How to obtain high-quality results with Fleur

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MAX DRIVING THE EXASCALE TRANSITION

cecam Centre Européen de Calcul Atomique et Moléculaire

JÜLICH Forschungszentrum

Outline

- Setting the parameters
- Semicore states and ghost bands
- The linearization error

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

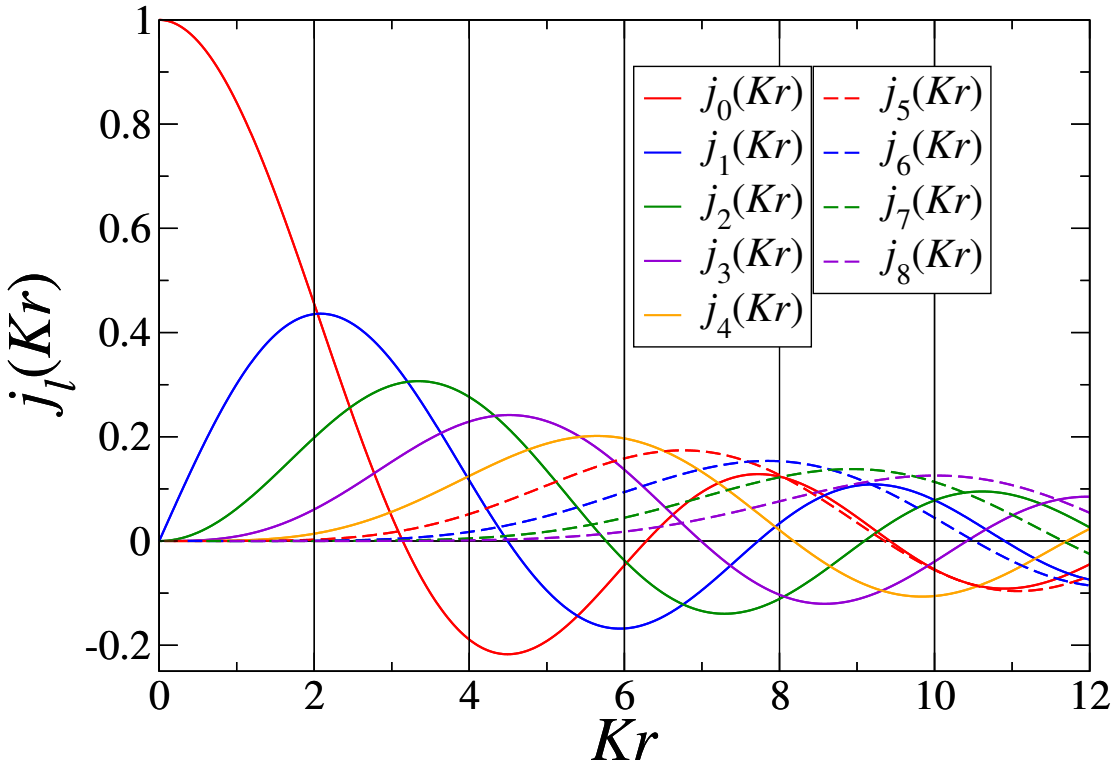
- Rayleigh expansion of planes waves at MT boundary:

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

- 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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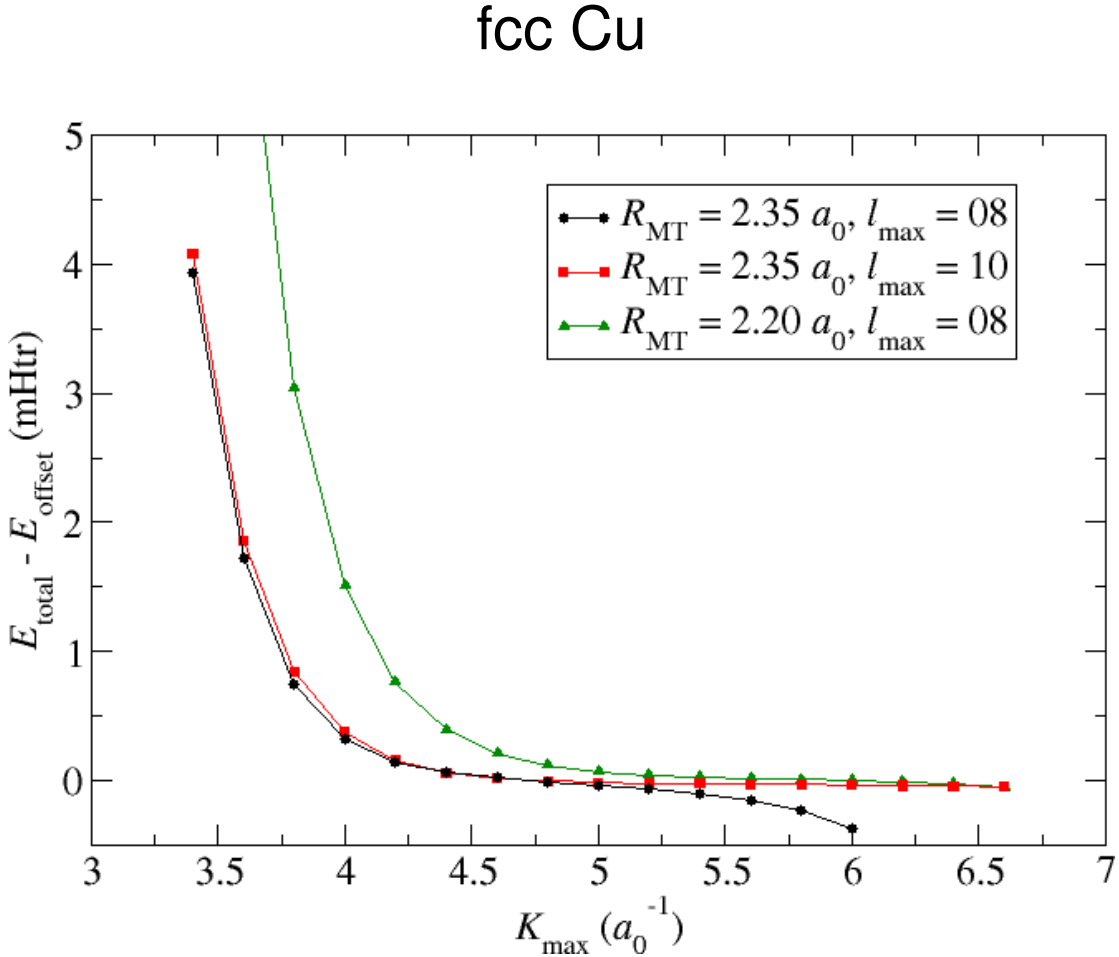
K_{max} parameter convergence

