MaX DRIVING THE EXASCALE TRANSITION

All-electron DFT using the FLEUR code

MaX "*Materials Design at the Exascale*", has received funding from the European Union's Horizon 2020 project call H2020-INFRAEDI-2018-1, grant agreement 824143

Topics

Introduction to FLEUR and FLAPW

Gregor Michalicek

Pushing FLEUR to the limits:

Large magnetic setups

Uliana Alekseeva

Getting FLEUR to run on your machine, Future of FLEUR

Daniel Wortmann

Remarks on questions

Use Q&A button during the talks to ask questions

You will also get questions on your background

Q&A session after the talks

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Introduction to FLEUR and FLAPW

Gregor Michalicek

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Outline

- **Theoretical background**
  - The FLAPW method and the LAPW basis
  - Separation of core electrons from valence electrons
  - Local orbitals
  - Film setups
- **Obtaining high-presision results**
  - Semicore states and ghost bands
  - Systematic convergence in MT spheres
- **Strengths, Challenges, and Features**
- **Using fleur**
- **Conclusion**

What is Fleur?

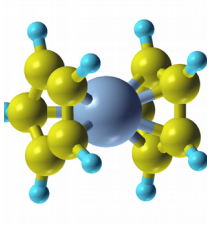
Features

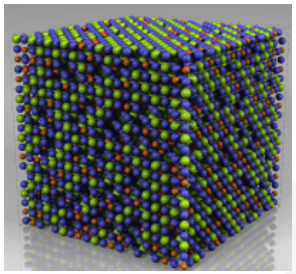
- FLAPW DFT code
- All electrons
- Full potential
- Linearized augmented plane waves
- Open source (MIT license)
- Spin-orbit coupling
- Noncollinear magnetism
- Many XC functionals
- Forces
- Unit cells several 1000 atoms

