The all-electron full-potential linearized augmented plane-wave method

Sep 9, 2019 | **Gregor Michalicek** | Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

MAX DRIVING THE EXASCALE TRANSITION

JÜLICH Forschungszentrum

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Outline

- **Theoretical background**
  - The FLAPW method and the LAPW basis
  - Separation of core electrons from valence electrons
  - Representation of density and potential
- **FLAPW in practice**
  - Setting the parameters
  - Semicore states and ghost bands
  - The linearization error
- **Using fleur**
  - The input file generator
  - The inp.xml file
- **Further reading**
- **Conclusion**

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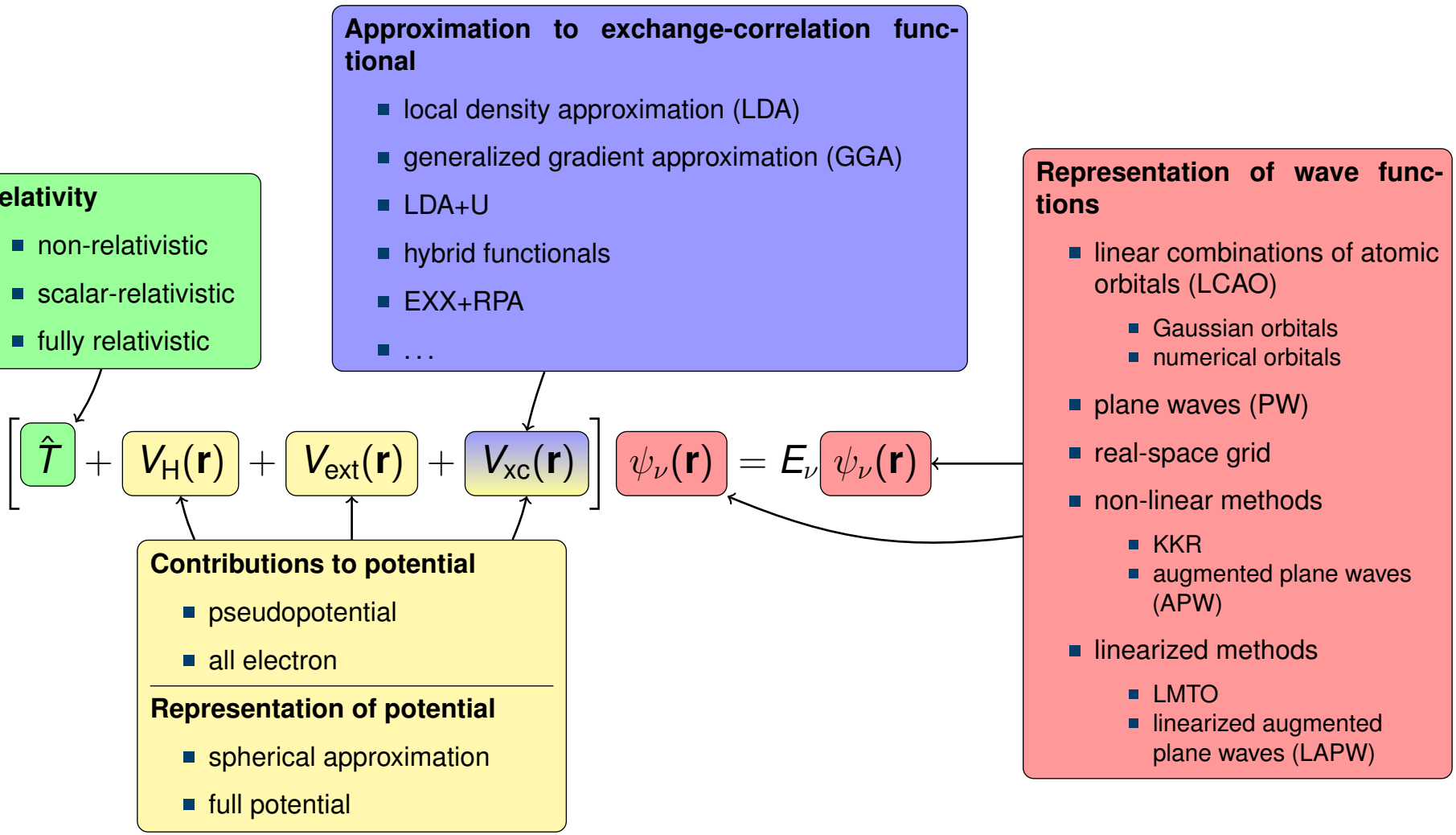
Motivation: FLAPW in zoo of electronic structure methods



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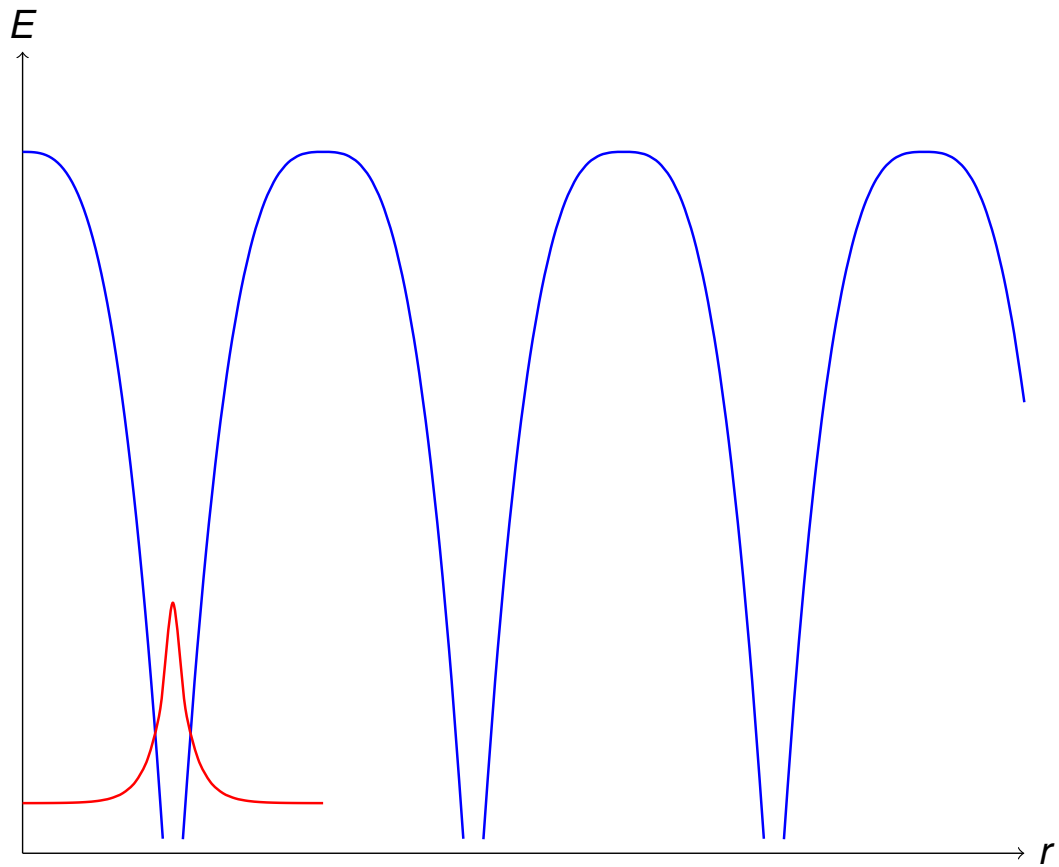
Potential and wave functions in a crystal



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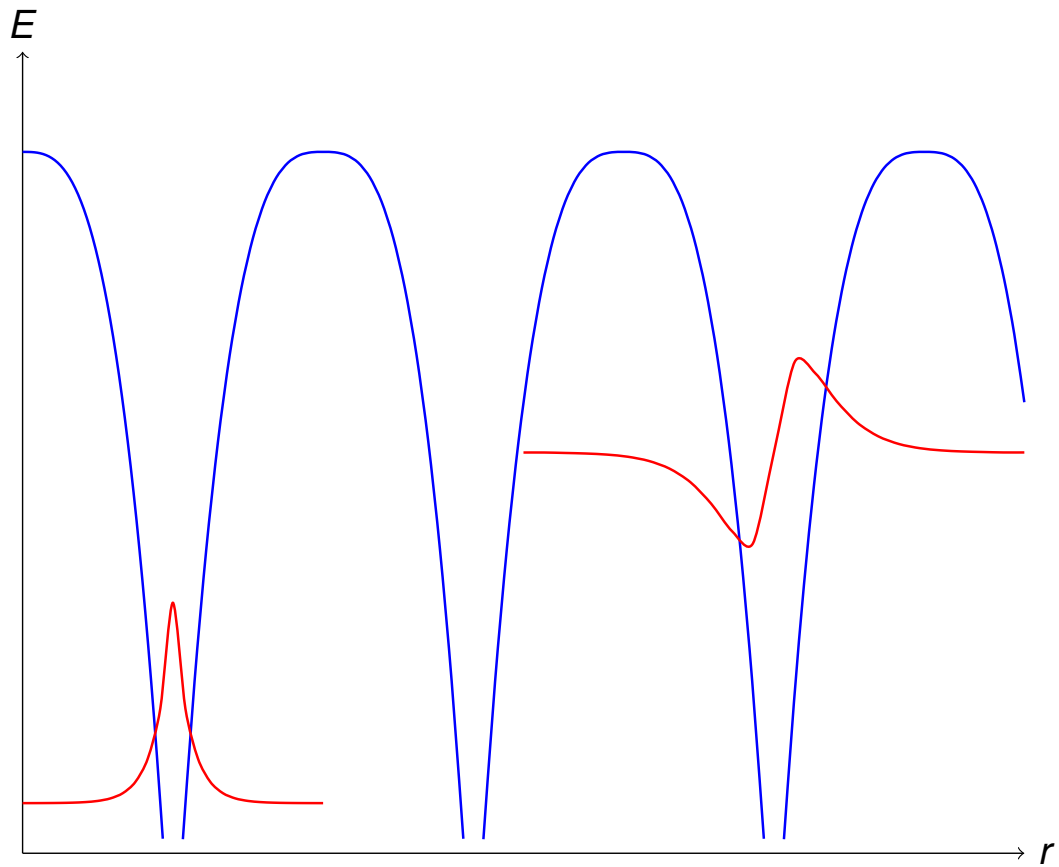