- LAPW basis is nearly linearly dependent.
  - There may be problems due to this when increasing K_{max}.
- If problems arise:
  - It may help to increase l_{max}.
  - It may help to reduce the MT radii.



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Choice of G_{max} and G_{maxXC}

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

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

- Rule

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

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

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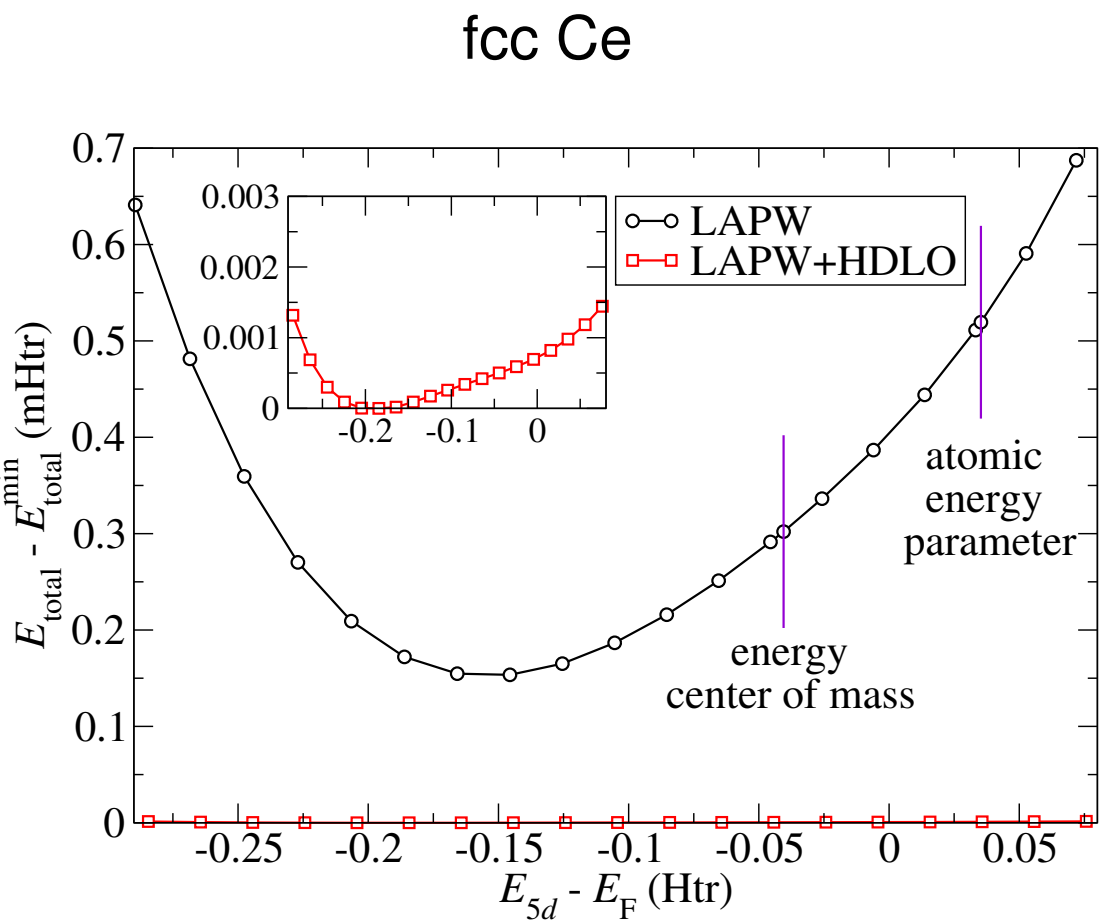
Choice of the energy parameters

