Introduction to the FlapwMBPT code

https://www.bnl.gov/cmpmsd/flapwmbpt/

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COMSCOPE
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Plan

- Hedin's set of equations as theoretical background
- Useful approximations (GW, QSGW, GW+Vertex)
- LAPW+LO/APW+lo basis set basics
- Details of GW implementation
- Details of GW+Vertex implementation
- Convergence issues
- Examples of the calculations
- Scalability
- Hands on training

Hedin's equations

$$\Gamma^{\alpha}(123) = \delta(12)\delta(13) + \sum_{\beta} \frac{\delta\Sigma^{\alpha}(12)}{\delta G^{\beta}(45)} G^{\beta}(46)\Gamma^{\beta}(673)G^{\beta}(75)$$

$$P(12) = \sum_{\alpha} G^{\alpha}(13)\Gamma^{\alpha}(342)G^{\alpha}(41)$$

$$W(12) = V(12) + V(13)P(34)W(42)$$

$$\Sigma^{\alpha}(12) = -G^{\alpha}(14)\Gamma^{\alpha}(425)W(51)$$

$$G^{\alpha}(12) = G_0^{\alpha}(12) + G_0^{\alpha}(13)\Sigma^{\alpha}(34)G^{\alpha}(42)$$

This system of equations is supposed to be solved self-consistently. As written, it is exact. In practice, approximations are needed.

L.Hedin
PR 139, A796 (1965)

G.Strinati
Rivista del Nuovo Cimento
11,1 (1988)

GW approximation

$$\Gamma^{\alpha}(123) = \delta(12)\delta(13)$$

$$P(12;\tau) = -G(12;\tau)G(21;\beta-\tau)$$

$$W(12;\nu) = V(12) + \int d(34)V(13)P(34;\nu)W(42;\nu)$$

$$\Sigma(12;\tau) = -G(12;\tau)W(21;\tau),$$

$$G(12;\omega) = G_0(12;\omega) + \int d(34)G_0(13;\omega)\Sigma(34;\omega)G(42;\omega)$$

The approximation was first considered by L. Hedin (1965) (electron gas). Applications to the real materials (non-self-consistent) first appeared in 1980's:

G. Strinati et al., Phys. Rev. B **25**, 2867 (1982).

M. S. Hybertsen and S. G. Louie, Phys. Rev. B **34**, 5390 (1986).

R. W. Godby et al., Phys. Rev. B **37**, 10159 (1988).

Quasiparticle GW approximation (QSGW)

$$G^{-1}_{\lambda\lambda'}(\mathbf{k};\omega) = (i\omega + \mu - \varepsilon^{\mathbf{k}}_{\lambda})\delta_{\lambda\lambda'} - \Sigma^{c}_{\lambda\lambda'}(\mathbf{k};\omega).$$

$$\Sigma^{c}_{\lambda\lambda'}(\mathbf{k};\omega) = \Sigma^{c}_{\lambda\lambda'}(\mathbf{k};\omega=0) + \frac{\partial\,\Sigma^{c}_{\lambda\lambda'}(\mathbf{k};\omega)}{\partial(i\omega)}|_{\omega=0}(i\omega)$$

$$G^{-1}_{\lambda\lambda'}(\mathbf{k};\omega) = Z^{-1}_{\lambda\lambda'}(\mathbf{k})(i\omega) + (\mu - \varepsilon^{\mathbf{k}}_{\lambda})\delta_{\lambda\lambda'} - \Sigma^{c}_{\lambda\lambda'}(\mathbf{k};0)$$

$$Z^{-1}_{\lambda\lambda'}(\mathbf{k}) = \delta_{\lambda\lambda'} - \frac{\partial\,\Sigma^{c}_{\lambda\lambda'}(\mathbf{k};\omega)}{\partial(i\omega)}|_{\omega=0}$$

$$\sum_{\lambda''\lambda'''} Z^{1/2}_{\lambda\lambda''}(\mathbf{k})G^{-1}_{\lambda''\lambda'''}(\mathbf{k};\omega)Z^{1/2}_{\lambda'''\lambda'}(\mathbf{k}) = i\omega\delta_{\lambda\lambda'}$$
$$+ \sum_{\lambda''\lambda'''} Z^{1/2}_{\lambda\lambda''}(\mathbf{k})[(\mu - \varepsilon^{\mathbf{k}}_{\lambda''})\delta_{\lambda''\lambda'''} - \Sigma^{c}_{\lambda''\lambda'''}(\mathbf{k};0)]Z^{1/2}_{\lambda'''\lambda'}(\mathbf{k}$$