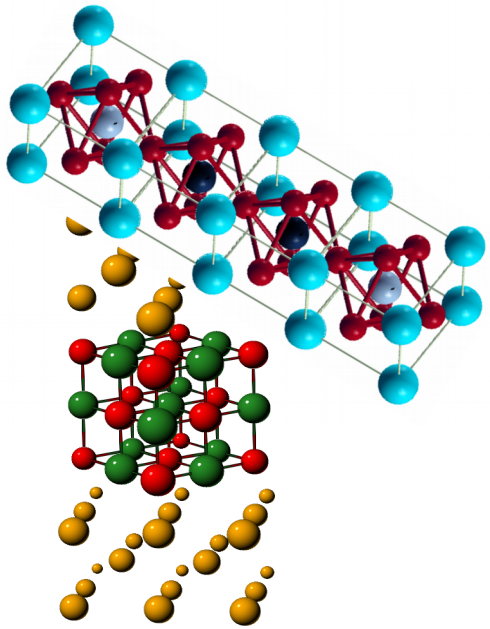
History

- Mainly developed in Jülich
- Complex magnetic systems, surface magnetism

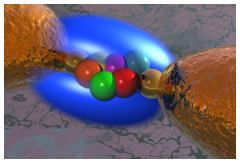
Environment of Applications

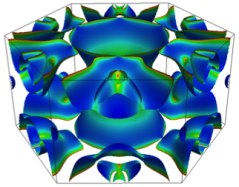






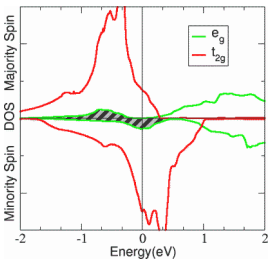
Atomic structure

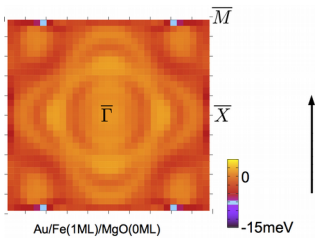


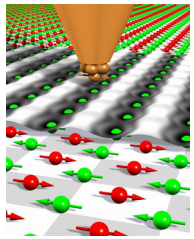


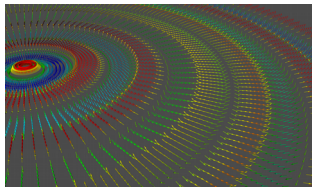
Electronic structure

Magnetic structure





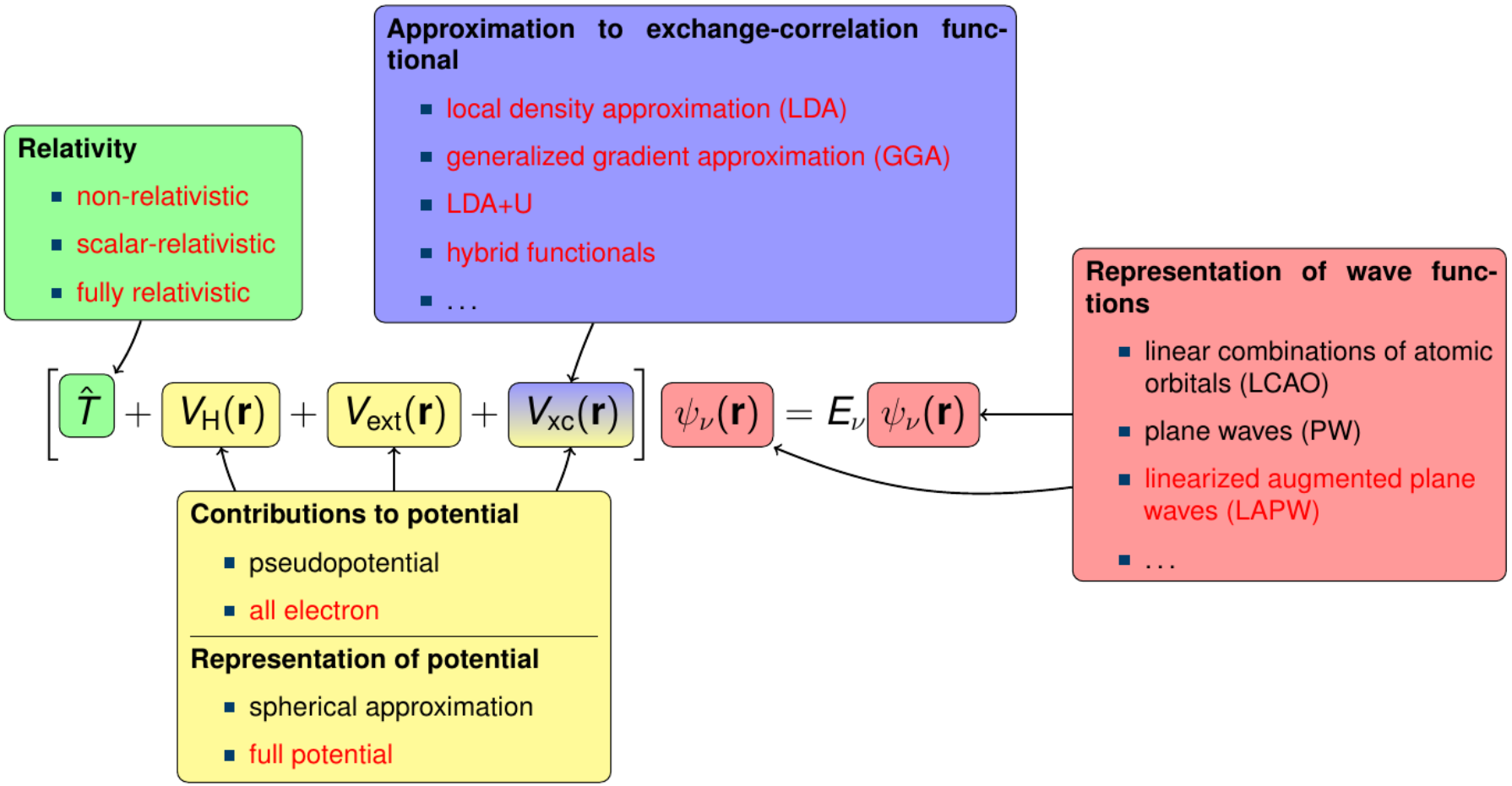




Outline

- **Theoretical background**
  - The FLAPW method and the LAPW basis
  - Separation of core electrons from valence electrons
  - Local orbitals
  - Film setups
- **Obtaining high-presision results**
  - Semicore states and ghost bands
  - Systematic convergence in MT spheres
- **Strengths, Challenges, and Features**
- **Using fleur**
- **Conclusion**

Where in MaX is FLEUR?

