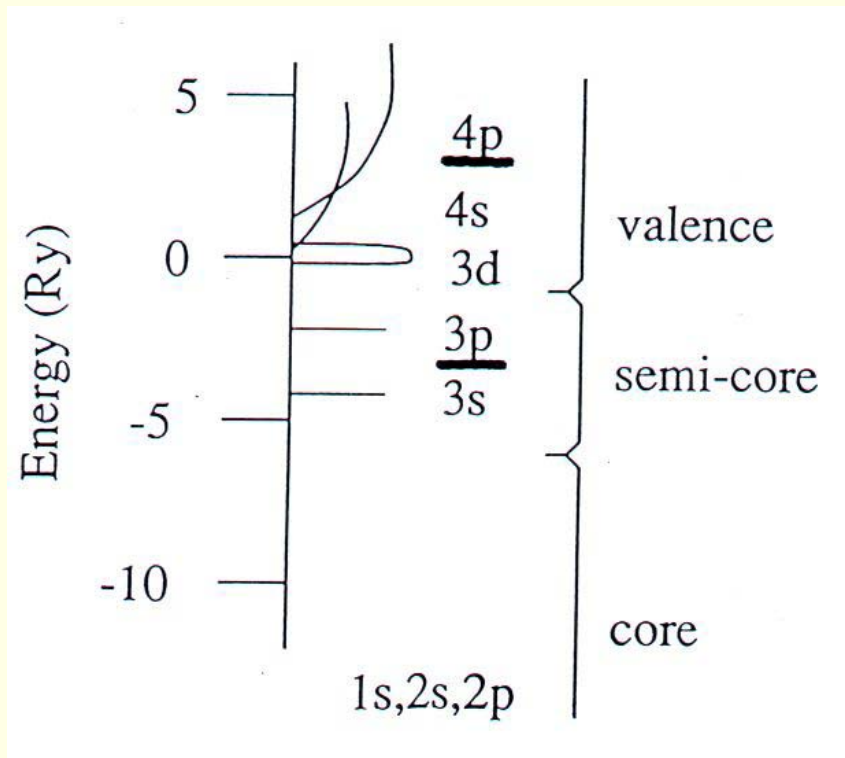




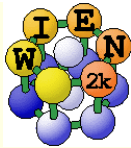
Relativistic treatment



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_{1/2})
- **Core states**
 - *Fully relativistic*
 - Dirac equation