$$\sum_{\lambda''\lambda'''} Z^{1/2}_{\lambda\lambda''}(\mathbf{k})G^{-1}_{\lambda''\lambda'''}(\mathbf{k};\omega)Z^{1/2}_{\lambda'''\lambda'}(\mathbf{k})$$
$$= \sum_{i} Q^{\mathbf{k}}_{\lambda i}\left[i\omega + \mu - E^{\mathbf{k}}_{i}\right]Q^{\dagger\mathbf{k}}_{i\lambda'},$$

$$Z^{\mathbf{k}}_{\lambda\lambda'} = \delta_{\lambda\lambda'}$$

$$G^{\mathbf{k}}_{\lambda\lambda'}(\omega) = \sum_{i} \frac{Q^{\mathbf{k}}_{\lambda i}Q^{\dagger\mathbf{k}}_{i\lambda'}}{i\omega + \mu - E^{\mathbf{k}}_{i}}$$

Approximations for GW+Vertex schemes

$$\Gamma^{\alpha}(123) = \delta(12)\delta(13) + \sum_{\beta} \frac{\delta\Sigma^{\alpha}(12)}{\delta G^{\beta}(45)} G^{\beta}(46)\Gamma^{\beta}(673)G^{\beta}(75)$$

$$P(12) = \sum_{\alpha} G^{\alpha}(13)\Gamma^{\alpha}(342)G^{\alpha}(41)$$

$$W(12) = V(12) + V(13)P(34)W(42)$$

$$\Sigma^{\alpha}(12) = -G^{\alpha}(14)\Gamma^{\alpha}(425)W(51)$$

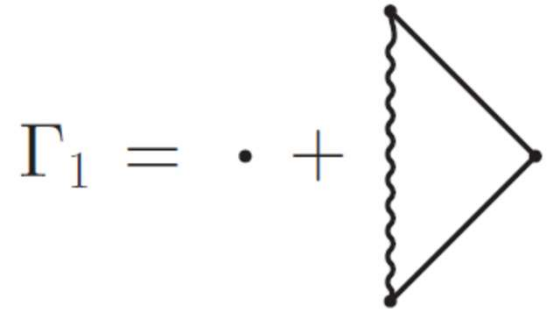
$$G^{\alpha}(12) = G_0^{\alpha}(12) + G_0^{\alpha}(13)\Sigma^{\alpha}(34)G^{\alpha}(42)$$

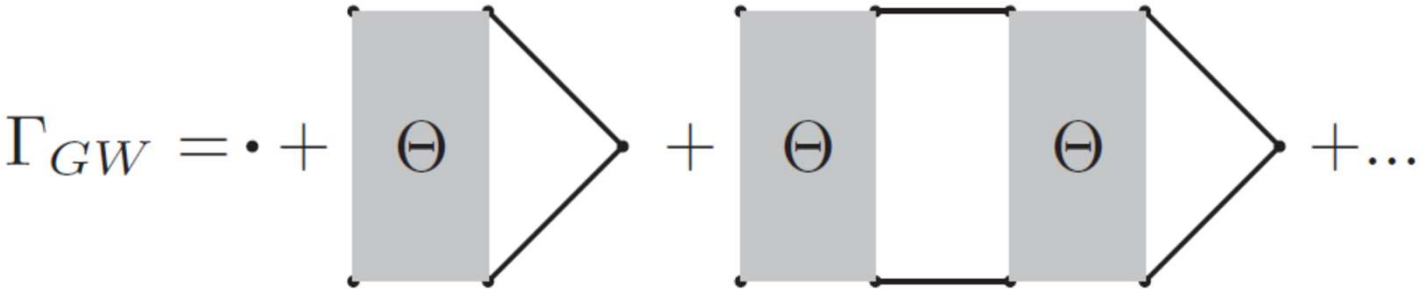
Two different routes to make approximations for the vertex are used.