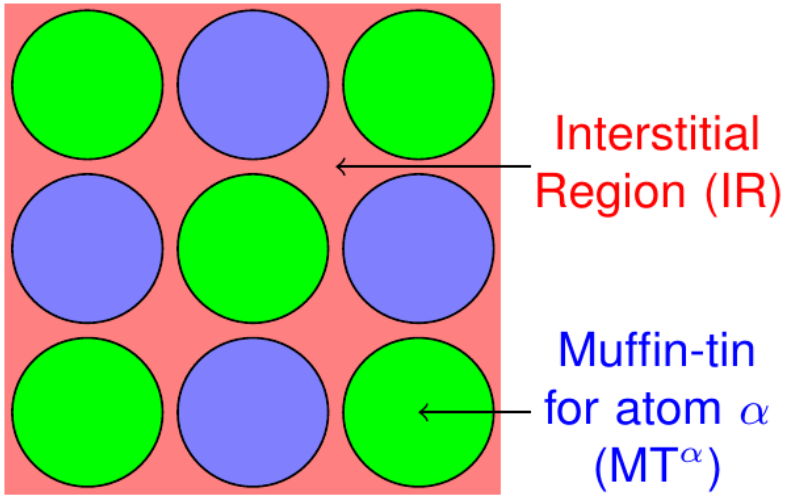


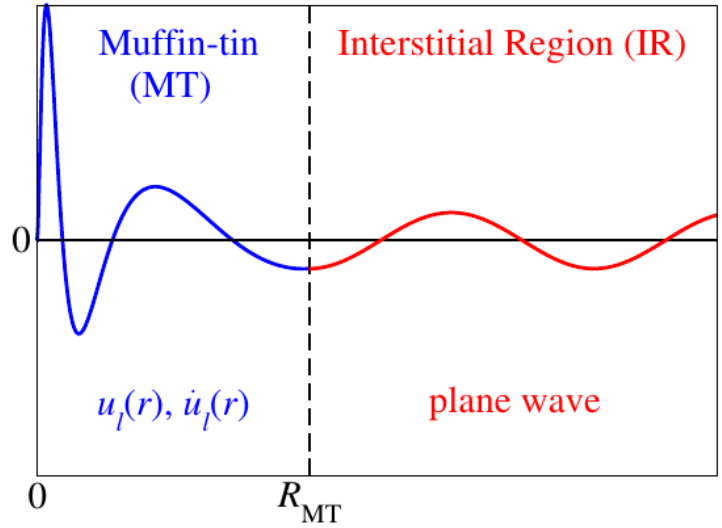
The LAPW basis

- 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





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.

Separation of core electrons from valence electrons

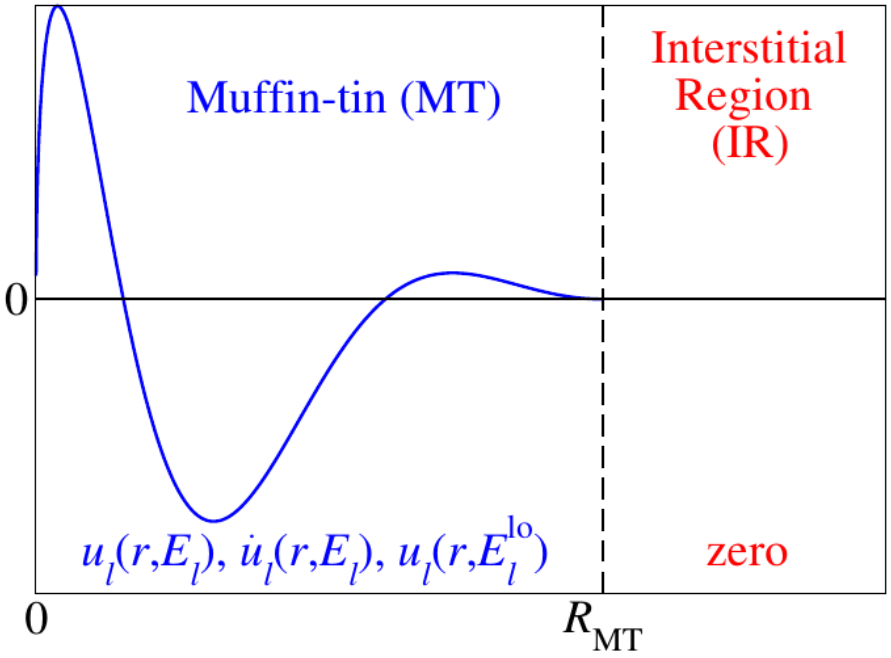
- The LAPW basis is orthogonal to core electron states.
  - (If core electron states vanish at MT sphere boundary)
  - Allows separate determination of core electron wave functions and energies
- Core electrons
  - Representation for each atom separately on radial mesh
  - Fully relativistic treatment
- Valence electrons
  - Representation by LAPW basis
  - Scalar-relativistic description in MT spheres
  - Optional inclusion of spin-orbit coupling
- Semicore states can lead to ghost bands