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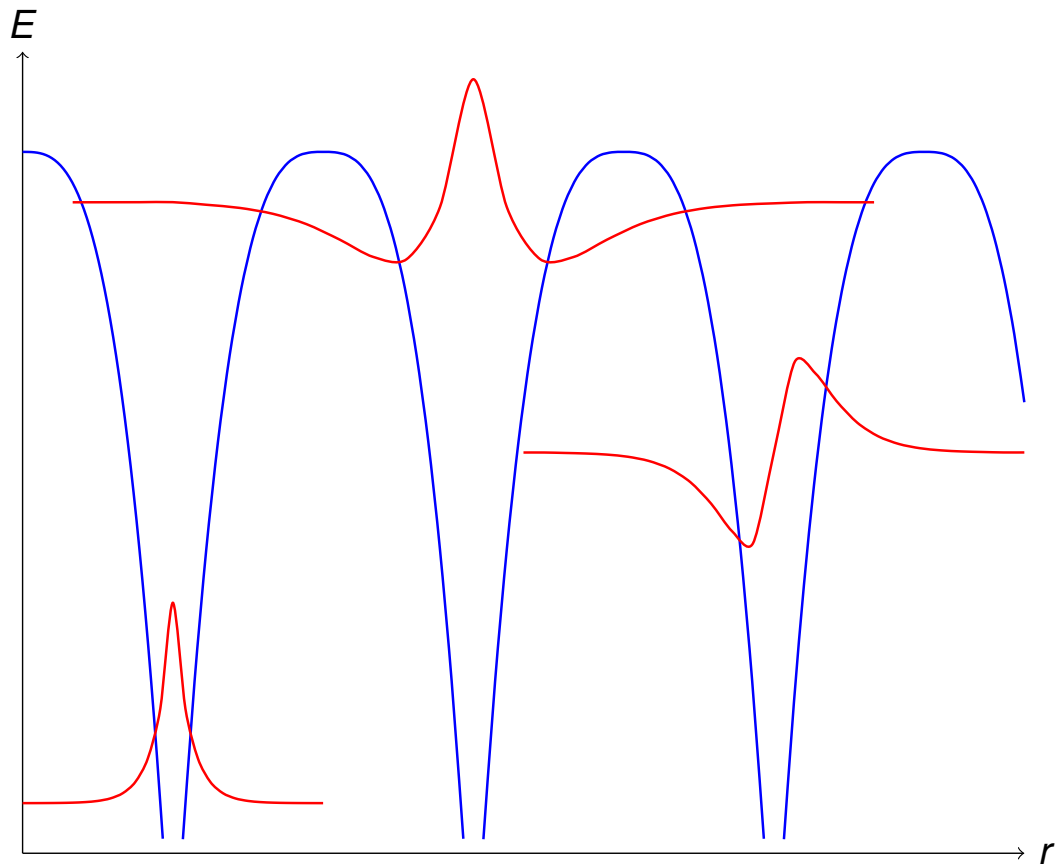

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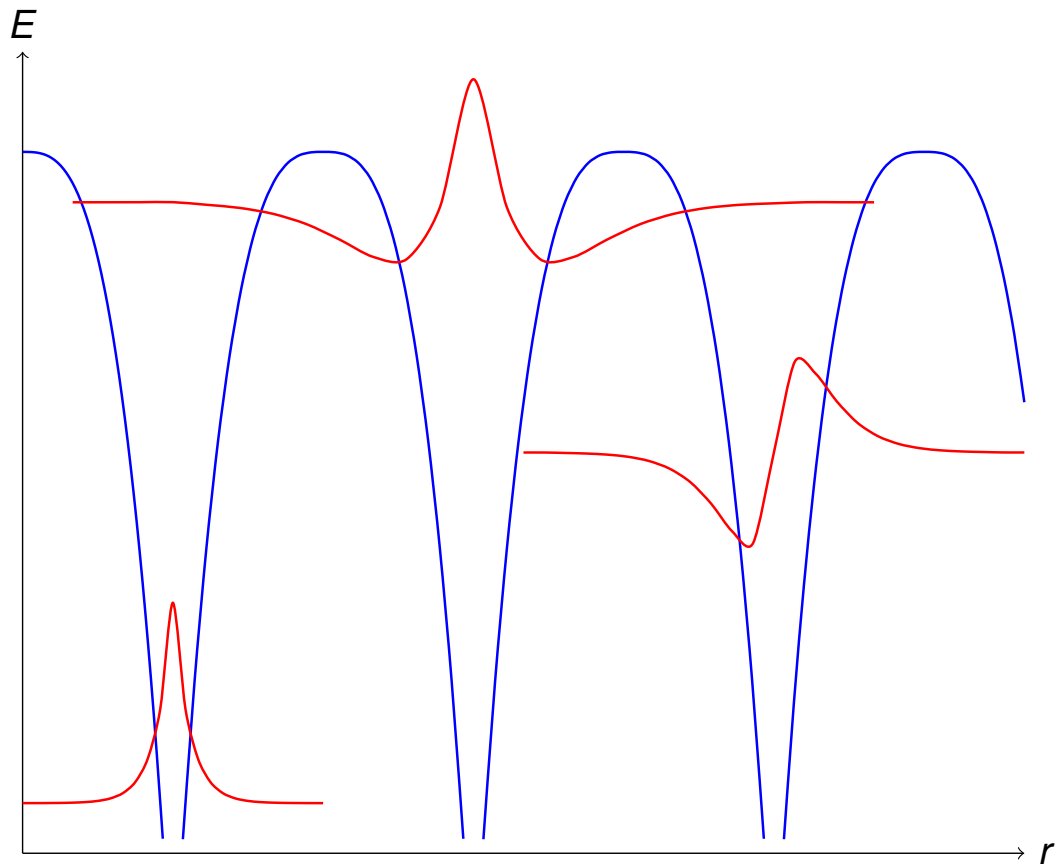

Valence electrons

Semicore electrons

Core electrons

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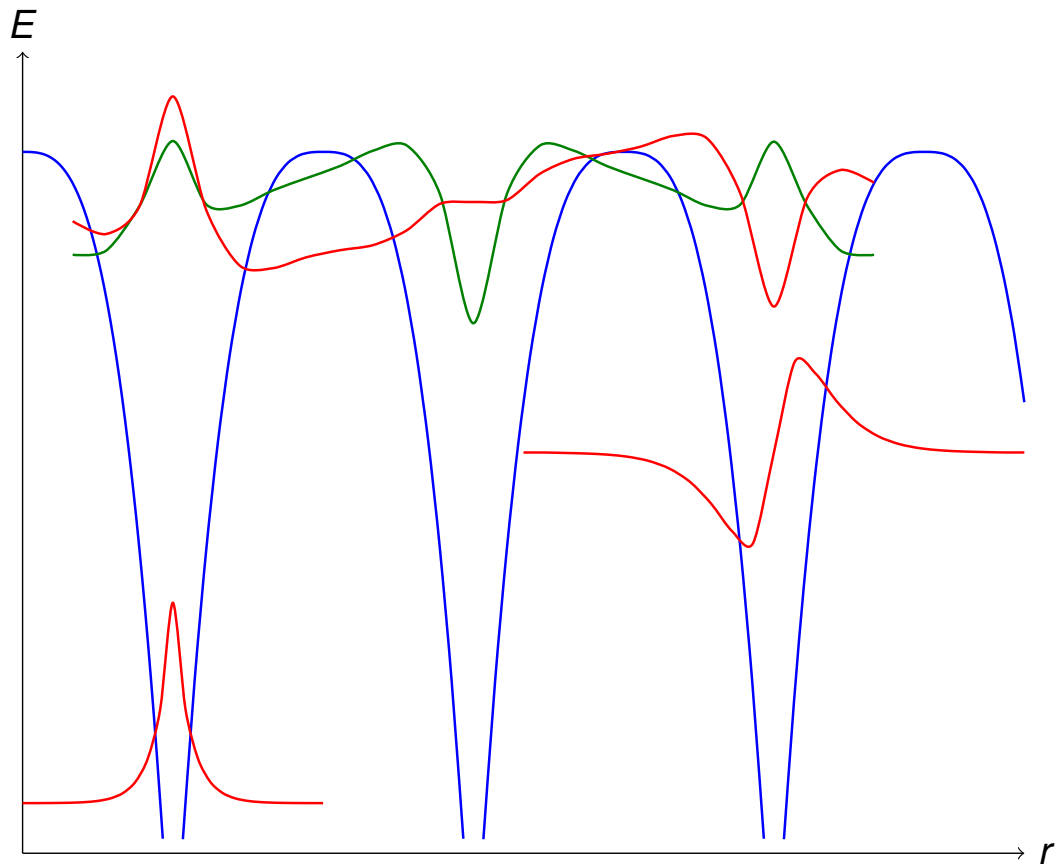

Bloch theorem:

If $V(\mathbf{r}) = V(\mathbf{r}+\mathbf{R})$:

$$\Psi(\mathbf{r}) = e^{i\mathbf{k}\mathbf{r}} \cdot u_{\mathbf{k}}(\mathbf{r}),$$

$$u_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r}+\mathbf{R})$$

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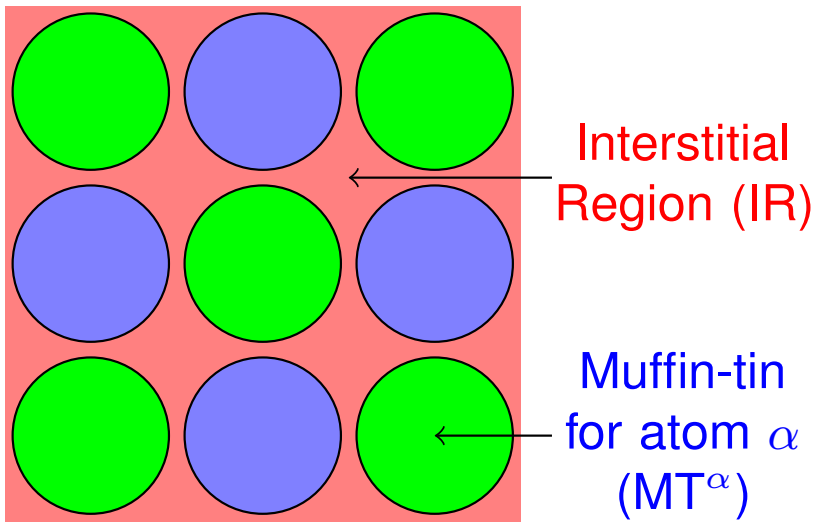
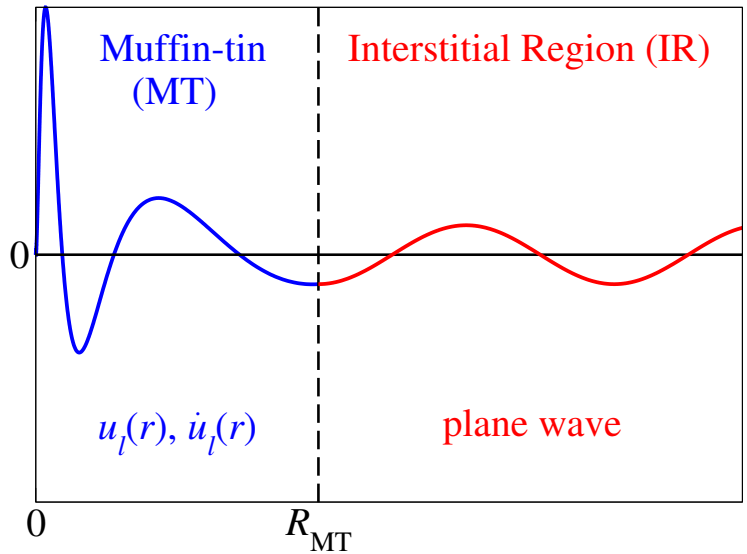
The LAPW basis