Relativistic semi-core states in fcc Th

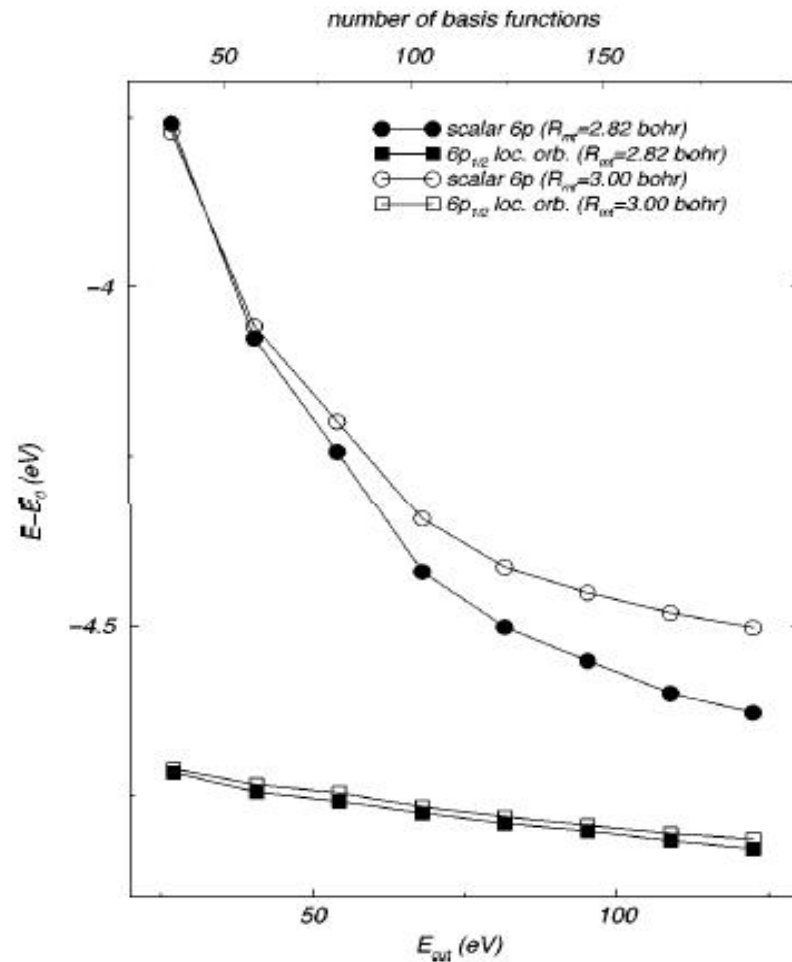


FIG. 1. The total energy E as a function of the second-variation cutoff energy E_{cut} (the approximate size of the second-variational-step basis, including spin, is marked on the top axis) for two different muffin-tin radii. The standard FLAPW results are marked with circles, the results obtained with 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 (2nd variational method)

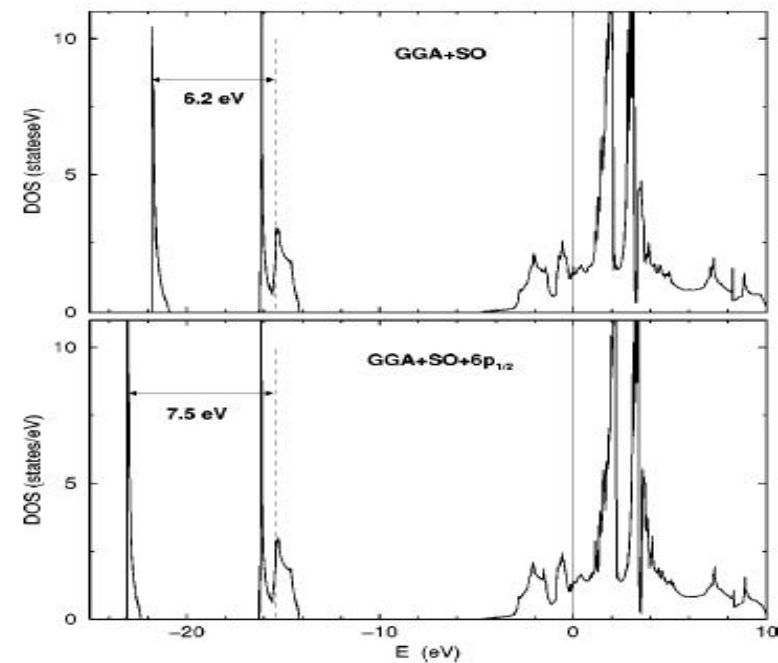
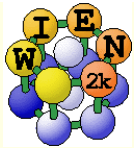


FIG. 2. Density of states calculated with the scalar relativistic basis (top panel) and with the $p_{1/2}$ local orbitals extended basis (bottom panel). The splitting between the centers of $6p_{1/2}$ and $6p_{3/2}$ bands is shown.

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 α :