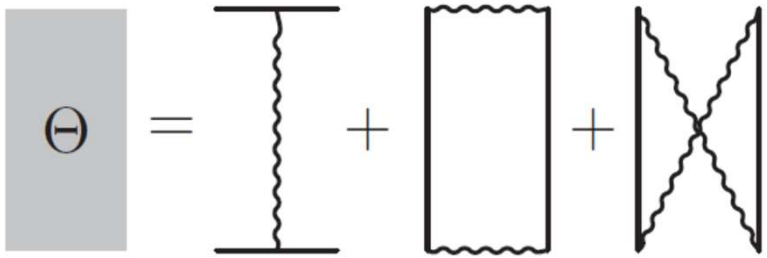
1) Finite order expansion of Γ in terms of W
2) Fixed diagrammatic approximations for Σ in the expression for the kernel of BSE

$$\frac{\delta\Sigma^{\alpha}(12)}{\delta G^{\beta}(45)}$$

Approximations for the vertex







LAPW+LO/APW+lo basis set

$$\psi_{\mathbf{G}}(\mathbf{k}) = \begin{cases} \exp(i(\mathbf{k}+\mathbf{G})\mathbf{r}) & \text{interstitial} \\ \sum_{l,m} \left(a_{lm}^{\mu,\mathbf{G}}(\mathbf{k}) u_l^{\mu}(r) + b_{lm}^{\mu,\mathbf{G}}(\mathbf{k}) \dot{u}_l^{\mu}(r)\right) Y_{lm}(\hat{\mathbf{r}}^{\mu}) & \text{muffin-tin } \mu \end{cases}$$

: LAPW

$$\sum_L a_L^{\mu\mathbf{G}}(\mathbf{k})\, u_l(R_{MT^\alpha}) Y_L(\hat{\mathbf{r}}) + b_L^{\mu\mathbf{G}}(\mathbf{k})\, \dot{u}_l(R_{MT^\alpha}) Y_L(\hat{\mathbf{r}})$$
$$= e^{i\mathbf{K}\boldsymbol{\tau}^{\mu}}\, 4\pi \sum_L i^l\, j_l(rK)\, Y_L^*(\mathbf{R}^{\mu}\hat{\mathbf{K}})\, Y_L(\hat{\mathbf{r}}),$$

$$\Phi_{lm}(r) = [a_l u(r) + b_l \dot{u}(r) + a_l \ddot{u}(r)] Y_{lm}(r)$$

: LO

$$\Psi_{\mathbf{G}}(\mathbf{k}) = \begin{cases} \exp[i(\mathbf{k}+\mathbf{G})r], & interstitial \\ \sum_{lm} \left[a_{tlm}^{G}(k) u_l^t(r)\right] Y_{lm}(\mathbf{r}), & MT\ sphere\ t \end{cases}$$

: APW

$$\Phi_{lm}(r) = [a_l u(r) + b_l \dot{u}(r)] Y_{lm}(r)$$

: lo

Product basis set

In order to perform GW (and beyond) calculations one needs not only LAPW basis set but also the basis set which represents sufficiently accurately the products of the one-electron wave functions. The choice for this basis set naturally comes from the MT geometry.

MT spheres: One constructs all products of radial functions inside a given MT sphere (for each L separately) and evaluates the overlap matrix between these products. Then one diagonalizes it. The linear combinations corresponding to non-zero eigen values are used as PB functions inside a given MT sphere.

Interstitial: In the interstitial region the products of one-electron functions are always some linear combinations of plane waves. Thus, natural choice for the PB in the interstitial region is PW basis set. Exact representation corresponds to the size of this PB being 8 times larger than the size of PW part of LAPW basis set. In practice, good choice is to take it 3-4 times larger (instead of 8).

Details of the GW implementation
Polarizability evaluation (Mt-Mt)

$$P(12;\tau) = -G(12;\tau)G(21;\beta-\tau)$$

$$G^{\alpha}(\mathbf{r};\mathbf{r}';\tau)|_{\mathbf{t}+\mathbf{R};\mathbf{t}'} = \sum_{LL'} \varphi_L^{\alpha\mathbf{t}}(\mathbf{r}) G^{\alpha\mathbf{R}}_{\mathbf{t}L;\mathbf{t}'L'}(\tau) \varphi_{L'}^{\alpha\mathbf{t}'}(\mathbf{r}')$$

$$G^{\alpha\mathbf{R}}_{\mathbf{t}L;\mathbf{t}'L'}(\tau) = \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{R}} \sum_{\lambda\lambda'} Z^{\alpha\mathbf{k}\lambda}_{\mathbf{t}L} G^{\alpha\mathbf{k}}_{\lambda\lambda'}(\tau) Z^{*\alpha\mathbf{k}\lambda'}_{\mathbf{t}'L'}$$