- Atom-centered functions in MT spheres matched in value and slope to plane waves in interstitial region (IR)

$$\phi_{\mathbf{kG}}(\mathbf{r}) = \begin{cases} \frac{1}{\sqrt{\Omega}} e^{i(\mathbf{k}+\mathbf{G})\mathbf{r}} & \text{for } \mathbf{r} \in \text{IR} \\ \sum_L \left[a_{\mathbf{kG}}^{L\alpha} u_l^\alpha(r_\alpha, E_l^\alpha) + b_{\mathbf{kG}}^{L\alpha} \dot{u}_l^\alpha(r_\alpha, E_l^\alpha) \right] Y_L(\hat{\mathbf{r}}_\alpha) & \text{for } \mathbf{r} \in \text{MT}^\alpha \end{cases}$$

- u_l^α and $\dot{u}_l^\alpha$ are solutions and energy derivatives for the spherical potential at energy parameters E_l^α





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- u_l^α and $\dot{u}_l^\alpha$ are solutions and energy derivatives for the spherical potential at energy parameters E_l^α

Parameters:

- $K_{\text{max}} = |\mathbf{k} + \mathbf{G}|_{\text{max}}$ reciprocal plane wave cutoff
- l_{max}^α angular momentum cutoff for sphere α
- R_{MT}^α radius for muffin-tin sphere α
- E_l^α energy parameter for u_l^α, $\dot{u}_l^\alpha$

Note: LAPW basis depends on atom positions and features discontinuities at MT boundaries

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Orthogonality of LAPW basis functions to core electron states (1)

- $u_l(r)$, $u_l^c(r)$ given by radial Schrödinger equation:

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial r^2} + \frac{l(l+1)}{2r^2} + V_{\text{eff}}^{\text{sphr}}(r)\right] r u_l(r) = E_l r u_l(r) \qquad (1)$$

- Multiply (1) for $u_l(r)$ by $ru_l^c(r)$ and vice versa, subtract the two resulting equations from each other, and integrate:

$$\int_0^{R_{\text{MT}}} -\frac{1}{2} r u_l^c(r) \frac{\partial^2}{\partial r^2} r u_l(r) + \frac{1}{2} r u_l(r) \frac{\partial^2}{\partial r^2} r u_l^c(r) \mathrm{d}r = (E_l - E_l^c) \int_0^{R_{\text{MT}}} u_l(r) r^2 u_l^c(r) \mathrm{d}r$$

- Assumption: $u_l^c(r)\big|_{R_{\text{MT}}} = 0$, $\frac{\partial}{\partial r} u_l^c(r)\big|_{R_{\text{MT}}} = 0$
- We obtain: $0 = \left\langle u_l^c \middle| u_l \right\rangle_{R_{\text{MT}}}$ and analogously $0 = \left\langle u_l^c \middle| \dot{u}_l \right\rangle_{R_{\text{MT}}}$

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Orthogonality of LAPW basis functions to core electron states (2)

- Orthogonality allows to determine core and valence electron energies and wave functions separately from each other
- Core electrons
  - Representation for each atom separately on radial mesh
  - Fully relativistic treatment
- Valence electrons
  - Representation by LAPW basis
  - Scalar-relativistic description in MT spheres
  - Optional inclusion of spin-orbit coupling
- But: assumption $u_l^c(r)\big|_{R_{\mathrm{MT}}} = 0,\ \frac{\partial}{\partial r} u_l^c(r)\big|_{R_{\mathrm{MT}}} = 0$ only approximately fulfilled
  - Semicore states can lead to ghost bands

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The linearization within the LAPW basis

- Description in MT spheres is not systematically improved by increasing the reciprocal cutoff parameter $K_{\max}$

Linearization of solutions u_l at arbitrary energy ϵ

- $u_l^\alpha(r_\alpha, \epsilon) = u_l^\alpha(r_\alpha, E_l^\alpha) + (\epsilon - E_l^\alpha)\dot{u}_l^\alpha(r_\alpha, E_l^\alpha) + \mathcal{O}\left[(\epsilon - E_l^\alpha)^2\right]$
- Due to the restriction to the function space spanned by $u_l^\alpha(r_\alpha, E_l^\alpha)$ and $\dot{u}_l^\alpha(r_\alpha, E_l^\alpha)$ we obtain a linearization error.
- This description is sufficient to obtain accurate results for many materials.

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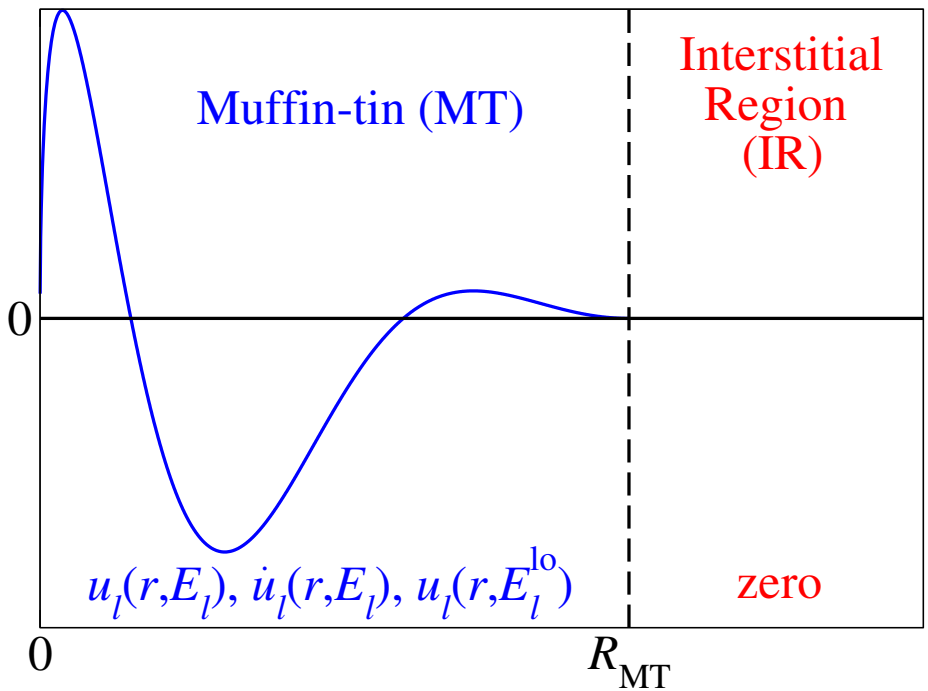
Extending the LAPW basis with local orbitals

Additional basis functions localized in MT spheres

$$\phi_L^{\mathrm{lo}}(\mathbf{r}) = \left[a_L^{\mathrm{lo}} u_l^{\alpha}(r_\alpha, E_l^{\alpha}) + b_L^{\mathrm{lo}} \dot{u}_l^{\alpha}(r_\alpha, E_l^{\alpha}) + c_L^{\mathrm{lo}} u_l^{\alpha}(r_\alpha, E_l^{\mathrm{lo}})\right] Y_L(\hat{\mathbf{r}}_\alpha)$$

- Mainly used to describe semicore states
- Determination of a_L^{lo}, b_L^{lo}, and c_L^{lo} by enforcing zero value and slope at the MT boundary, as well as a normalization condition on the local orbital



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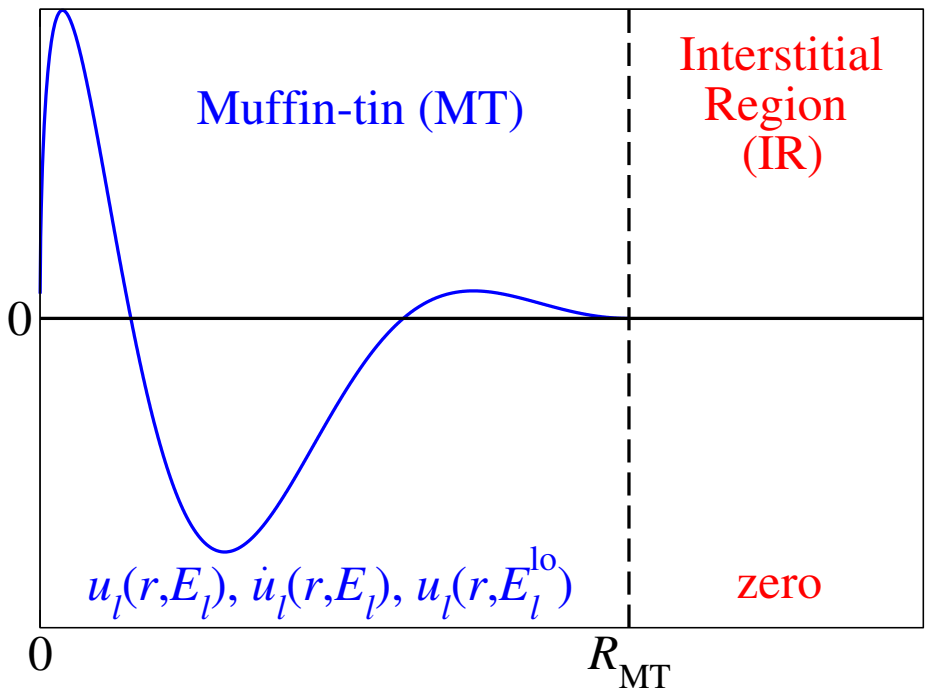
- Semicore states (SCLO)
  - Choose E_l^{lo} to be energy of semicore state
- Unoccupied orbitals (HELO)
  - Choose E_l^{lo} above Fermi energy
- Higher derivative LOs (HDLO)
  - Choose $\ddot{u}_l^{\alpha}(r_\alpha, E_l^{\alpha})$ instead of $u_l^{\alpha}(r_\alpha, E_l^{\mathrm{lo}})$