- 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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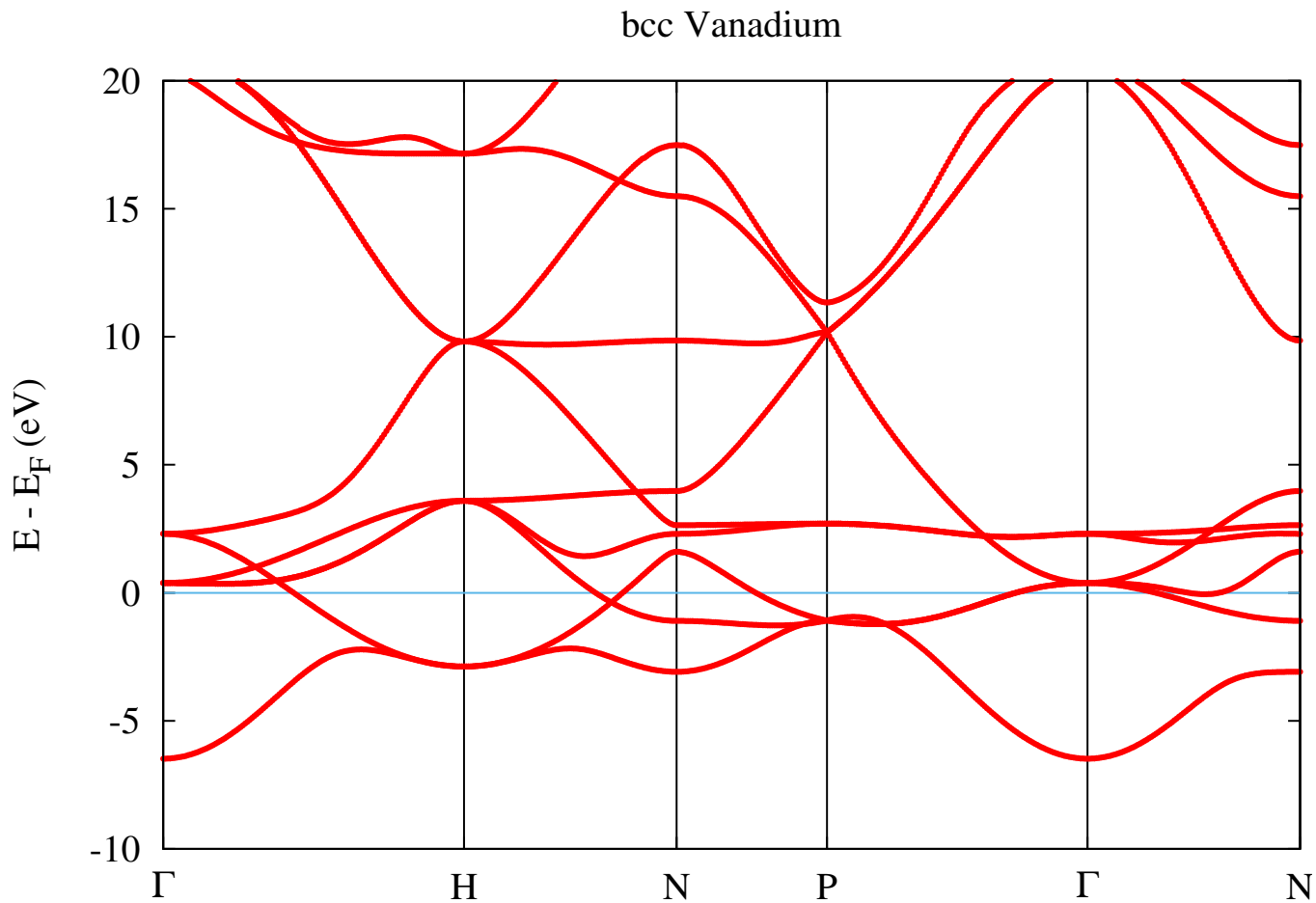
Semicore states and ghost bands