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

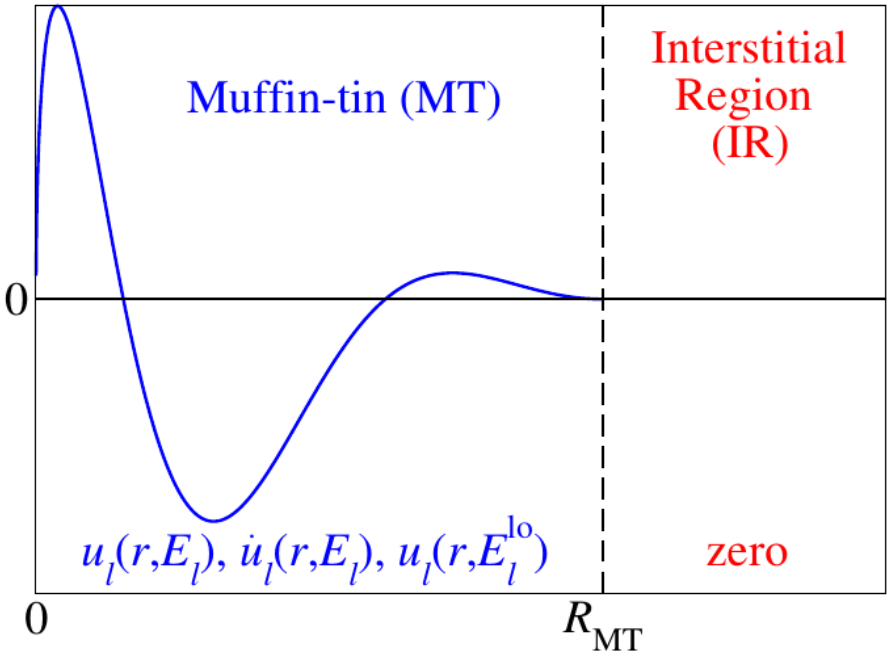


Extending the LAPW basis with local orbitals

Additional basis functions localized in MT spheres

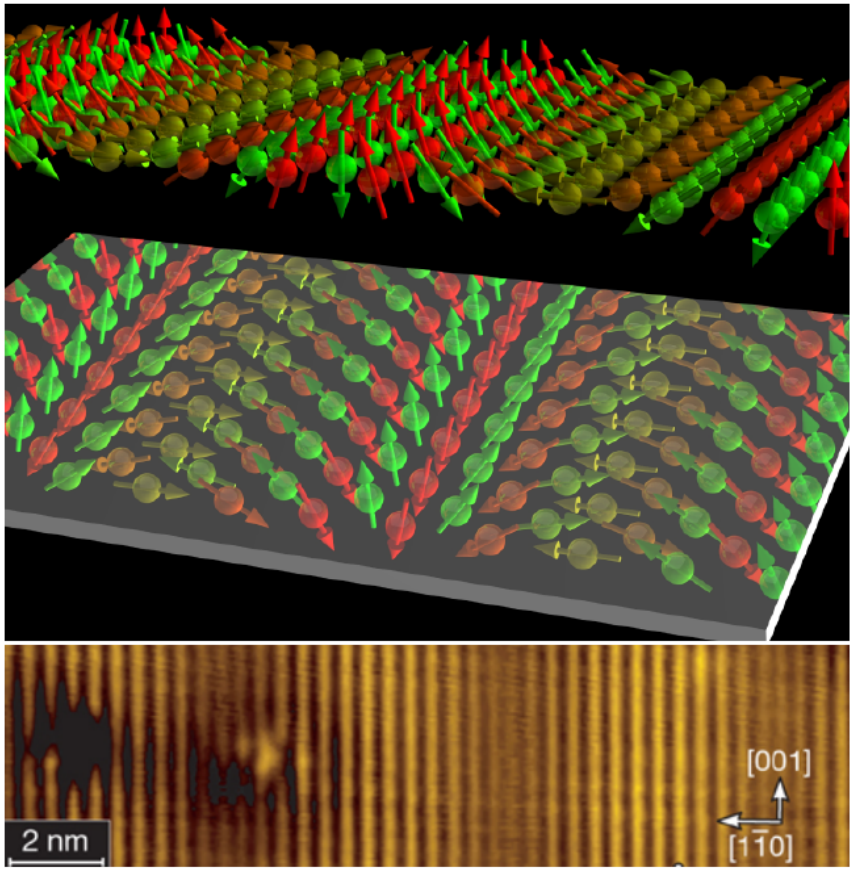
$$\phi_L^{\mathrm{lo}}(\mathbf{r}) = \left[a_L^{\mathrm{lo}} u_l^{\alpha}(r_\alpha, E_l^{\alpha}) + b_L^{\mathrm{lo}} \dot{u}_l^{\alpha}(r_\alpha, E_l^{\alpha}) + c_L^{\mathrm{lo}} u_l^{\alpha}(r_\alpha, E_l^{\mathrm{lo}})\right] Y_L(\hat{\mathbf{r}}_\alpha)$$

- 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 $u_l^{\alpha}(r_\alpha, E_l^{\mathrm{lo}})$



Describing films and surfaces

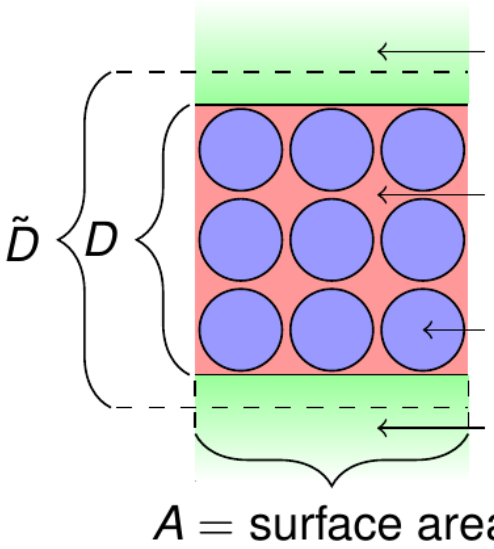
- Film setups break periodicity in one direction
- Description by basis sets with built-in periodicity:
  - Periodic slab calculations
  - Adapt basis set (Fleur)
- Simulate surfaces by increasing film thickness