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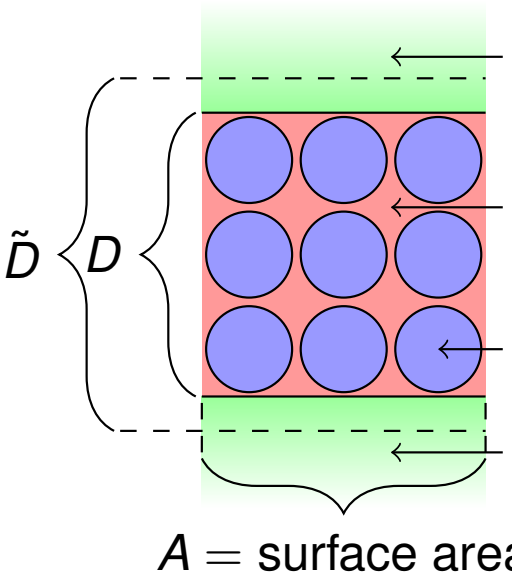
The LAPW basis for films

$$\phi_{\mathbf{k}_\parallel \mathbf{G}}(\mathbf{r}) = \begin{cases} \frac{1}{\sqrt{\Omega}} e^{i(\mathbf{k}_\parallel + \mathbf{G})\mathbf{r}} & \text{for } \mathbf{r} \in \text{IR} \\ \sum_L \left[a^{L\alpha}_{\mathbf{k}_\parallel \mathbf{G}} u^\alpha_l(r_\alpha, E^\alpha_l) + b^{L\alpha}_{\mathbf{k}_\parallel \mathbf{G}} \dot{u}^\alpha_l(r_\alpha, E^\alpha_l) \right] Y_L(\hat{\mathbf{r}}_\alpha) & \text{for } \mathbf{r} \in \text{MT}^\alpha \\ \left[a^{\text{vac}}_{\mathbf{k}_\parallel \mathbf{G}} u^{\text{vac}}_{\mathbf{k}_\parallel \mathbf{G}_\parallel}(z, E^{\text{vac}}) + b^{\text{vac}}_{\mathbf{k}_\parallel \mathbf{G}} \dot{u}^{\text{vac}}_{\mathbf{k}_\parallel \mathbf{G}_\parallel}(z, E^{\text{vac}}) \right] & \\ \times \frac{1}{\sqrt{A}} e^{i(\mathbf{k}_\parallel + \mathbf{G}_\parallel)\mathbf{r}_\parallel} & \text{for } \mathbf{r} \in \text{VR}^{\text{vac}} \end{cases}$$



Vacuum Region 1 (VR^1)

Interstitial Region (IR)

Muffin-tin (MT)

Vacuum Region 2 (VR^2)

- $u^{\text{vac}}_{\mathbf{k}_\parallel \mathbf{G}_\parallel}, \dot{u}^{\text{vac}}_{\mathbf{k}_\parallel \mathbf{G}_\parallel}$: solutions, energy derivatives to vacuum potential at energy parameters E^{vac}
- $G_\perp = 2\pi n / \tilde{D}$

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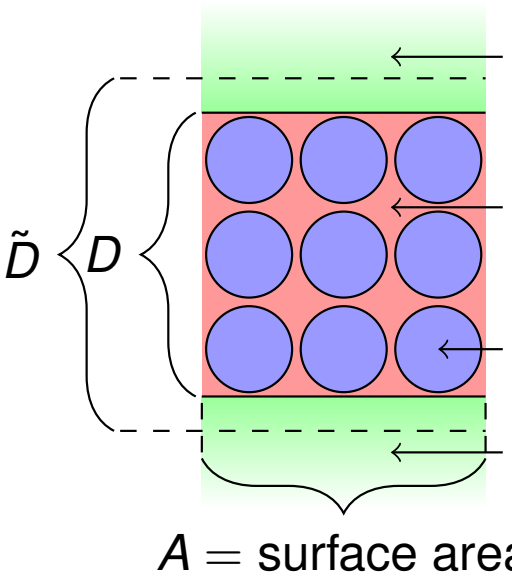

Vacuum Region 1 (VR^1)

Interstitial Region (IR)

Muffin-tin (MT)

Vacuum Region 2 (VR^2)

Parameters:

- D - vacuum boundary
- $\tilde{D}$ - determination of $G_\perp$
- E^{vac} - vacuum energy parameters

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Representation of density and potential

Plane-wave part

$$\rho^{\mathrm{PW}}(\mathbf{r}) = \sum_{\mathbf{G}}^{G_{\max}} \rho_{\mathbf{G}} \cdot e^{i\mathbf{G}\mathbf{r}}$$

- Actually represented by stars
  - Linear combinations of plane waves according to symmetry

MT sphere α

$$\rho^{\alpha}(\mathbf{r}) = \sum_{L}^{L^{\alpha}_{\max}} \rho^{\alpha}_{L}(r_{\alpha})\, Y_{L}(\hat{\mathbf{r}}_{\alpha})$$

- Actually represented by lattice harmonics
  - Linear combinations of spherical harmonics according to symmetry

Parameters:

- $G_{\max}$ reciprocal plane-wave cutoff for density, potential
- $G_{\max \mathrm{XC}}$ reduced cutoff for exchange correlation potential

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Choice of $K_{\max}$, $l^{\alpha}_{\max}$, and $l^{\alpha}_{\text{nonsphr}}$

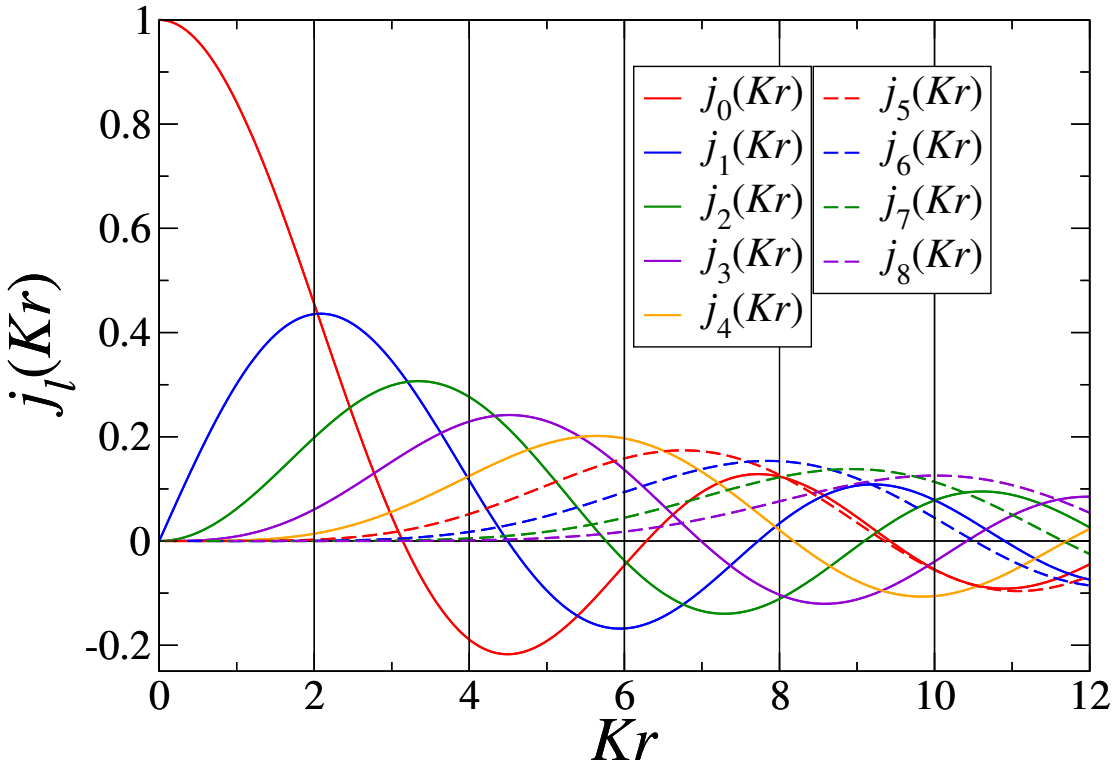
- Rayleigh expansion of planes waves at MT boundary:

$$e^{i\mathbf{K}\mathbf{r}} = 4\pi e^{i\mathbf{K}\tau_\alpha} \sum_L i^l Y_L^*(\hat{\mathbf{K}}) j_l(Kr_\alpha) Y_L(\hat{\mathbf{r}}_\alpha) \Big|_{r_\alpha = R^\alpha_{\text{MT}}}$$

- Rule of thumb:

$$l^{\alpha}_{\max} \approx K_{\max} \cdot R^{\alpha}_{\text{MT}} \approx 8 - 12$$

- Determination of $K_{\max}$ based on $R^{\alpha,\min}_{\text{MT}}$
- $l^{\alpha}_{\text{nonsphr}} \approx \min(8, l^{\alpha}_{\max} - 2)$



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Choice of G_{max} and G_{maxXC}

- G_{max} is cutoff for different functions
  - Plane wave part of charge density $\rho^{\mathrm{PW}}(\mathbf{r})$
  - Plane wave part of potential $V_{\mathrm{eff}}^{\mathrm{PW}}(\mathbf{r})$
  - Step function $\Theta(\mathbf{r})$ indicating the interstitial region
- $V_{\mathrm{eff}}^{\mathrm{PW}}(\mathbf{r})$ and $\Theta(\mathbf{r})$ have infinitely many plane-wave coefficients.
- Interstitial potential contribution to Hamilton matrix:

$$\left\langle \phi_{\mathbf{kG}} \middle| \Theta(\mathbf{r})\, V_{\mathrm{eff}}^{\mathrm{PW}}(\mathbf{r}) \middle| \phi_{\mathbf{kG'}} \right\rangle$$

- Rule

$$G_{\mathrm{max}} \geq G_{\mathrm{maxXC}} \geq 2 \cdot K_{\mathrm{max}}$$

- typically $G_{\mathrm{max}} \approx 3 \cdot K_{\mathrm{max}}$, $G_{\mathrm{maxXC}} \approx 2.5 \cdot K_{\mathrm{max}}$

