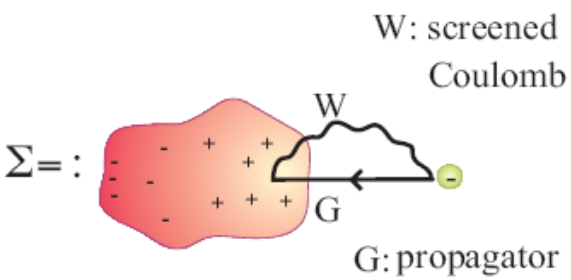
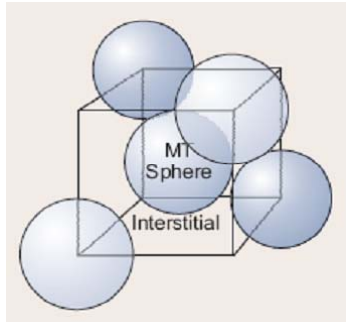




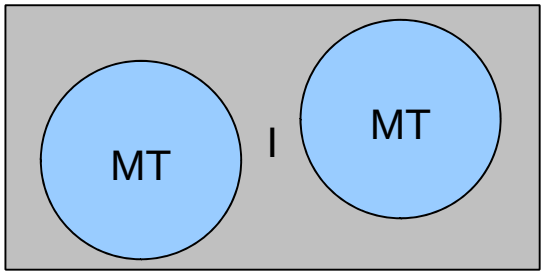
All-electron *GW* based on LAPW approach

Hong Jiang

R. I. Gomez-Abal, X. Li, H. Jiang, C. Meisenbichler, C. Ambrosch-Draxl and M. Scheffler, *The G_0W_0 approach based on the full-potential linearized augmented planewave method,* to be submitted to *Comp. Phys. Comm*.

LAPW basis

APW (J. C. Slater, 1937)



$$\tilde{\Phi}^{\vec{k}}_{\vec{G}}(\vec{r};E)=\begin{cases}\dfrac{1}{\sqrt{\Omega}}e^{i\left(\vec{k}+\vec{G}\right)\cdot\vec{r}} & \vec{r}\in I\\ \displaystyle\sum_{l=0}^{l_{max}}\sum_{m=-l}^{+l}\left[A^a_{lm}(\vec{k}+\vec{G})u_l(r^a,E)\right]Y_{lm}(\hat{r}^a) & \vec{r}\in MT_a\end{cases}$$

- Small basis set size and accurate (with full-potential treatment)
- non-linear problem, numerically difficult to solve

LAPW (O. K. Anderson, 1975)

$$\tilde{\Phi}^{\vec{k}}_{\vec{G}}(\vec{r})=\begin{cases}\dfrac{1}{\sqrt{\Omega}}e^{i\left(\vec{k}+\vec{G}\right)\cdot\vec{r}} & \vec{r}\in I\\ \displaystyle\sum_{l=0}^{l_{max}}\sum_{m=-l}^{+l}\left[A^a_{lm}(\vec{k}+\vec{G})u_l(r^a,E_l)+B^a_{lm}(\vec{k}+\vec{G})\dot{u}_l(r^a,E_l)\right]Y_{lm}(\hat{r}^a) & \vec{r}\in MT_a\end{cases}$$

- Larger number of plane waves than APW
- linear problem: numerically easy to solve

LAPW basis: extension

Local orbital (LO) for semicore states (D.J. Singh, 1991)

$$\tilde{\Phi}^{LO}_{LAPW}(\mathbf{r}) = \begin{cases} 0 & \mathbf{r} \in I \\ \left[A^a_{lm} u_l(r^a, E_l) + B^a_{lm} \dot{u}_l(r^a, E_l) + C^a_{lm} u^{(2)}_l(r^a)\right] Y_{lm}(\hat{r}^a) & \mathbf{r} \in MT_a \end{cases}$$

APW+lo (E. Sjoestedt, L. Nordstroem, D.J. Singh, 2000)

$$\tilde{\Phi}^{\mathbf{k}}_{\mathbf{G}}(\mathbf{r}) = \begin{cases} \frac{1}{\sqrt{\Omega}} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} & \mathbf{r} \in I \\ \sum_{l=0}^{l_{max}} \sum_{m=-l}^{+l} A^a_{lm}(\mathbf{k}+\mathbf{G}) u_l(r^a, E_l) Y_{lm}(\hat{r}^a) & \mathbf{r} \in MT_a \end{cases}$$