M. Bode *et al.*, Nature **447**, 190 (2007)

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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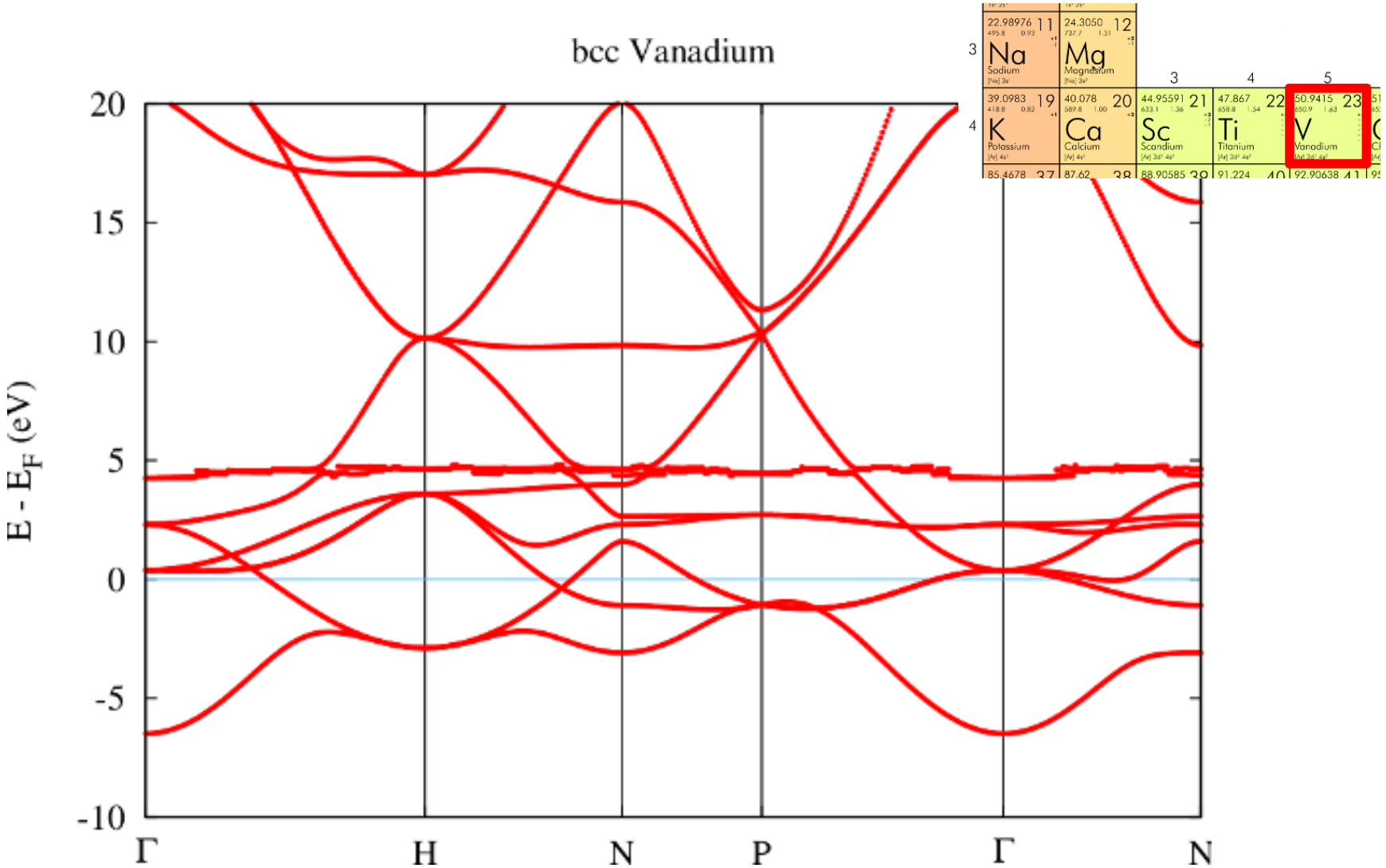
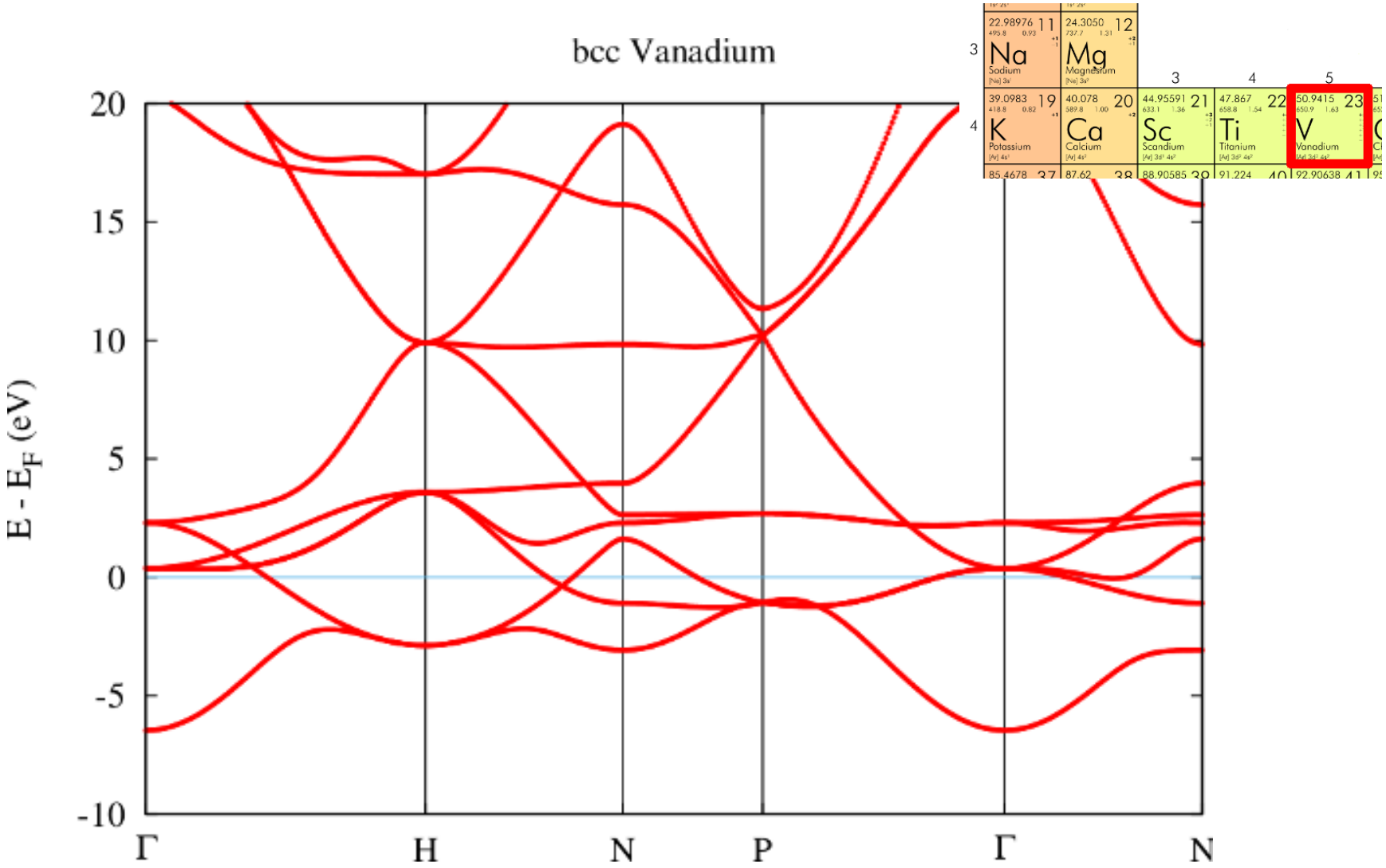
Parameters in FLEUR