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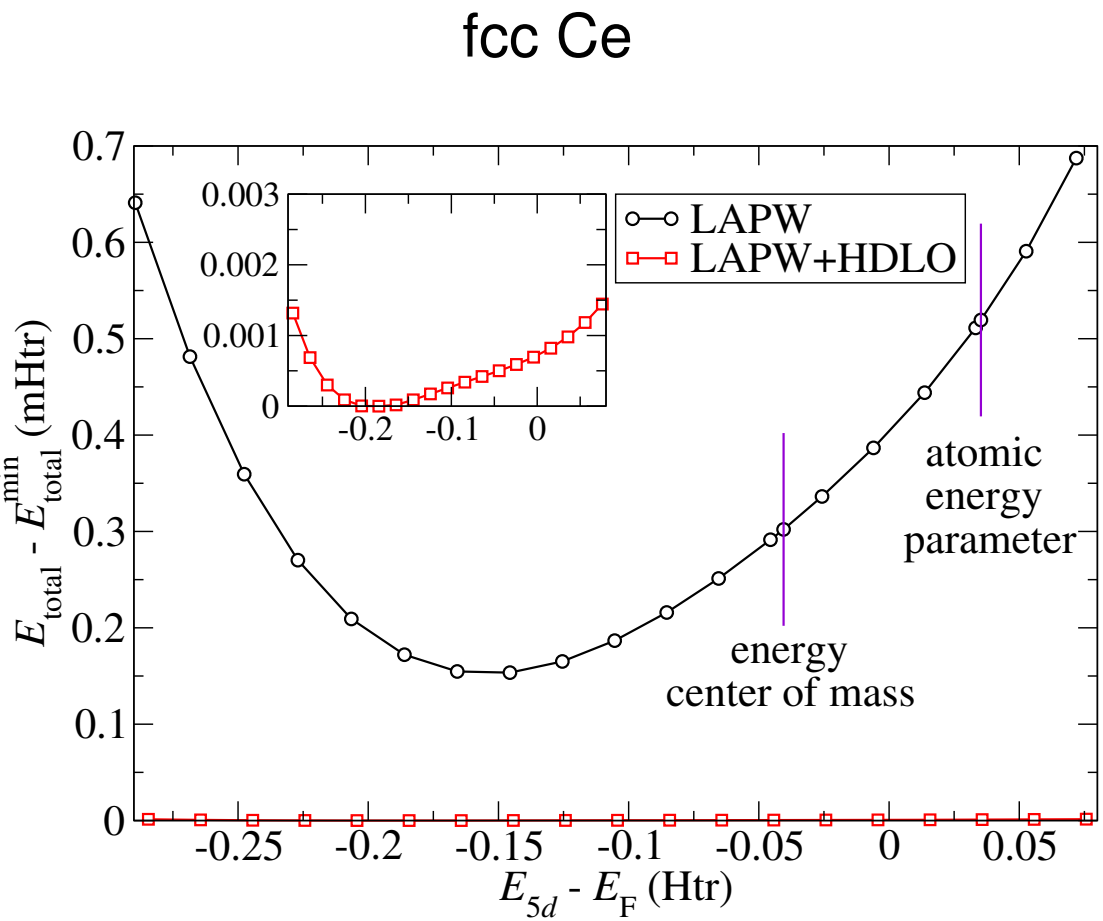
Choice of the energy parameters

- energy center of mass of the *l*-projected DOS
  - minimizes quadratic error weighted by charge in each eigenstate
- atomic solutions
  - yields more friendly convergence behavior



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Choice of MT radii

- Due to different bonding lengths in different materials the R_{MT} are material dependent.
- If calculations have to be compared identical MT radii should be chosen.

Large MT radii

- Faster calculations
- Larger linearization error
- Fewer SCLOs needed
- Some quantities only evaluated in MT

Small MT radii

- Slower calculations
- More stable calculations
- Smaller linearization error
- More SCLOs needed
- More space available for structural relaxations

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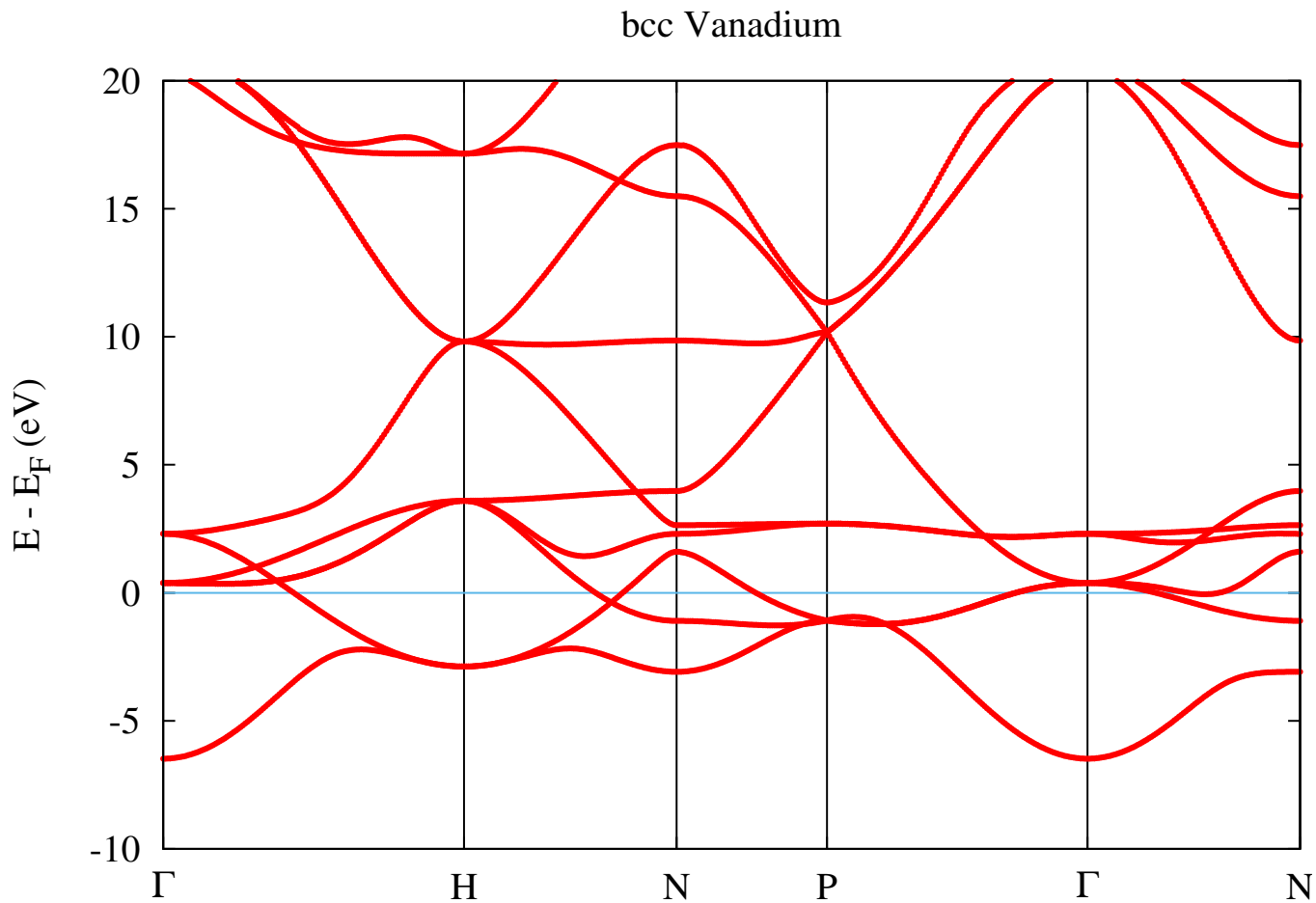
Semicore states and ghost bands



- $R_{MT} = 2.25\ a_0$, lostElectrons $= 0.086$

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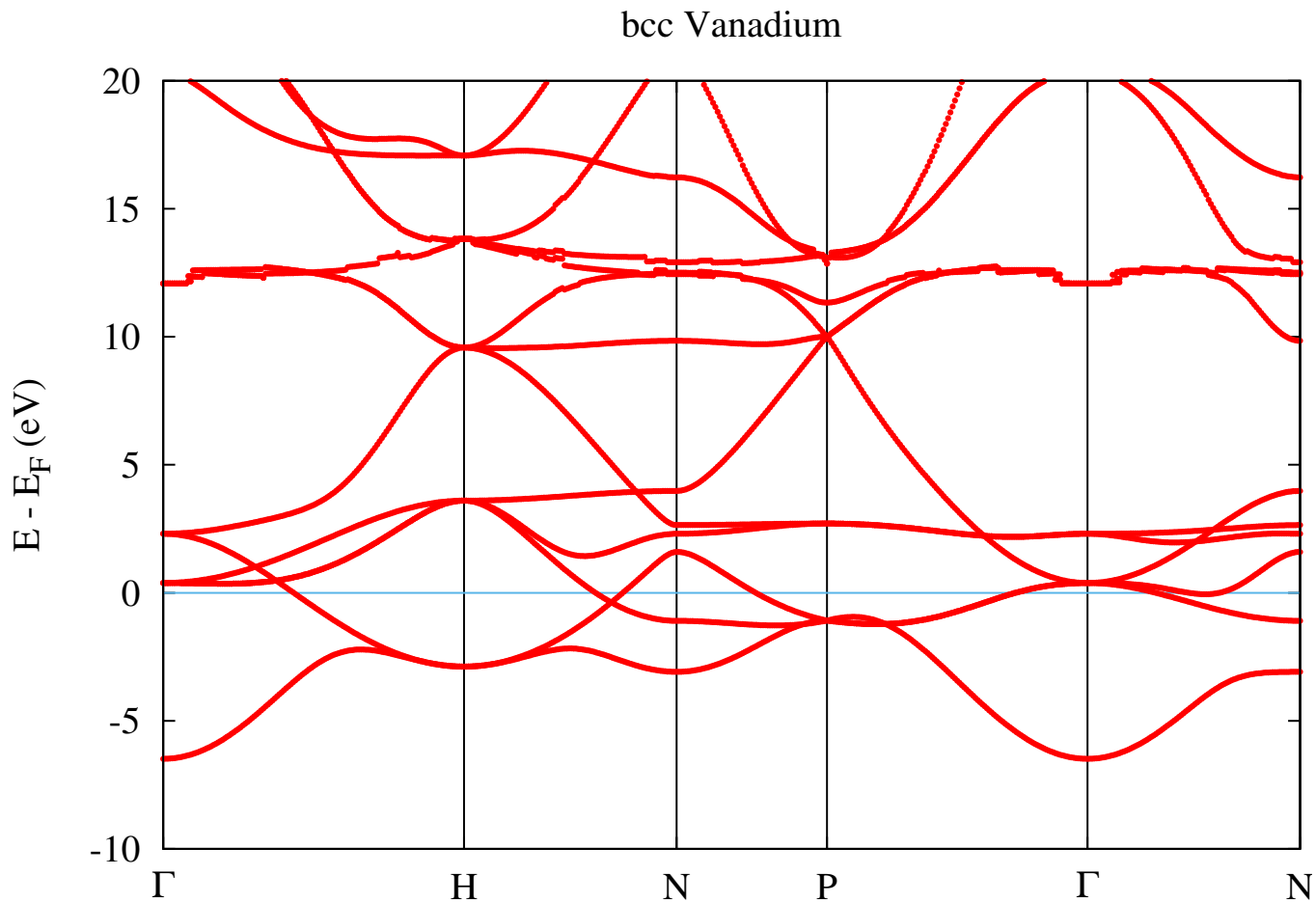
Semicore states and ghost bands