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

Hellmann-Feynman-force

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

Pulay corrections

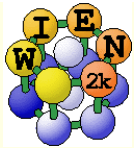
- Core
- Valence

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

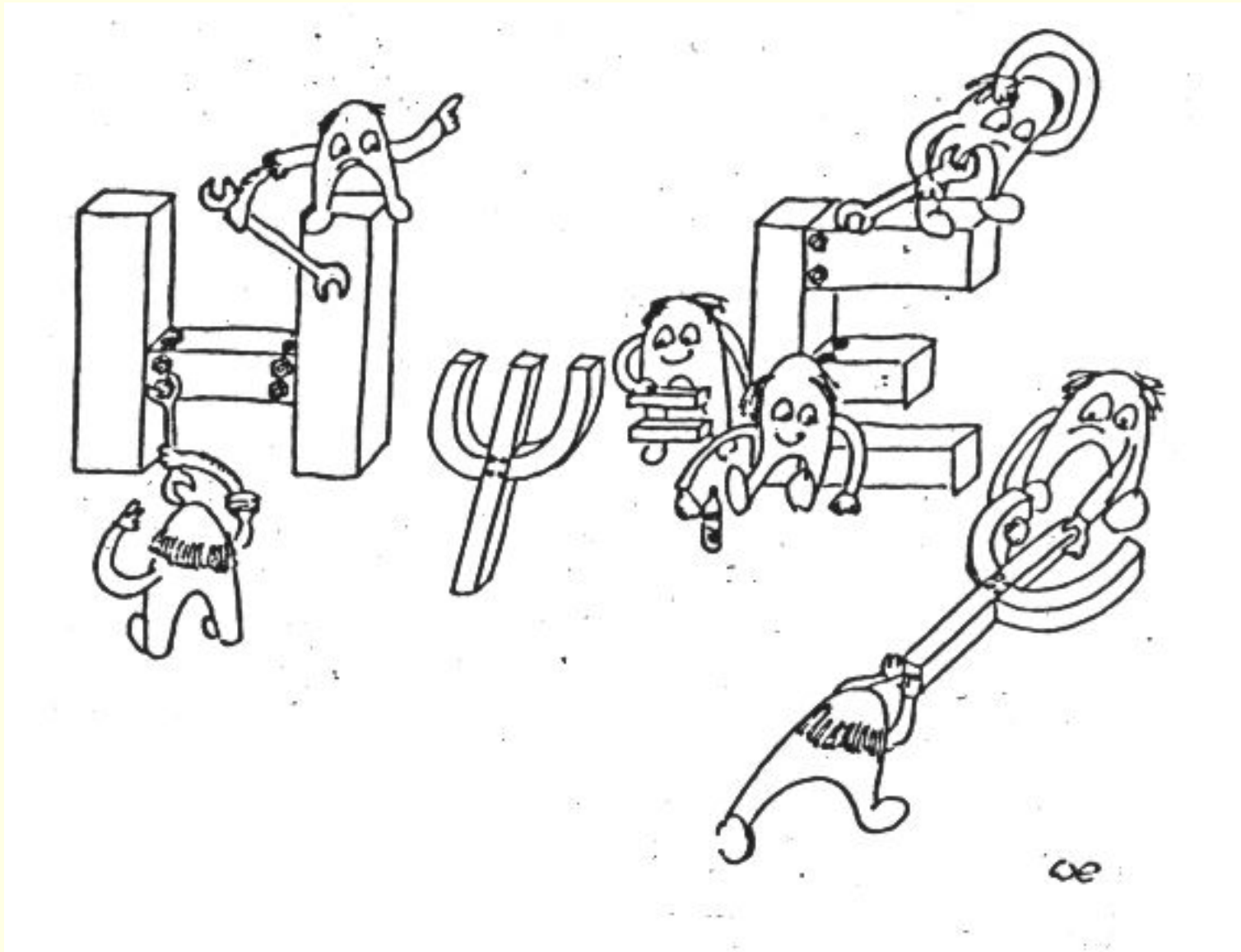
- expensive, contains a summation of matrix elements over all occupied states

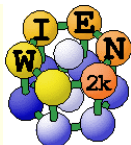
$$F_{val}^{\alpha} = \int_{\alpha} V_{eff}(r) \nabla_{\alpha} \rho_{val}(r) d\vec{r} + \sum_{k,i} n_i \sum_{K,K'} c_i^*(K') c_i(K) \times$$

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

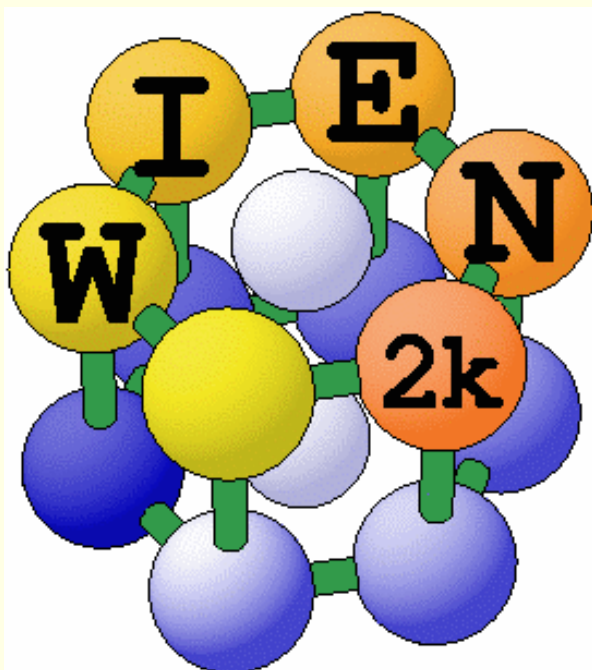


Quantum mechanics at work





WIEN2k software package



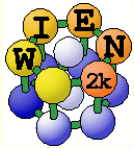
WIEN97: ~500 users
WIEN2k: ~500 users
mailinglist: 800 users