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

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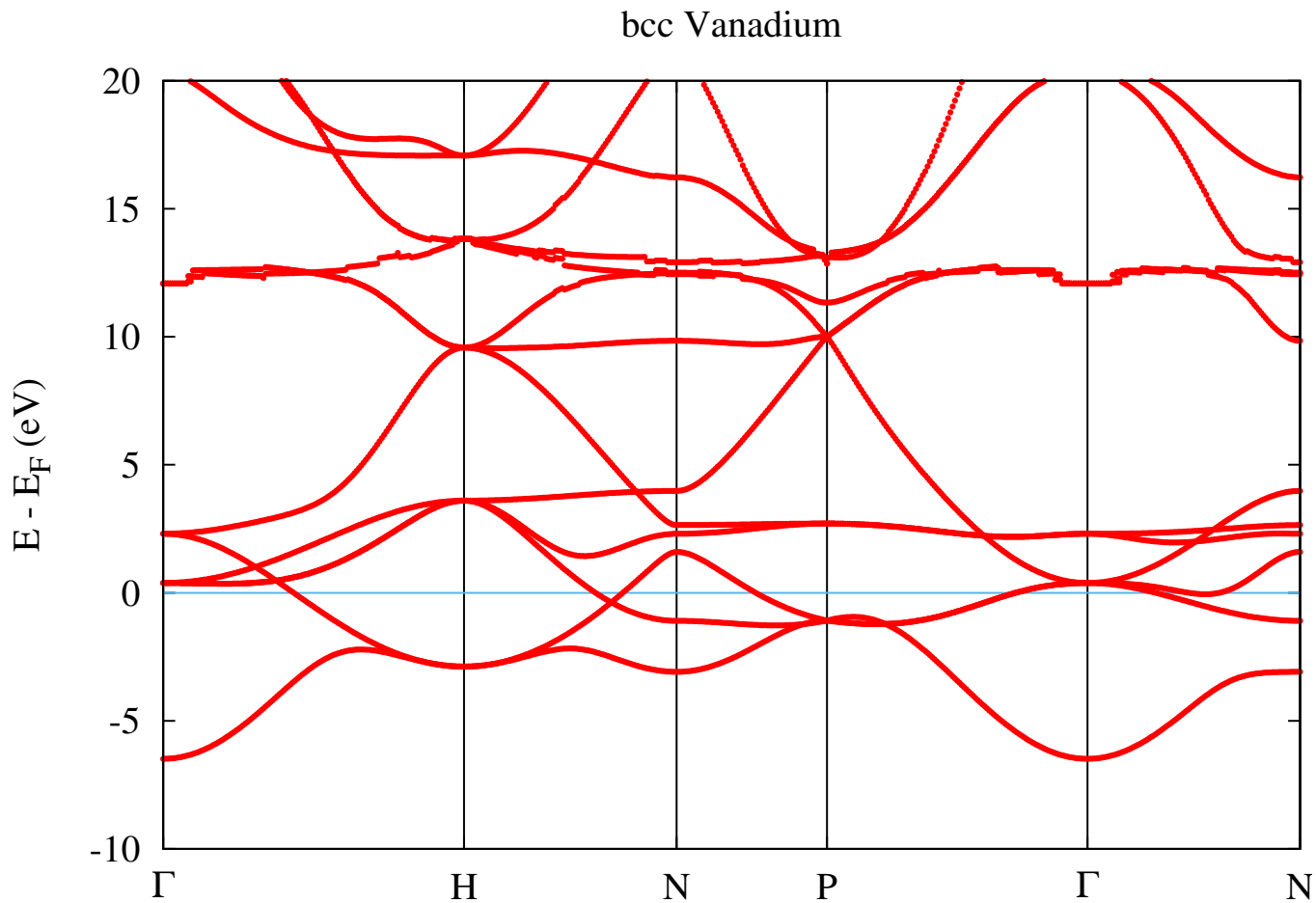
Semicore states and ghost bands



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

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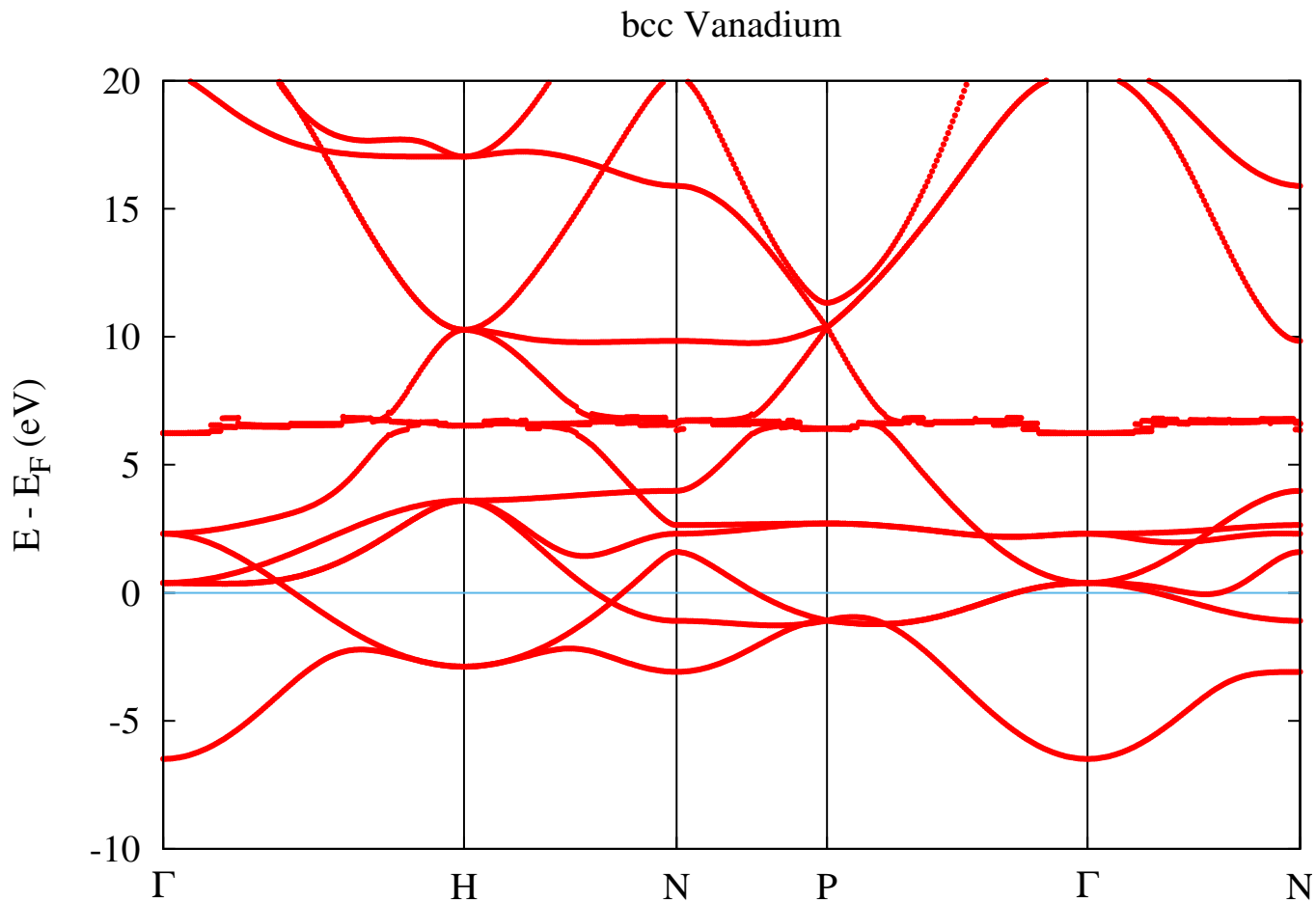
Semicore states and ghost bands