- $R_{MT} = 2.20\ a_0$, lostElectrons $= 0.100$

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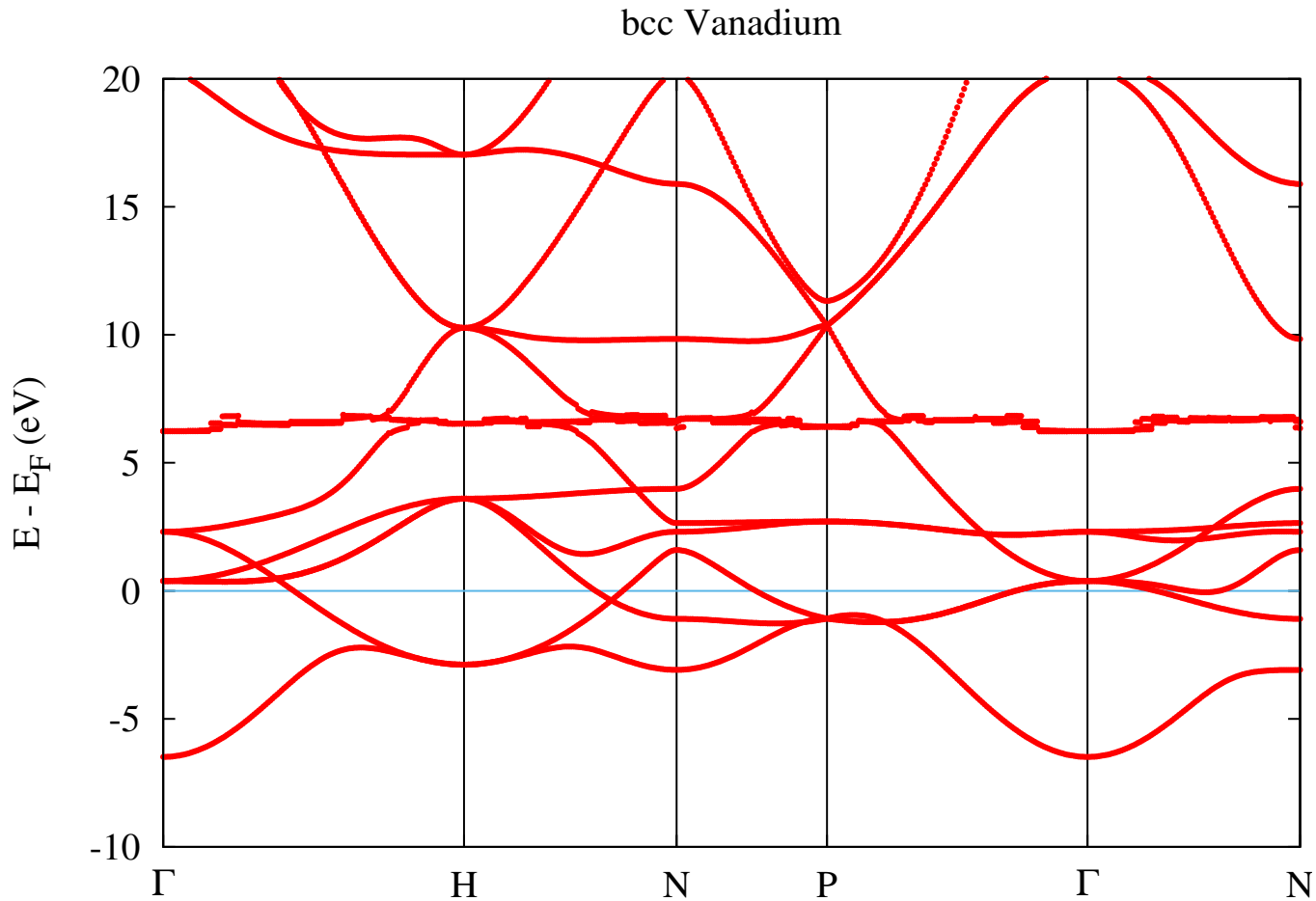
Semicore states and ghost bands



- $R_{MT} = 2.17\ a_0$, lostElectrons $= 0.109$

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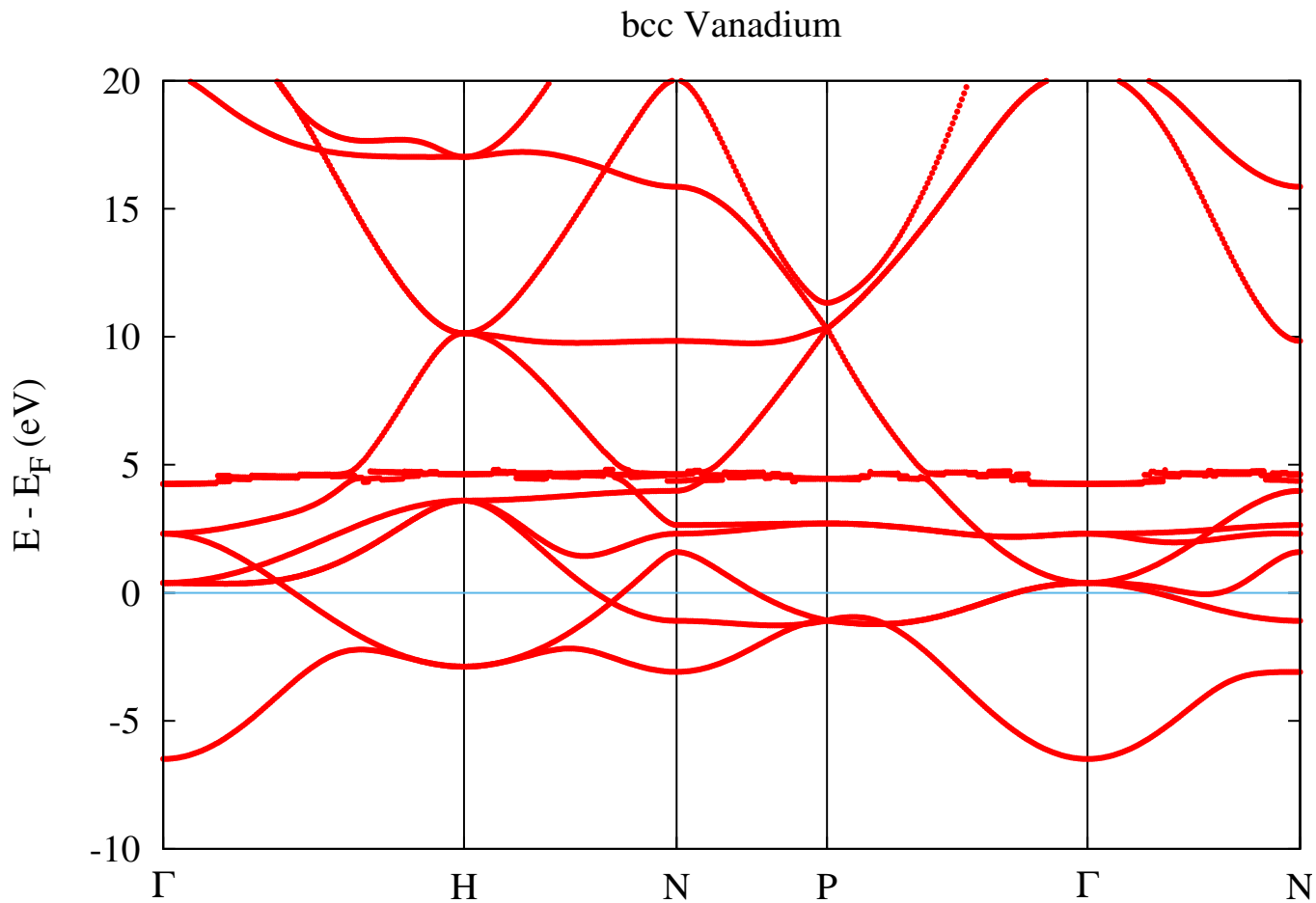
Semicore states and ghost bands



- $R_{MT} = 2.16\ a_0$, lostElectrons $= 0.112$

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Semicore states and ghost bands

```
**************juDFT-Error*****************
Error message:differ 2: problems with solving dirac equation
Error occurred in subroutine:differ
Error from PE:0/1
****************************************
 Last kown location:
 Last timer:Updating energy parameters
 Timerstack:
 Timer:eigen
 Timer:gen. of hamil. and diag. (total)
 Timer:Iteration
 Timer:Total Run
 ****************************************
```

- $R_{\mathrm{MT}} = 2.15\ a_0$, lostElectrons $= 0.123$
- This error message can also have other causes.
- Other error messages are also possible.

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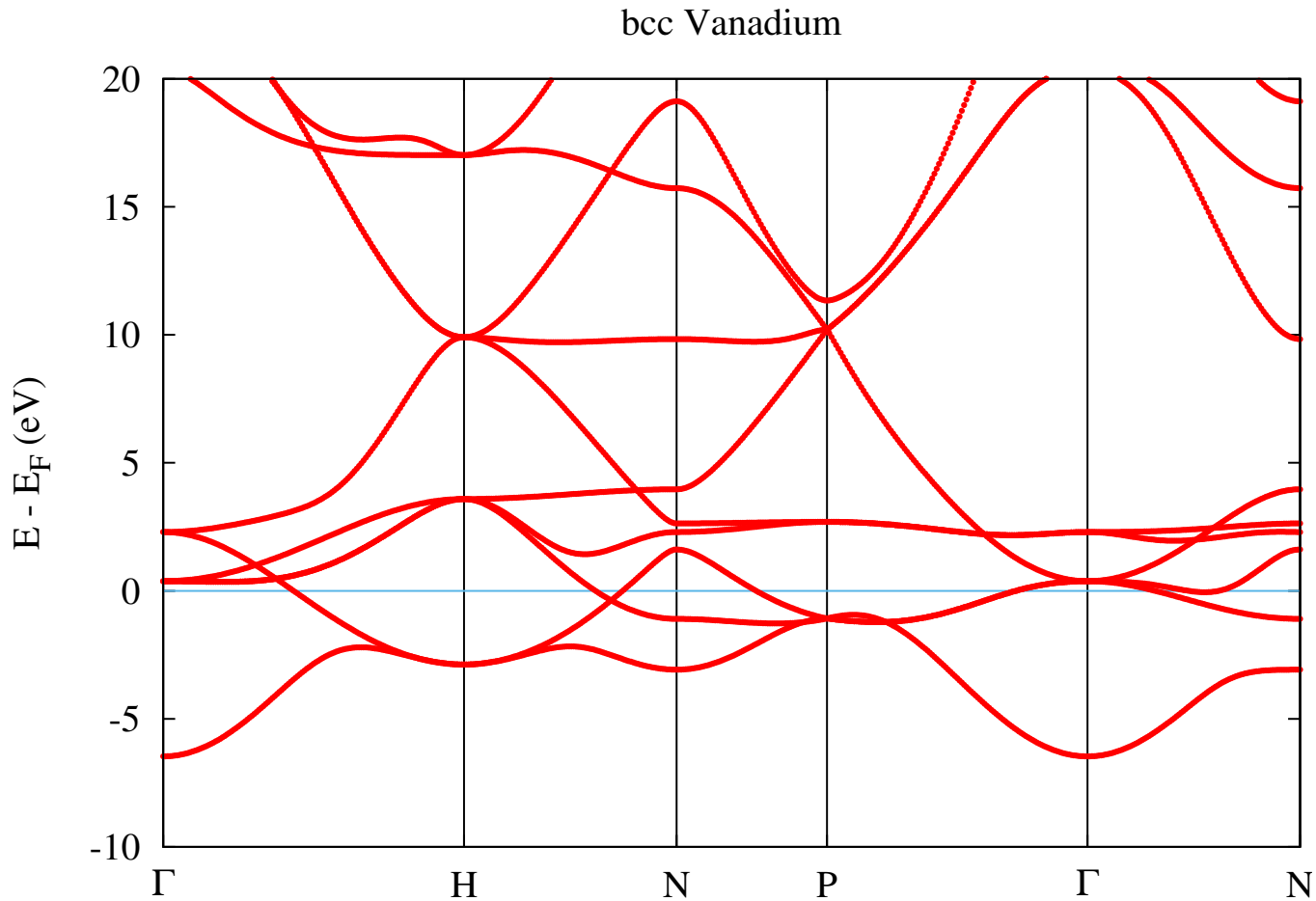
Semicore states and ghost bands - with SCLO