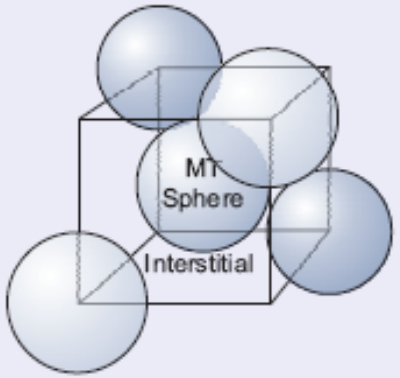
$$\tilde{\Phi}^{lo}_{APW}(\mathbf{r}) = \begin{cases} 0 & \mathbf{r} \in I \\ \left[A^a_{lm} u_l(r^a, E_l) + B^a_{lm} \dot{u}_l(r^a, E_l)\right] Y_{lm}(\hat{r}^a) & \mathbf{r} \in MT_a \end{cases}$$

Basis functions for *GW*: mixed basis

$$M^{i}_{nm}(\vec{k},\vec{q}) \equiv \int_{\Omega} \chi_i^{\vec{q}*}(\vec{r})\Psi_{n\vec{k}}(\vec{r})\Psi^{*}_{m\vec{k}-\vec{q}}(\vec{r})d^3r$$

$$\tilde{\psi}_{n\mathbf{k}}(\mathbf{r}) = \sum_{a\nu lm} A^{n\mathbf{k}}_{a\nu lm} u_{a\nu l}(r^a) Y_{lm}(\hat{r}^a) + \sum_{\mathbf{G}} Z^{n\mathbf{k}}_{\mathbf{G}} \tilde{P}^{\mathbf{k}}_{\mathbf{G}}(\mathbf{r})$$

$$\chi_i^{\mathbf{q}}(\mathbf{r}) = \begin{cases} \sum_{\mathbf{R}a} e^{i\mathbf{k}\cdot(\mathbf{R}+\mathbf{r}_a)} \upsilon_{NL}(r) Y_{LM}(\hat{r}) & \mathbf{r} \in \text{MT-spheres} \\ \frac{1}{\sqrt{V}} \sum_{\mathbf{G}} S_{i,\mathbf{G}} e^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}} & \mathbf{r} \in \text{Interstitial} \end{cases}$$



Radial functions $\upsilon_{NL}(r)$ for each *L* are constructed by orthogonalizing all products of radial functions $u_{\nu l}(r)u_{\nu' l'}(r)$ that fulfill the condition $|l-l'| \le L \le l+l'$ and removing all redundant ones due to linear dependency.

Aryasetiawan and Gunnarsson(1994); Kotani and van Schilfgaarde (2002); R. Gomez-Abal et al. (2009)

Basis functions for *GW*: Extension

***v*-diagonalized basis**: eigenvectors of the bare Coulomb matrix as represented by original mixed-basis (C. Friedrich *et al.* (2009))

- almost equivalent to the original mixed-basis, except for **q**=0
- reduce the number of matrix multiplication
- Γ point treated more accurately [e.g. dielectric anisotropy (C. Freysoldt *et al*. (2007)]
- can be reduced in size by removing those corresponding to small eigen-values of v
- but: all basis functions become “global”

$$\varepsilon_{ij}(\mathbf{q},i\omega) = \delta_{ij} - N_c^{-1} \sum_{\mathbf{k}}^{BZ} \sum_{n}^{\text{occ}} \sum_{m}^{\text{unocc}} F_{nm\mathbf{k}}(\mathbf{q},\omega) \sum_{kl} v_{ik}^{\frac{1}{2}}(\mathbf{q}) M_{nm}^{k}(\mathbf{k},\mathbf{q}) \left[M_{nm}^{l}(\mathbf{k},\mathbf{q})\right]^{*} v_{lj}^{\frac{1}{2}}(\mathbf{q})$$

$$\Rightarrow \quad \varepsilon_{ij}^{b}(\mathbf{q},\omega) = \delta_{ij} - N_c^{-1} \sum_{\mathbf{k}}^{BZ} \sum_{n}^{\text{occ}} \sum_{m}^{\text{unocc}} F_{nm\mathbf{k}}(\mathbf{q},\omega)(0,\omega) v_{i}^{\frac{1}{2}} M_{nm}^{i}(\mathbf{k},\mathbf{q}) \left[v_{j}^{\frac{1}{2}} M_{nm}^{j}(\mathbf{k},\mathbf{q})\right]^{*}$$