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

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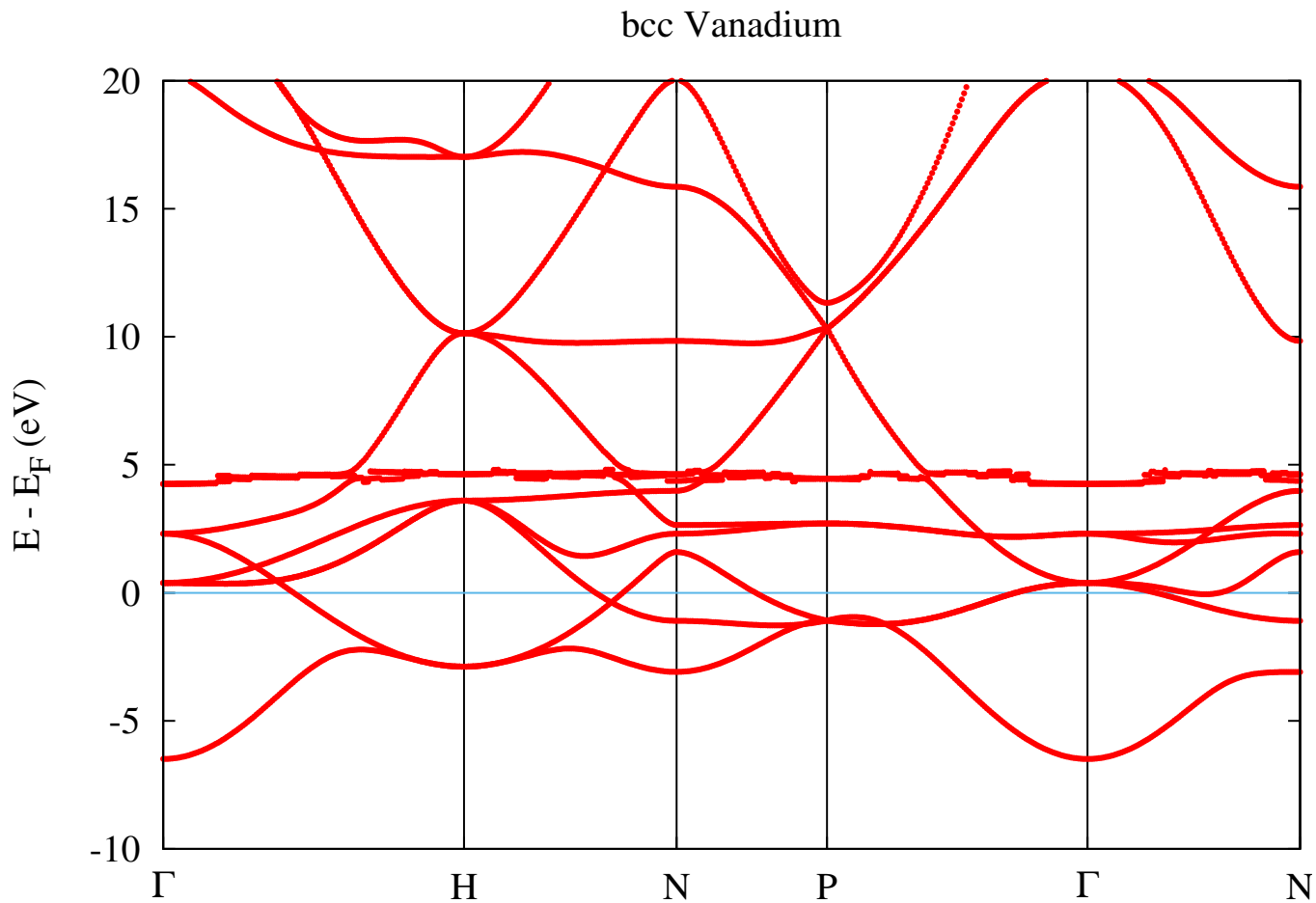
Semicore states and ghost bands