$K_{\max}$	reciprocal plane-wave cutoff for LAPW basis
$l^{\alpha}_{\max}$	cutoffs for l expansion of LAPW basis in MT spheres
R^{α}_{MT}	MT radii
E^{α}_{l}	energy parameters
$G_{\max}$	reciprocal plane-wave cutoff for density and potential
D, $\tilde{D}$	vacuum boundary for film setups
...	...

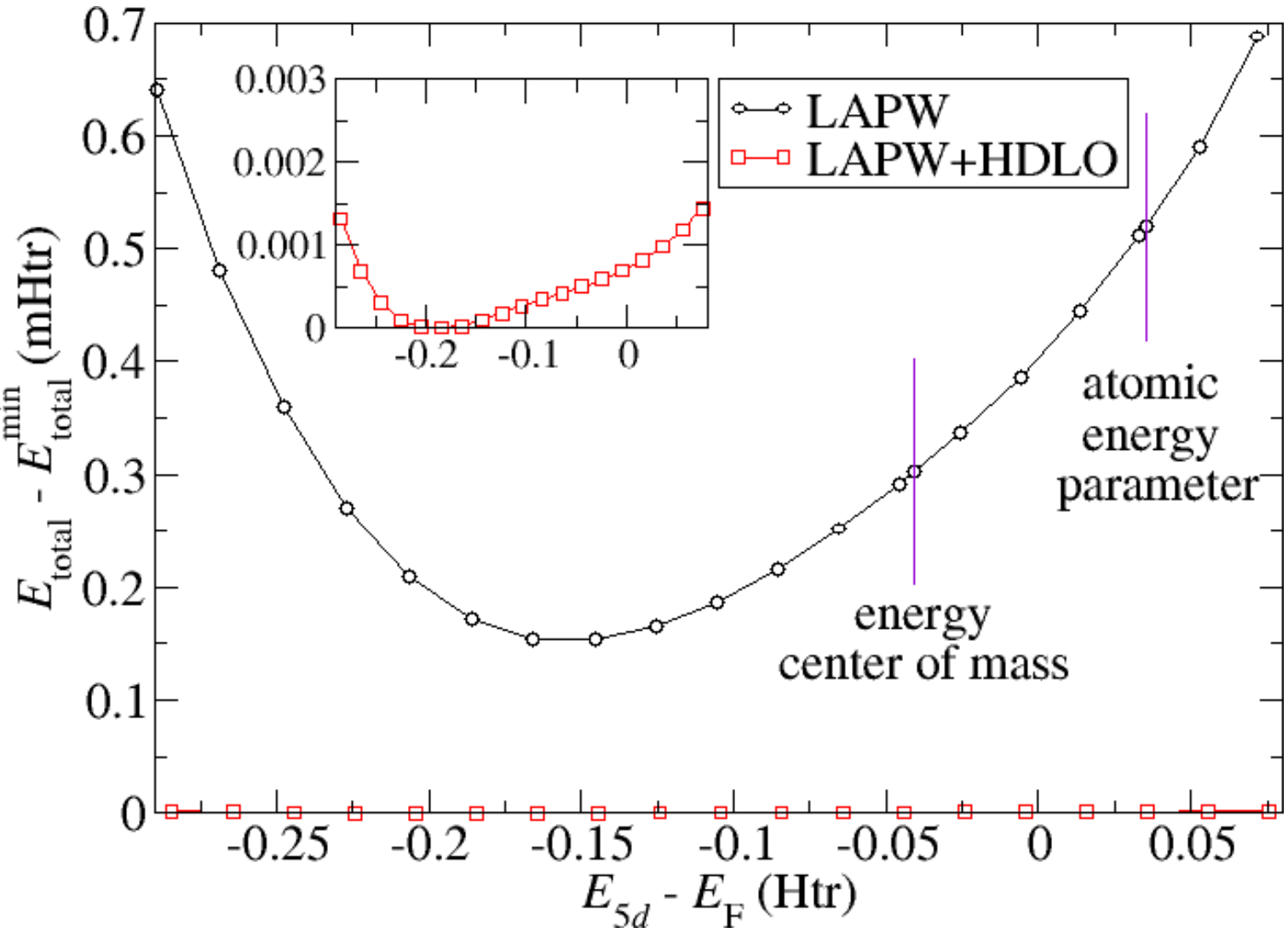
Semicore states and ghost bands



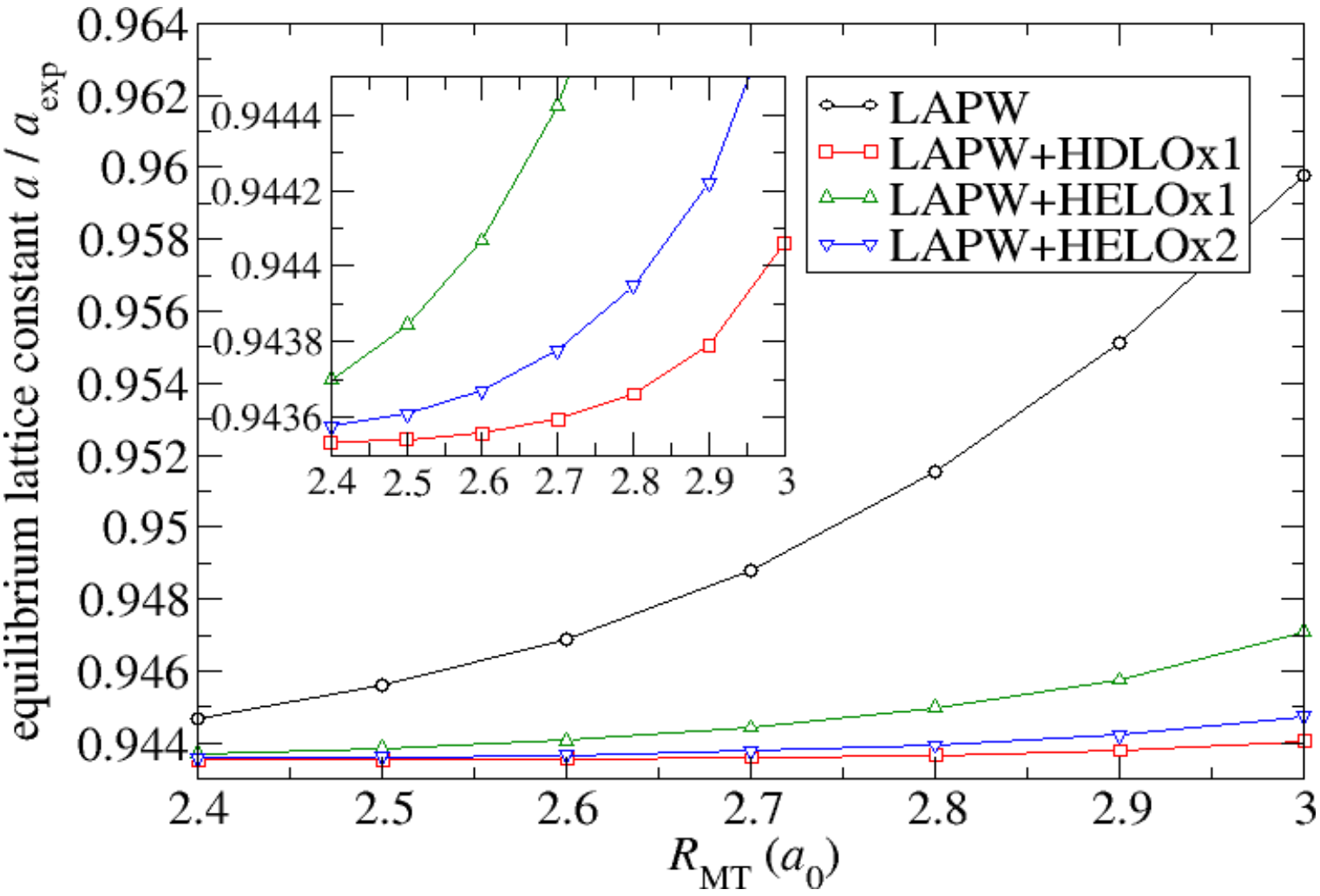
Semicore states and ghost bands – with SCLO



Choice of the energy parameter (fcc Ce)



Systematic convergence in MT spheres (fcc Ce)



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Strengths and Challenges for Fleur

Strengths:

- Possibility to produce precise reference results
- Everything where the core electron spectrum is of direct relevance
- Elements including *f* electrons in valence shell
- Complex magnetism, spin-orbit coupling
  - Example in following talk by Uliana Alekseeva

Challenges in LAPW:

- Complicated expressions due to sophisticated basis
  - Stress tensor
  - Phonons
- Constraint of non-overlapping MT spheres

FLEUR features

- Noncollinear magnetism
- Spin-orbit coupling