Γ-point singularity

Symmetrized dielectric function

$$\tilde{\varepsilon}_{ij}(\mathbf{q},\omega) = \sum_{lm} v_{il}^{\frac{1}{2}}(\mathbf{q}) P_{lm}(\mathbf{q},\omega) v_{mj}^{\frac{1}{2}}(\mathbf{q})$$

Screened Coulomb interaction

$$W_{ij}(\mathbf{q},\omega) = \sum_{lm} v_{il}^{\frac{1}{2}}(\mathbf{q}) \tilde{\varepsilon}_{lm}^{-1}(\mathbf{q},\omega) v_{mj}^{\frac{1}{2}}(\mathbf{q})$$

$$v_{ij}^{\frac{1}{2}}(\mathbf{q}\to 0) = \frac{v_{ij}^{s\frac{1}{2}}}{|\mathbf{q}|} + \tilde{v}_{ij}^{\frac{1}{2}}$$

$$\tilde{\varepsilon}_{ij}(0,\omega) = \tilde{\varepsilon}_{ij}^{H}(0,\omega) + \tilde{\varepsilon}_{ij}^{W}(0,\omega) + \tilde{\varepsilon}_{ij}^{B}(0,\omega)$$

$$W_{ij}^{c}(\mathbf{q}\to 0,\omega) = \frac{1}{|\mathbf{q}|^2} W_{ij}^{cs2}(\omega) + \frac{1}{|\mathbf{q}|} W_{ij}^{cs1}(\omega) + \tilde{W}_{ij}^{c}(\omega)$$

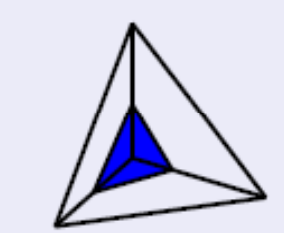
***v*-diag. basis**

$$\boldsymbol{\varepsilon} = \begin{bmatrix} \mathcal{E}_{00}^{\mathrm{H}} & \mathcal{E}_{0i}^{\mathrm{W}} \\ \mathcal{E}_{i0}^{\mathrm{W}} & \mathcal{E}_{ij}^{\mathrm{B}} \end{bmatrix} \qquad \mathbf{W} = \begin{bmatrix} W_{00}^{\mathrm{H}}/q^2 & W_{0i}^{\mathrm{W}}/q \\ W_{i0}^{\mathrm{W}}/q & W_{ij}^{\mathrm{B}} \end{bmatrix}$$