- $R_{MT} = 2.16\ a_0$, 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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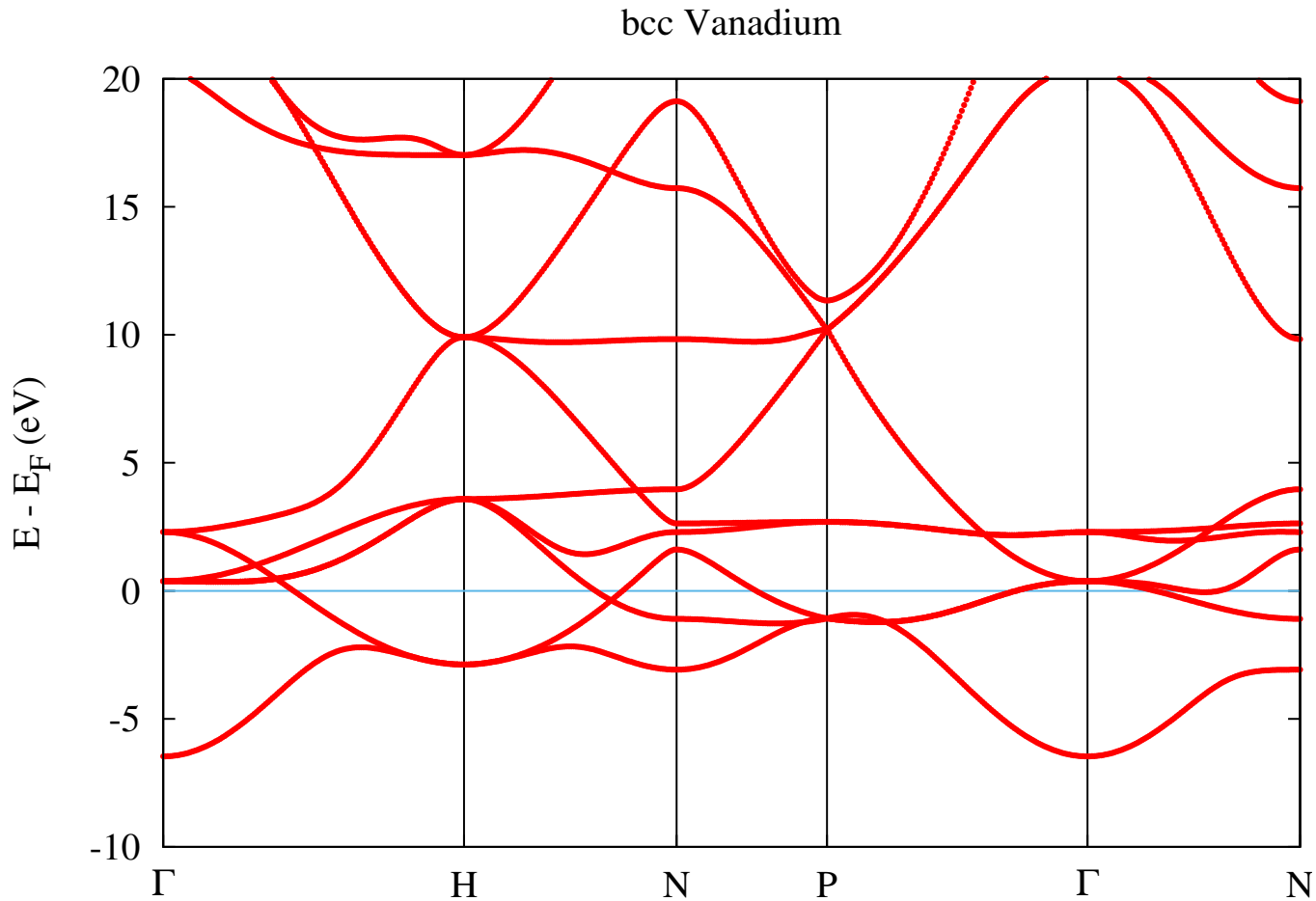
Semicore states and ghost bands - with SCLO



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

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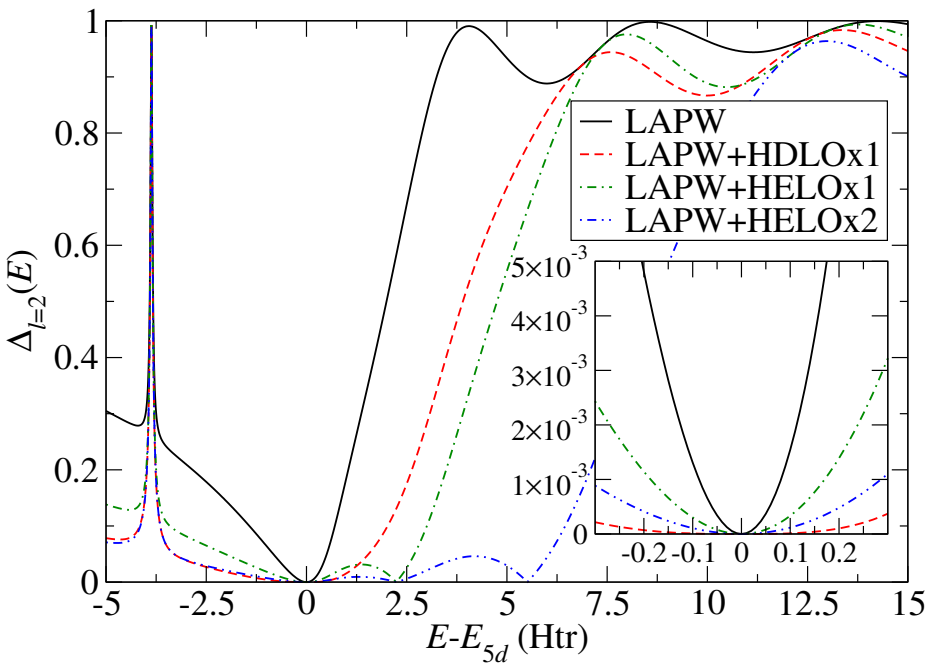
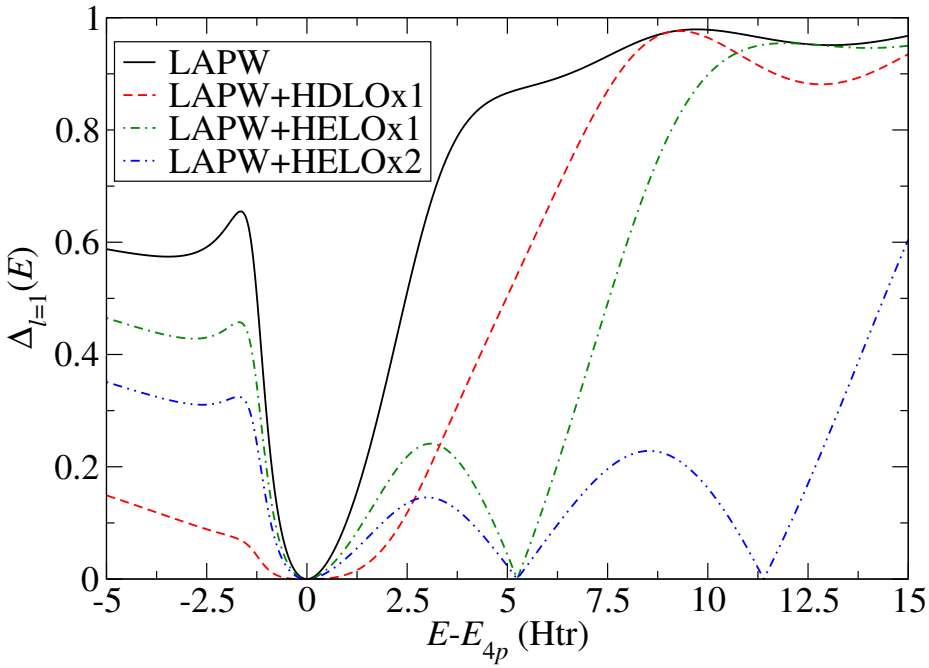
Linearization error depending on energy mismatch