**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



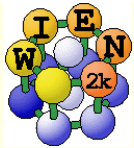
■ Authors of WIEN2k

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

■ Other contributions to WIEN2k

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

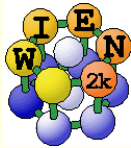
■ and many others



International co-operations



- **More than 500 user groups worldwide**
 - *Industries* (Canon, Eastman, Exxon, Fuji, A.D.Little, Mitsubishi, Motorola, NEC, Norsk Hydro, Osram, Panasonic, Samsung, Sony, Sumitomo).
 - *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**
 - *400/4000 Euro for Universities/Industries*
 - *code download via www (with password), updates, bug fixes, news*
 - *usersguide, faq-page, mailing-list with help-requests*

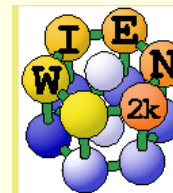


WIEN2k- hardware/software



- WIEN2k runs on any **Unix/Linux** platform from PCs, workstations, clusters to supercomputers
- **Fortran90** (dynamical allocation)
- many individual **modules**, linked together with **C-shell** or perl-scripts
- **f90 compiler**, **BLAS-library**, perl5, ghostview, gnuplot, Tcl/Tk (Xcrysden), pdf-reader, www-browser

- web-based GUI – **w2web**
- **real/complex** version (inversion)
- 10 atom cells on **128Mb 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 (>50 atoms) and **fast** network
- installation support for most platforms



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Session: TiC User: **pblaha**
/susi/pblaha/lapw/TiC

Thu Nov 29 13:22:25 2001
STATUS: idle
[refresh](#) [noefresh](#)

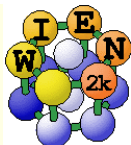
w2web, the fully web-enabled interface to WIEN2k

Session Name:	TiC
Session ID:	599582
Directory:	/susi/pblaha/lapw/TiC
Last changed:	Wed Nov 21 10:12:17 2001
Comments:	

- spin polarized calculation
- AFM calculation
- complex calculation (no inversion)
- parallel calculation

Change session information





■ Based on **www**

- *WIEN2k can be managed remotely via w2web*
- *Secure (Password)*

■ Important steps:

- *start w2web on all your hosts*
- *use your favorite browser and connect to the master host*
- *define a session on the desired host*

Welcome to *w2web*
the fully web-enabled interface to WIEN2k

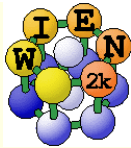
Select stored session:

- Fccni
- tic**
- TiO2
- bccw
- fcccu_ldau
- fcccu
- fccyb_sp
- fccyb
- he_surf_0
- nibnn
- si_goessl
- test
- tic_goessl
- tic_puls
- tio_puls

Create new session:

on host-node

- master node**
- http://jupiter:10000
- http://homer:10000
- http://pauli:10000
- http://fp98.zserv:10000
- http://hal.zserv:10000



GUI (Graphical user interface)



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

Session: TiC User: pblaha /susi/pblaha/lapw/TiC

The Nov 29 13:23:41 2001 STATUS: idle refresh none#

StructEdit /susi/pblaha/lapw/TiC

StructGen™

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

Save Structure

Title: TiC

Treatment of core: relativistic

Lattice:
Type: F
P
F
B
inequivalent Atoms: 2

Lattice parameters in Å

a= 4.46770858 b= 4.46770858 c= 4.46770858
a= 90.000000 b= 90.000000 g= 90.000000

Atom 1: Ti x= 0.000000000 y= 0.000000000 z= 2.2.0 [remove atom](#)

NPT= 781 RMT= 2.000 RO= 0.00005 Non-cubic

Pos 1: x= 0.000000000 y= 0.000000000 z= 0.000000000 [remove](#)
[add position](#)

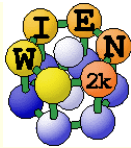
Atom 2: C x= 0.500000000 y= 0.500000000 z= 0.500000000 [remove atom](#)

NPT= 781 RMT= 1.900 RO= 0.00010 Non-cubic

Pos 1: x= 0.500000000 y= 0.500000000 z= 0.500000000 [remove](#)
[add position](#)
[add an atom](#)