Brillouin zone integration

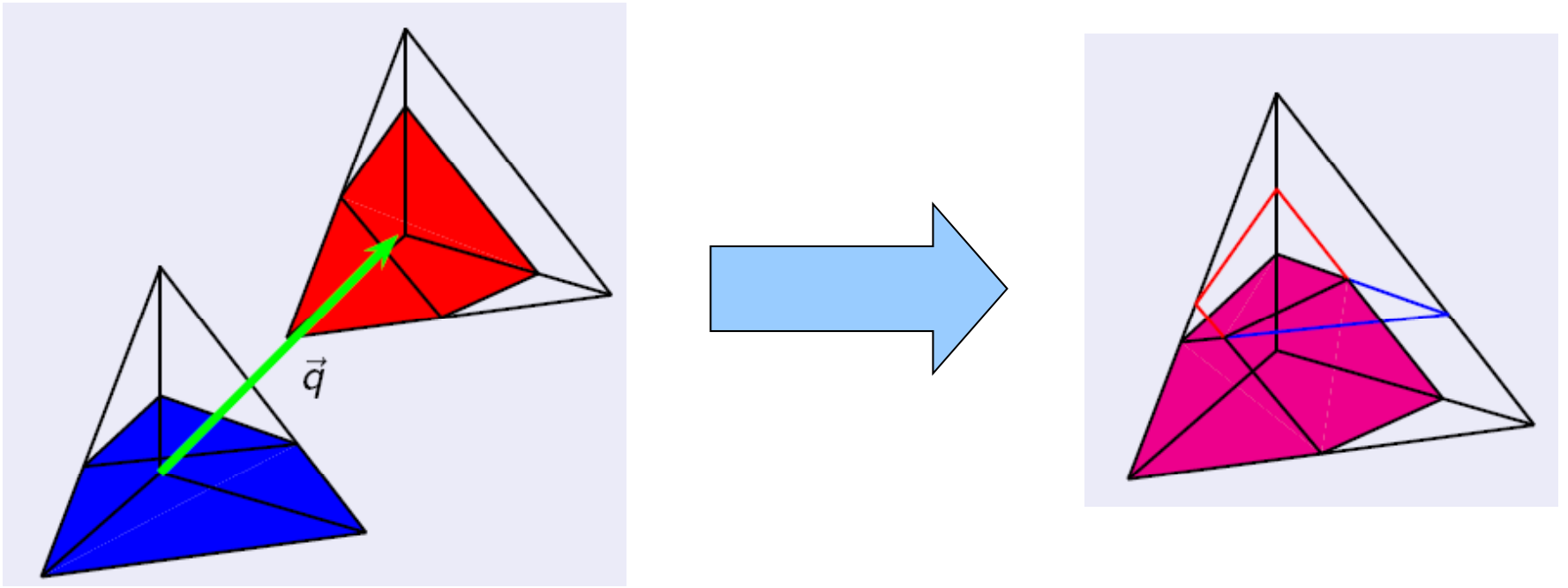
The Linear Tetrahedron method

$$\langle X \rangle = \frac{1}{\Omega} \sum_n \int_\Omega X_n(\mathbf{k}) f(\epsilon_n(\mathbf{k})) d^3k \longrightarrow \langle X \rangle = \sum_n \sum_i X_n(\mathbf{k_i}) w_n(\mathbf{k_i})$$



q-dependent Linear Tetrahedron Method

$$P_{ij}(\mathbf{q},\omega) = \int_{BZ} \sum_{nm} \left\{ \frac{M^i_{nm}(\mathbf{k},\mathbf{q})\left[M^j_{nm}(\mathbf{k},\mathbf{q})\right]^*}{\omega - \epsilon_{m\mathbf{k}-\mathbf{q}} + \epsilon_{n\mathbf{k}} + i\eta} - \frac{M^i_{nm}(\mathbf{k},\mathbf{q})\left[M^j_{nm}(\mathbf{k},\mathbf{q})\right]^*}{\omega - \epsilon_{n\mathbf{k}} + \epsilon_{m\mathbf{k}-\mathbf{q}} - i\eta} \right\} f(\epsilon_{\mathbf{k}})[1 - f(\epsilon_{\mathbf{k}-\mathbf{q}})] d^3\mathbf{k}$$



Frequency integration

$$\Sigma(\mathbf{r}_1,\mathbf{r}_2;\omega) = \frac{i}{2\pi}\int G_0(\mathbf{r}_1,\mathbf{r}_2;\omega+\omega')W_0(\mathbf{r}_2,\mathbf{r}_1;\omega')d\omega'$$

$$\Downarrow \text{ Analytic continuation}$$

$$\Sigma(\mathbf{r}_1,\mathbf{r}_2;i\omega) = \frac{i}{2\pi}\int G_0(\mathbf{r}_1,\mathbf{r}_2;i\omega+i\omega')W_0(\mathbf{r}_2,\mathbf{r}_1;i\omega')di\omega'$$

$$\boxed{\Sigma_{n\mathbf{k}}(i\omega) = -\sum_{\mathbf{q}}\sum_{ij}\sum_{n'} M^{i}_{nn'}(\mathbf{k},\mathbf{q})\frac{1}{\pi}\int_0^\infty \frac{W_{ij}(\mathbf{q};i\omega')d\omega'}{(i\omega-\epsilon_{n,\mathbf{k}'})^2+\omega'^2} M^{*j}_{n'n}(\mathbf{k},\mathbf{q})}$$

Non linear least squares

$$\Sigma_{n\mathbf{k}}(i\omega) = \sum_{j=1}^{n}\frac{a_j}{i\omega-b_j}$$

$$\Downarrow \text{ Analytic continuation}$$

$$\Sigma_{n\mathbf{k}}(\omega) = \sum_{j=1}^{n}\frac{a_j}{\omega-b_j}$$

Other features

- **Spin-polarization => Magnetic systems**
- **G_0W_0@LDA+*U***

$$\left[-\frac{1}{2}\nabla^2 + V^{\mathrm{LDA}}(\vec{r}) + \delta\hat{V}^{\mathrm{LDA+U}}\right]\Psi_{n\vec{k}}(\vec{r}) = \varepsilon_{n\vec{k}}\Psi_{n\vec{k}}(\vec{r})$$

$$\varepsilon_{n\vec{k}}^{\mathrm{QP-LDA+U}} = \varepsilon_{n\vec{k}}^{\mathrm{LDA+U}} + Z_{n\vec{k}}\left(\varepsilon_{n\vec{k}}^{\mathrm{LDA+U}}\right)\left[\Sigma_{n\vec{k}}\left(\varepsilon_{n\vec{k}}^{\mathrm{LDA+U}}\right) - V_{n\vec{k}}^{\mathrm{XC}} - \delta V_{n\vec{k}}^{\mathrm{LDA+U}}\right]$$