fcc Cerium



bcc Vanadium



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

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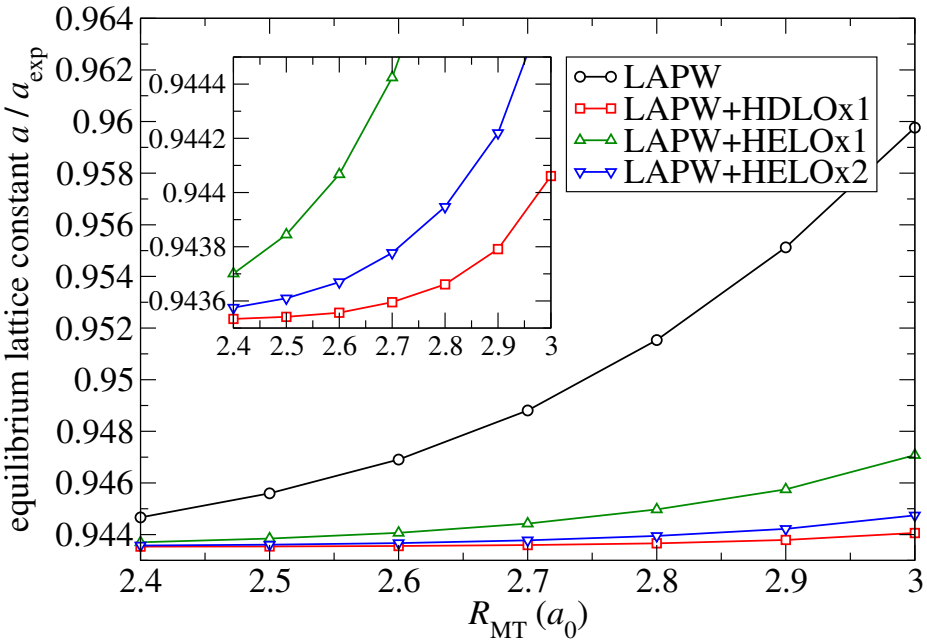
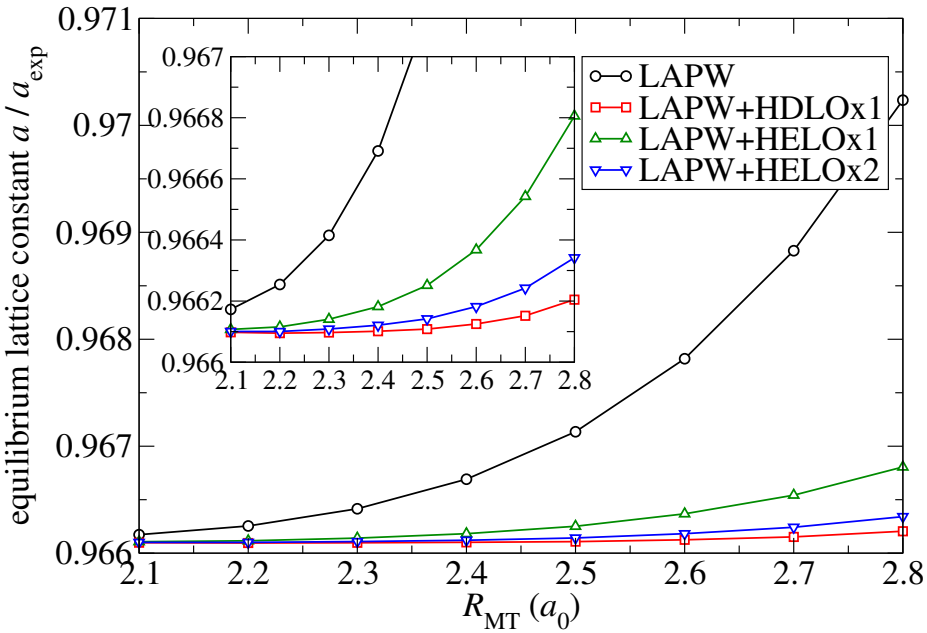
The linearization error and MT radii