Number of symmetry operations: 48

Idea and realization by [Lutz J. J.](#) ©2001



Program structure of WIEN2k

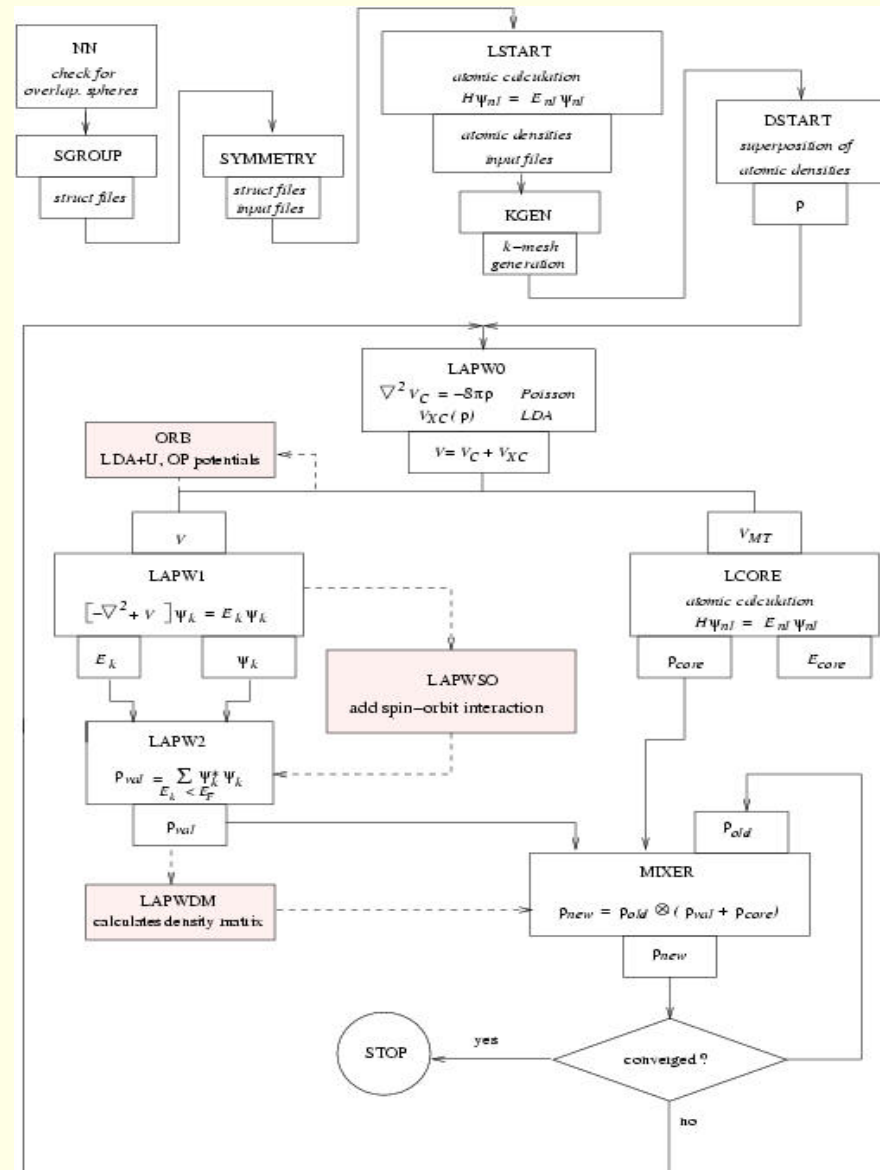


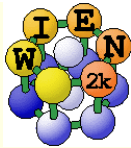
■ `init_lapw`

- *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)*

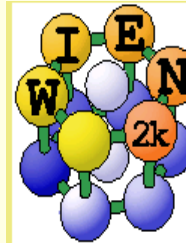




Task for electron density plot



- A task consists of
 - *a series of steps*
 - *that must be executed*
 - *to generate a plot*
- For electron density plot
 - *select states (e.g. valence e^-)*
 - *select plane for plot*
 - *generate 3D or contour plot with gnuplot or Xcrysden*



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Session: TiC User: pblaha
/susi/pblaha/lapw/TiC

Thu Nov 25 13:26:30 2004
STATUS: idle
[re@esh](#) [nore@esh](#)