- Spin spirals (with generalized Bloch theorem)
- Extraction of parameters for (extended) Heisenberg model
  - exchange coupling parameters, Dzyaloshinskii-Moriya interaction, ...
  - Magnetic force theorem
- LDA+U, Hybrid functional
- Application of external fields
- EELS
- Magnetic circular dichroism
- Band unfolding
- Vacuum DOS (for STM images)
- With Fleur-SPEX: GW approximation to MBPT, ...
- ...

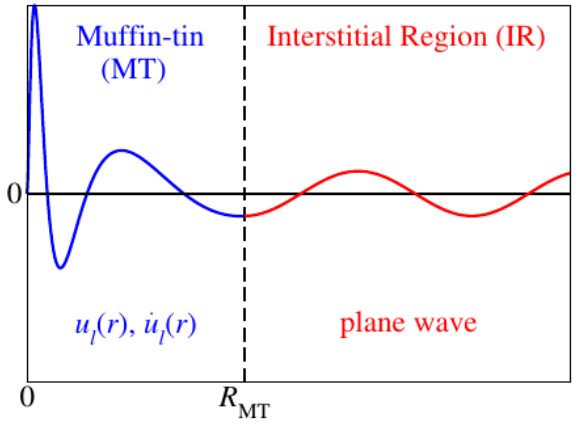
Using Fleur

- Complex parametrization cannot be performed solely by the user
- Usage of an input generator
  - Requires only basic structural input for the unit cell
  - Generates Fleur input with material-adapted default parameters
- Fleur input file (inp.xml)
  - Can be modified by the user...
  - ...to increase cutoff parameters
  - ...activate special calculation modes
- Automatization with AiiDA
- More on this in the talk by Daniel Wortmann

Conclusion

Discussed:

- LAPW basis, local orbitals, film setups
- Obtaining high-precision results
- Strengths, Challenges, and Features
- Fleur input files



More on www.flapw.de:

- Get the code
- Extensive documentation
- References