- $R_{MT} = 2.16\ a_0$, lostElectrons $= 0.012$, SCLO for $3p$ state

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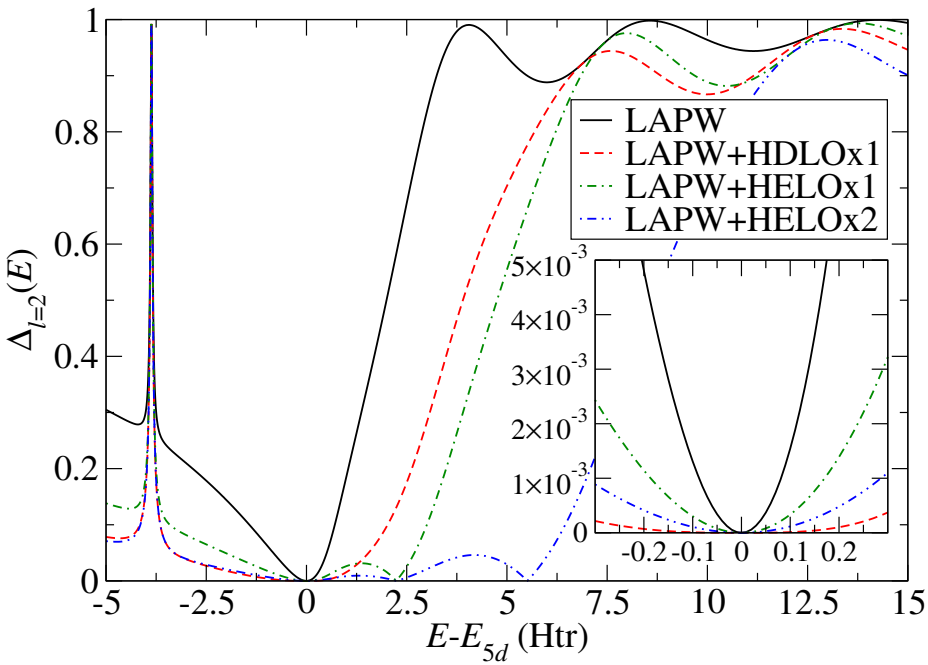
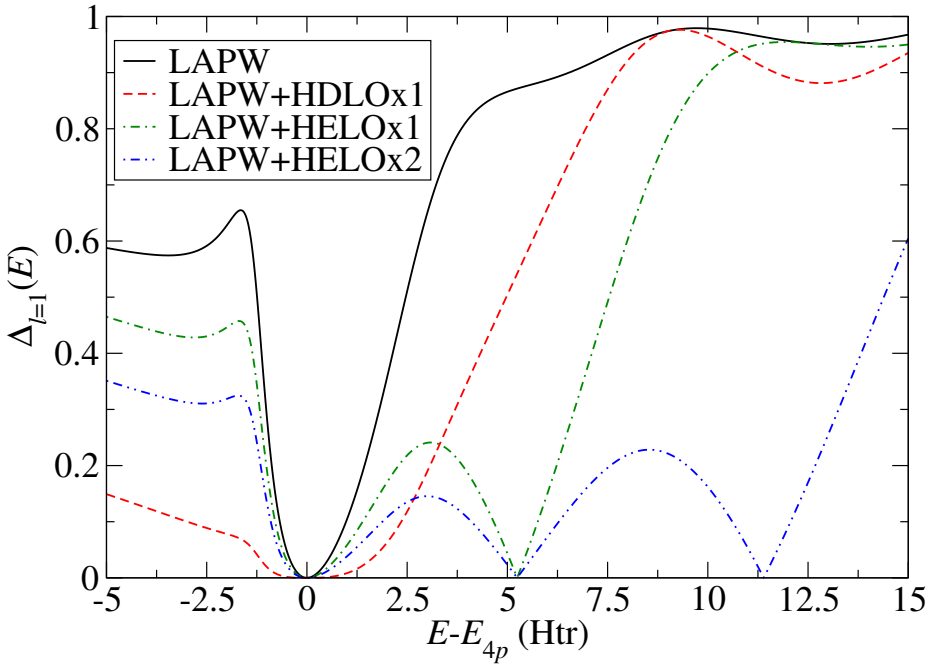
Linearization error depending on energy mismatch

fcc Cerium



bcc Vanadium



- $\Delta_l = \sqrt{\| u_l(r,\epsilon) - \tilde{u}_l(r,\epsilon) \|^2}$

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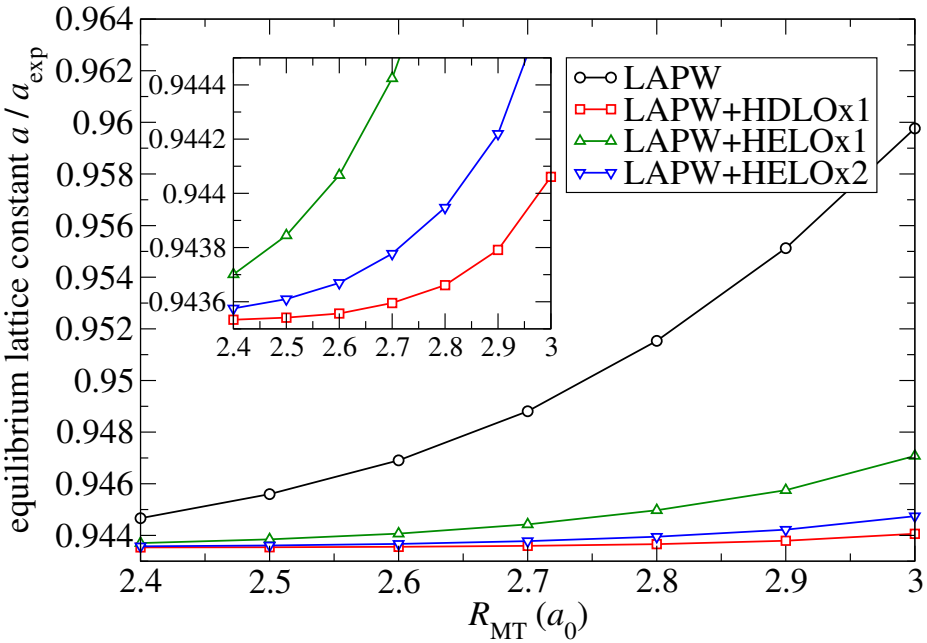
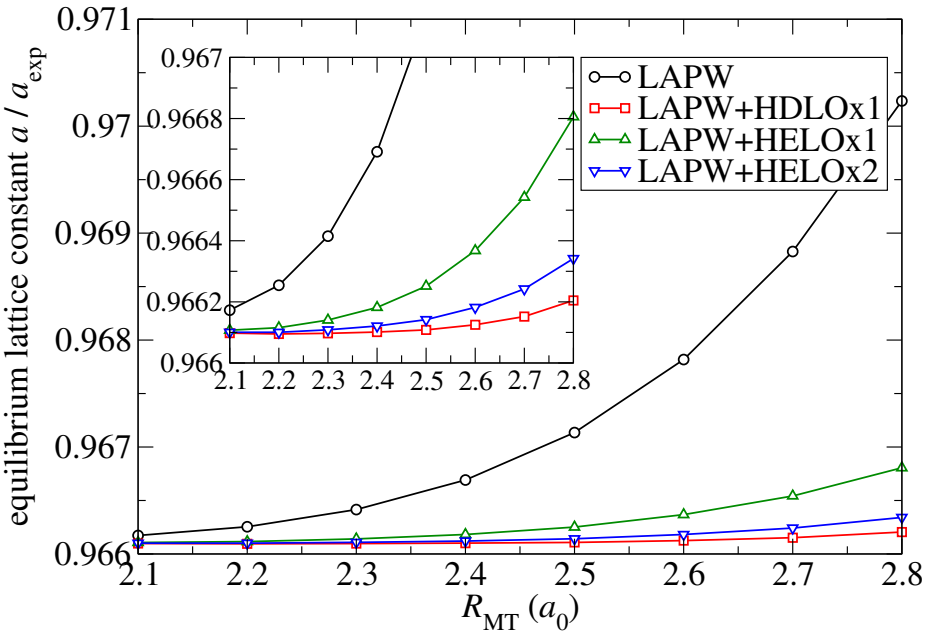
The linearization error and MT radii