Electron density plots

edit TiC.in2 change EMIN

x lapw2 Calculate clmval

Calculate density with XCrysden

edit TiC.in5 Edit input-file

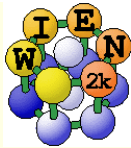
x lapw5 Calculate partial DOS

Preview density with XCrysden

rhplot Plot DOS

edit TiC.in2 reset EMIN

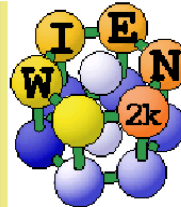
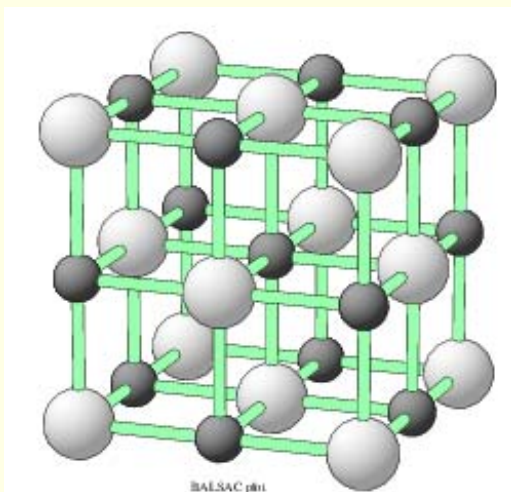




TiC electron density



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



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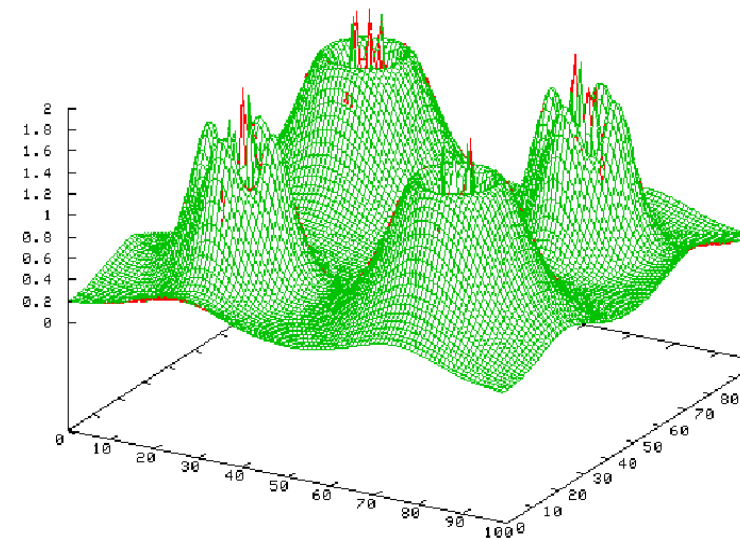
Session: TiC User: pblaha
/susi/pblaha/lapw/TiC

The Oct 25 16:53:31 2001
STATUS: idle
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Electron density plots

[Show full menu](#)

We are in rplot mode



[Download hardcopy in PostScript format](#)

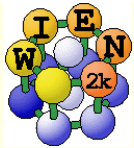
Min Max



Properties with WIEN2k - I



- **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)*
- **Electron density, potential**
 - *total-, valence-, difference-, spin-densities, ρ 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 / LDA+U)*
- **Hyperfine parameters**
 - *hyperfine fields (contact + dipolar + orbital contribution)*
 - *Isomer shift*
 - *Electric field gradients*



Properties with WIEN2k - II

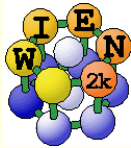


■ Total energy and forces

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

■ Spectroscopy

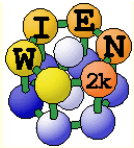
- *core levels (with core holes)*
- *X-ray emission, absorption, electron-energy-loss (core-valence/conduction bands including matrix elements and angular dep.)*
- *optical properties (dielectric function, JDOS including momentum matrix elements and Kramers-Kronig)*
- *fermi surface (2D, 3D)*



Properties with WIEN2k - III



- **New developments (in progress)**
 - *non-linear optics*
 - *non-collinear magnetism*
 - *transport properties (Fermi velocities, Seebeck, conductivity, thermoelectrics, ..)*
 - *Compton profiles*
 - *linear response (phonons, E-field) (C.Ambrosch-Draxl)*
 - *stress tensor (C.Ambrosch-Draxl)*
 - *exact exchange, GW, ... ??*
 - *grid-computing*



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
- + 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 (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



**Thank you for
your attention !**