- **Energy-only self-consistent *GW*$_0$**

$$\Sigma_{n\vec{k}}^{c}(i\omega) = \frac{1}{\pi}\sum_{\vec{q}}^{BZ}\sum_{n'}\sum_{ij}\left[M_{nn'}^{i}(\vec{k},\vec{q})\right]^{*}\int_0^{\infty}\frac{(\varepsilon_{n'\vec{k}+\vec{q}} - i\omega)W_{ij}^{c}(\vec{q},i\omega')}{(i\omega - \varepsilon_{n'\vec{k}+\vec{q}})^2 + \omega'^2}d\omega' M_{nn'}^{j}(\vec{k},\vec{q})$$

$$\boxed{\Sigma_{n\vec{k}}^{c}(i\omega) = \frac{1}{\pi}\sum_{\vec{q}}^{BZ}\sum_{n'}\int_0^{\infty}\frac{(\varepsilon_{n'\vec{k}+\vec{q}} - i\omega)X_{nn'}(\vec{k},\vec{q},\omega')}{(i\omega - \varepsilon_{n'\vec{k}+\vec{q}})^2 + \omega'^2}d\omega'}$$

Applications: AE vs PP *GW*

PRL **101,** 106404 (2008) PHYSICAL REVIEW LETTERS week ending 5 SEPTEMBER 2008

Influence of the Core-Valence Interaction and of the Pseudopotential Approximation on the Electron Self-Energy in Semiconductors

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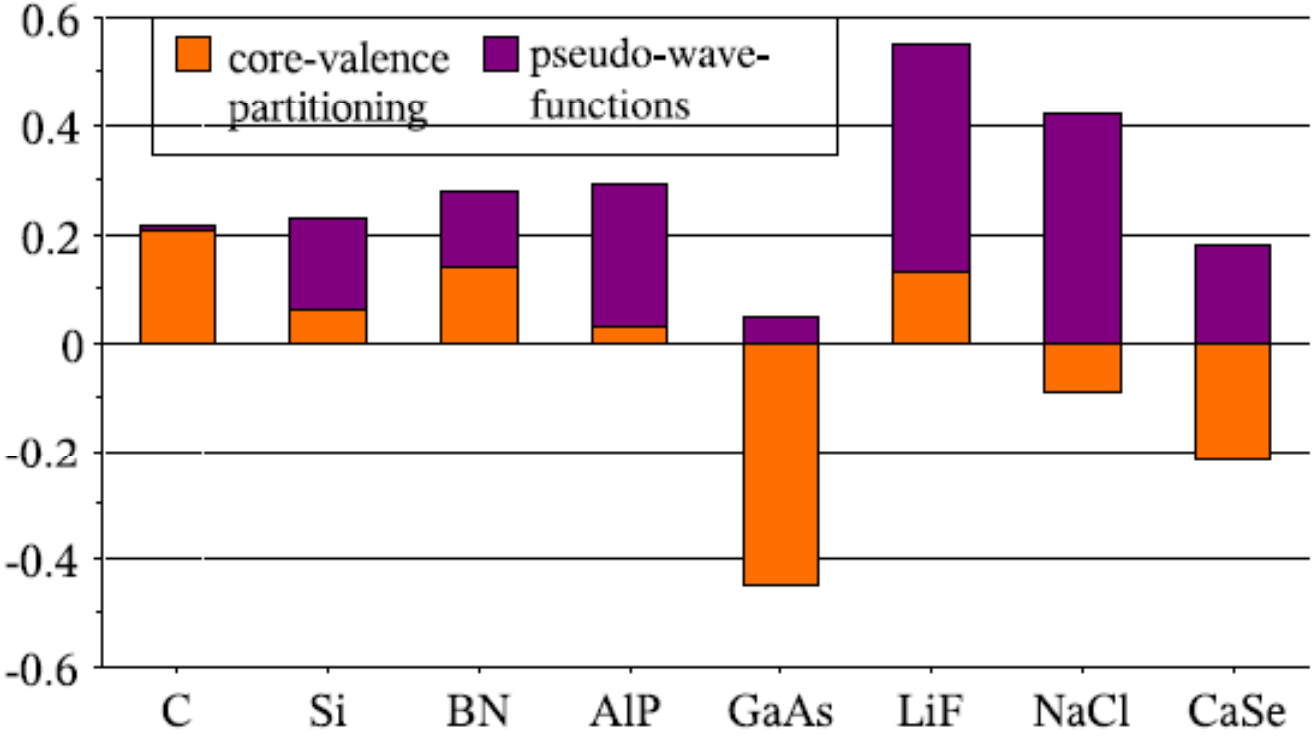