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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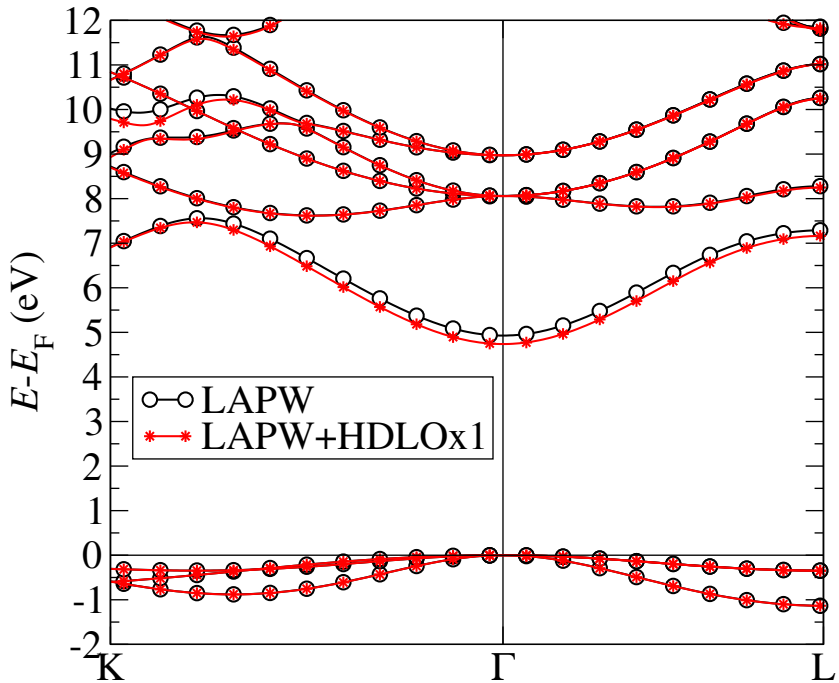
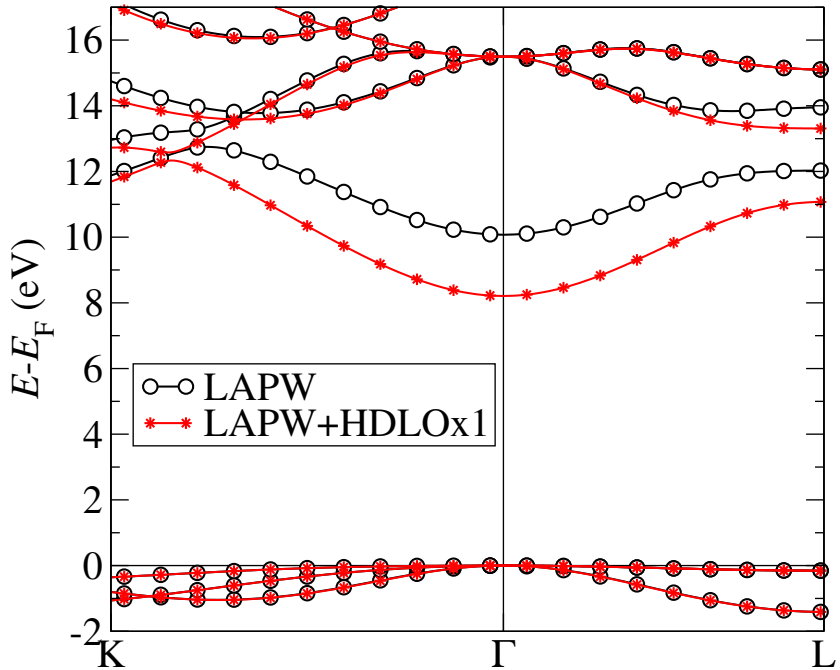
The linearization error and unoccupied states





- 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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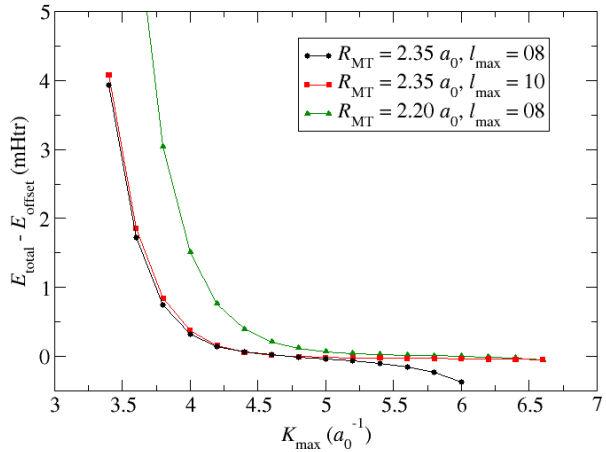
Conclusions

- 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
- Not discussed
  - General numerical DFT parameters, e.g., k point set, Fermi smearing, ...



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