fcc Ce



- lattice constant changes by 1.6% when MT radius is reduced

rock-salt KCl



- lattice constant changes by 0.4% when MT radii are reduced

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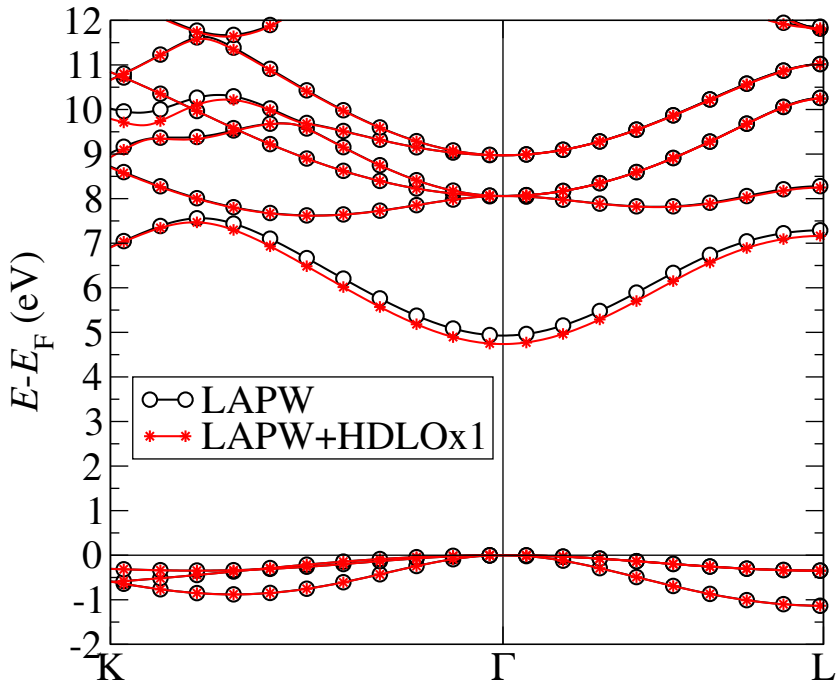
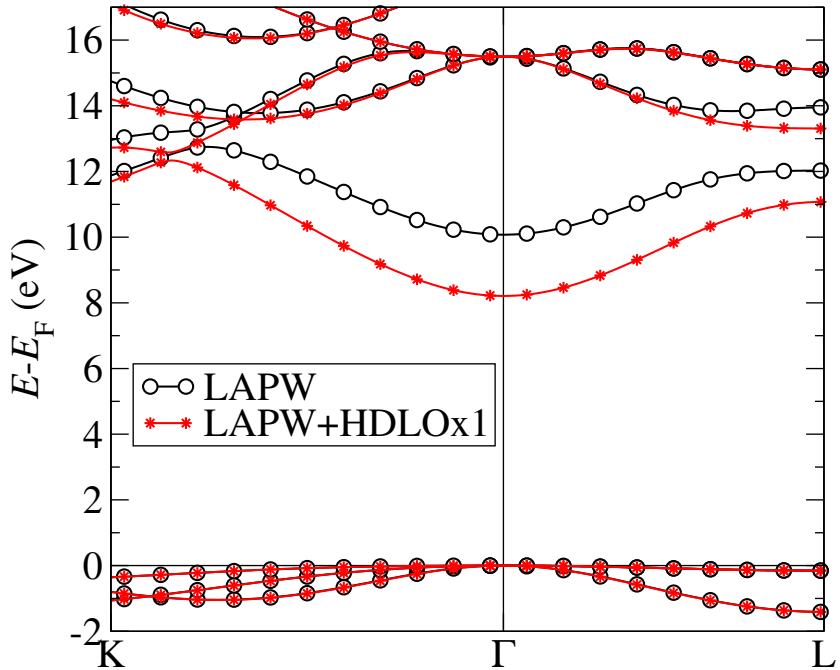
The linearization error and unoccupied states





- KS band gap for rock-salt KCl is reduced by 4% by adding one set of HDLOs
- KS band gap for fcc Ar is reduced by 19% by adding one set of HDLOs

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Outline

- **Theoretical background**
  - The FLAPW method and the LAPW basis
  - Separation of core electrons from valence electrons
  - Representation of density and potential
- **FLAPW in practice**
  - Setting the parameters
  - Semicore states and ghost bands
  - The linearization error
- **Using fleur**
  - The input file generator
  - The inp.xml file
- **Further reading**
- **Conclusion**

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The input file generator

- Fleur uses complex input
  - Input file with default parameters is generated by input file generator **inpgen**
  - Simple structural input needed for inpgen
- Example input for inpgen

```
NaCl bulk

&lattice latsys='fcc' a0=10.62026 /

  2
  11 0.0 0.0 0.0
  17 0.5 0.5 0.5
```

- Usage: inpgen < myInputFile.txt

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Input file generator - command line options

- **-h** write out list of command line options
- Optional Input to be generated
  - **-explicit** add some optional input direcly to **inp.xml** file.
    - List of k points
    - Symmetry operations (otherwise if needed in **sym.out** file)
    - Noncollinear magnetism input
  - **-noco** generate noncollinear magnetism input in inp.xml
  - **-genEnpara** generate **enpara** file for more energy parameter options
  - ...

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Fleur input: the inp.xml file

```
<?xml version="1.0" encoding="UTF-8" standalone="no"?>
<fleurInput fleurInputVersion="0.30">
   <comment> Fleur is cool </comment>
   <calculationSetup> ... </calculationSetup>
   <cell> ... </cell>
   <xcFunctional> ... </xcFunctional>
   <atomSpecies> ... </atomSpecies>
   <atomGroups> ... </atomGroups>
   <output> ... </output>
</fleurInput>
```

- Usage: fleur
- **-h** command line option to display all fleur modes

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The inp.xml file - calculationSetup

```
<calculationSetup>
   <cutoffs Kmax="3.6" Gmax="10.7" GmaxXC="8.9"
            numbands="0"/>
   <scfLoop itmax="15" minDistance=".0"
            imix="Anderson" alpha=".05"/>
   <coreElectrons ctail="T" frcor="F" kcrel="0"/>
   <magnetism jspins="1" l_noco="F"/>
   <bzIntegration valenceElectrons="16.0" mode="hist"
                  fermiSmearingEnergy=".001">
      <kPointCount count="15" gamma="F"/>
   </bzIntegration>
</calculationSetup>
```

+ Optional input, e.g., nocoParams, geometryOptimization

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The inp.xml file - cell, xcFunctional

```
<cell>
   <symmetryFile filename="sym.out"/>
   <bulkLattice scale="1.000" latnam="any">
      <bravaisMatrix>
         <row-1> 0.00000 5.31013 5.31013</row-1>
         <row-2> 5.31013 0.00000 5.31013</row-2>
         <row-3> 5.31013 5.31013 0.00000</row-3>
      </bravaisMatrix>
   </bulkLattice>
</cell>
<xcFunctional name="pbe"
              relativisticCorrections="F"/>
```


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The inp.xml file - atomSpecies

```
<atomSpecies>
   <species name="Na-1" element="Na" atomicNumber="11"
            coreStates="1" magMom=".00" flipSpin="T">
      <mtSphere radius="2.80" gridPoints="925"
                logIncrement=".0120"/>
      <atomicCutoffs lmax="10" lnonsphr="8"/>
      <energyParameters s="3" p="3" d="3" f="4"/>
      <lo type="SCLO" l="0" n="2" eDeriv="0"/>
      <lo type="SCLO" l="1" n="2" eDeriv="0"/>
   </species>
   <species name="Cl-2" element="Cl" atomicNumber="17"
            coreStates="4" magMom=".00" flipSpin="T">
      ...
   </species>
</atomSpecies>
```


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The inp.xml file - atomGroups

```
<atomGroups>
   <atomGroup species="Na-1">
      <relPos> .000000 .000000 .000000</relPos>
      <force calculate="T" relaxXYZ="TTT"/>
   </atomGroup>
   <atomGroup species="Cl-2">
      <relPos> 1.0/2.0 1.0/2.0 1.0/2.0</relPos>
      <force calculate="T" relaxXYZ="TTT"/>
   </atomGroup>
</atomGroups>
```

+ Optional input, e.g., nocoParams

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The inp.xml file - output

```
<output dos="F" band="F" vacdos="F" slice="F">
   <densityOfStates ndir="0" minEnergy="-.50"
                    maxEnergy=".50" sigma=".015"/>
</output>
```

+ Optional input, e.g., vacuumDOS, plotting, chargeDensitySlicing

- Full documentation of inp.xml file on www.flapw.de

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Overview on files

with HDF5

- inp.xml
- (sym.out)
- enpara (optional)
- cdn.hdf
- mixing_history.*
- input for special calculations
- out, inf, out.xml

without HDF5

- inp.xml
- (sym.out)
- enpara (optional)
- cdn1, cdn??, cdnc
- mixing_history.*
- stars, wkf2
- input for special calculations
- out, inf, out.xml

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Further reading

- The FLAPW method
  - Overview book - Singh *et al.*, *Planewaves, Pseudopotentials, and the LAPW Method*, Springer
  - Initial publication - Andersen, PRB **12**, 3060 (1975)
  - FLAPW for films - Krakauer *et al.*, PRB **19**, 1706 (1979)
  - Potential calculation - Weinert, J.Math.Phys. **22**, 2433 (1981)
  - Predecessor (APW) - Slater, Phys.Rev. **51**, 846 (1937)
- Local orbitals
  - SCLOs - Singh, PRB **43**, 6388 (1991)
  - HELOs - Betzinger *et al.*, PRB **83**, 045105 (2011)
  - HDLOs - Friedrich *et al.*, PRB **74**, 045104 (2006)
  - Linearization error - Michalicek *et al.*, CPC **184**, 2670 (2013)

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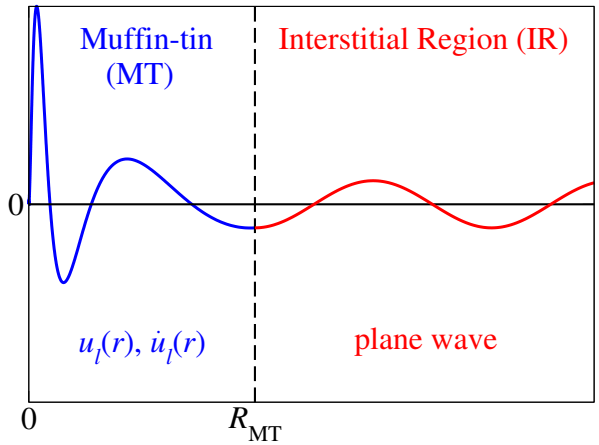
Conclusions

- LAPW basis + local orbitals
- Guidelines for setting parameters
  - $K_{\max}$, $l^{\alpha}_{\max}$, $l^{\alpha}_{\text{nonsphr}}$
  - R^{α}_{MT}, E^{α}_{l}
  - $G_{\max}$, $G_{\max\text{XC}}$
- Semicore states and ghost bands
- The linearization error
- Fleur input files
- Not discussed
  - General numerical DFT parameters, e.g., k point set, Fermi smearing, ...



$$l^{\alpha}_{\max} \approx K_{\max} \cdot R^{\alpha}_{\text{MT}}$$