Applications: *GW* for *f*-electron systems

PRL **102,** 126403 (2009) PHYSICAL REVIEW LETTERS week ending 27 MARCH 2009

Localized and Itinerant States in Lanthanide Oxides United by *GW* @ LDA + *U*

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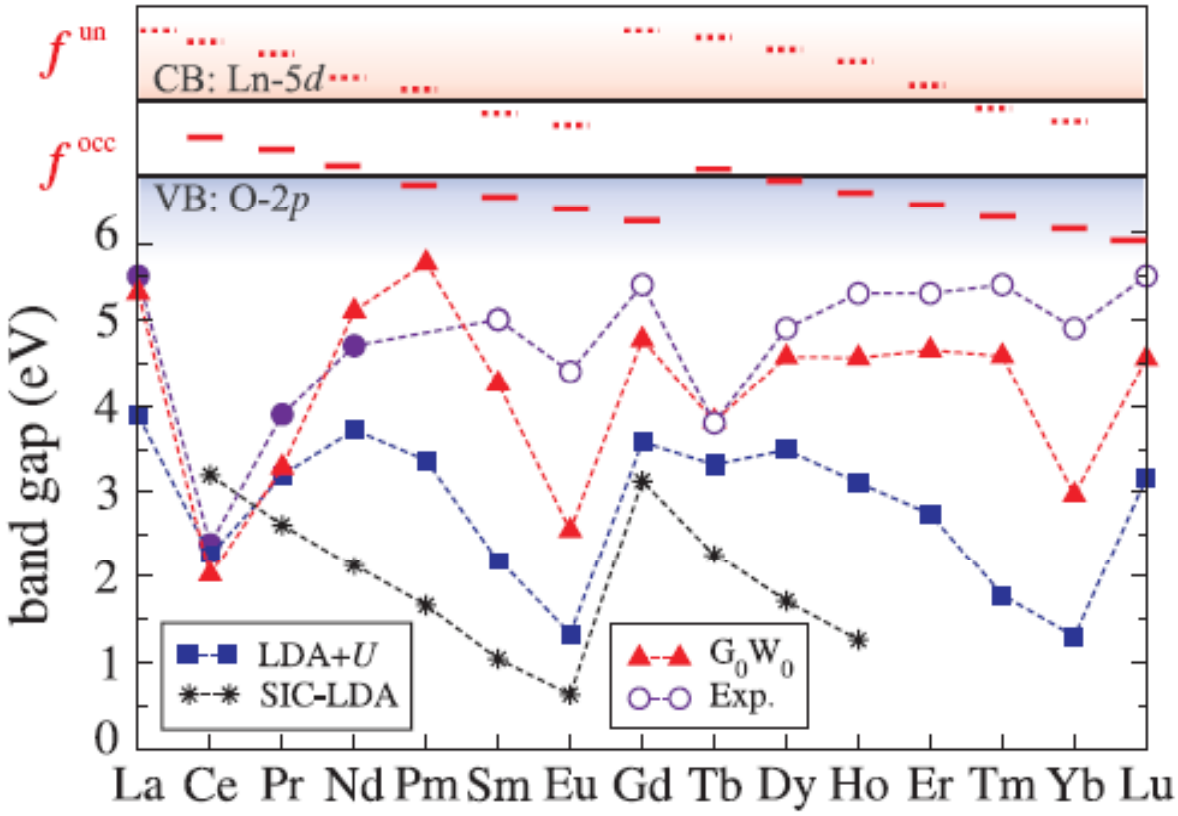

On-going and to-do list

- Interfacing with different LAPW packages (WIEN2k, EXCITING …)
- (approximate and/or full?) self-consistent *GW*
- G_0W_0 with spin-orbit coupling
- *GW*+BSE for *d/f*-electron systems
- RPA @ LAPW
- Beyond *GW*: vertex correction