$$\begin{aligned} P^{\mathbf{R}}_{\mathbf{t}K;\mathbf{t}'K'}(\tau) = &- \sum_{\alpha} \sum_{LL''} \langle M_K^{\mathbf{t}} | \varphi_L^{\alpha\mathbf{t}} \varphi_{L''}^{\alpha\mathbf{t}} \rangle \\ &\times \sum_{L'} G^{\alpha\mathbf{R}}_{\mathbf{t}L;\mathbf{t}'L'}(\tau) \sum_{L'''} G^{\alpha;\mathbf{R}}_{\mathbf{t}L'';\mathbf{t}'L'''}(\beta-\tau) \\ &\times \langle \varphi_{L'}^{\alpha\mathbf{t}'} \varphi_{L'''}^{\alpha\mathbf{t}'} | M_{K'}^{\mathbf{t}'} \rangle . \end{aligned}$$

$$P^{\mathbf{q}}_{\mathbf{t}K;\mathbf{t}'K'}(\tau) = \sum_{\mathbf{R}} e^{-i\mathbf{q}\mathbf{R}} P^{\mathbf{R}}_{\mathbf{t}K;\mathbf{t}'K'}(\tau)$$

Details of the GW implementation
Polarizability evaluation (Mt-Int)

$$G^{\alpha}(\mathbf{r};\mathbf{r}';\tau)|^{\mathbf{r}\in\mathbf{t}+\mathbf{R}}_{\mathbf{r}'\in Int} = \sum_{L} \varphi^{\alpha\mathbf{t}}_{L}(\mathbf{r}) G^{\alpha\mathbf{R}}_{\mathbf{t}L;\mathbf{r}'}(\tau)$$

$$G^{\alpha\mathbf{k}}_{\mathbf{t}L;\mathbf{G}'}(\tau) = \frac{1}{\sqrt{\Omega_0}} \sum_{\lambda\lambda'} Z^{\alpha\mathbf{k}\lambda}_{\mathbf{t}L} G^{\alpha\mathbf{k}}_{\lambda\lambda'}(\tau) A^{*\alpha\mathbf{k}\lambda'}_{\mathbf{G}'}$$

$$G^{\alpha\mathbf{R}}_{\mathbf{t}L;\mathbf{r}'}(\tau) = \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{R}} \sum_{\mathbf{G}'} e^{-i(\mathbf{k}+\mathbf{G}')\mathbf{r}'} G^{\alpha\mathbf{k}}_{\mathbf{t}L;\mathbf{G}'}(\tau)$$

$$P^{\mathbf{R}}_{\mathbf{t}K;\mathbf{r}'}(\tau) = -\sum_{\alpha} \sum_{LL'} \langle M^{\mathbf{t}}_{K} | \varphi^{\alpha\mathbf{t}}_{L} \varphi^{\mathbf{t}}_{L'} \rangle G^{\alpha\mathbf{R}}_{\mathbf{t}L;\mathbf{r}'}(\tau) G^{\alpha\mathbf{R}}_{\mathbf{t}L';\mathbf{r}'}(\beta-\tau)$$

$$\widetilde{P}^{\mathbf{q}}_{\mathbf{t}K;\mathbf{G}'}(\tau) = \frac{1}{N_{\mathbf{r}}} \sum_{\mathbf{r}'} e^{i(\mathbf{q}+\mathbf{G}')\mathbf{r}'} \sum_{\mathbf{R}} e^{-i\mathbf{q}\mathbf{R}} P^{\mathbf{R}}_{\mathbf{t}K;\mathbf{r}'}(\tau)$$

$$P^{\mathbf{q}}_{\mathbf{t}K;K'}(\tau) = \sum_{\mathbf{G}'} \widetilde{P}^{\mathbf{q}}_{\mathbf{t}K;\mathbf{G}'}(\tau) \langle e^{i(\mathbf{q}+\mathbf{G}')\mathbf{r}'} | M^{\mathbf{q}}_{K'} \rangle_{Int}$$

Details of the GW implementation
Polarizability evaluation (Int-Int)

$$G^{\alpha\mathbf{k}}_{\mathbf{G};\mathbf{G}'}(\tau) = \frac{1}{\Omega_0}\sum_{\lambda\lambda'} A^{\alpha\mathbf{k}\lambda}_{\mathbf{G}} G^{\alpha\mathbf{k}}_{\lambda\lambda'}(\tau) A^{*\alpha\mathbf{k}\lambda'}_{\mathbf{G}'}$$

$$G^{\alpha\mathbf{R}}_{\mathbf{r};\mathbf{r}'}(\tau) = \frac{1}{N_{\mathbf{k}}}\sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{R}} \sum_{\mathbf{G};\mathbf{G}'} e^{i(\mathbf{k}+\mathbf{G})\mathbf{r}} G^{\alpha\mathbf{k}}_{\mathbf{G};\mathbf{G}'}(\tau) e^{-i(\mathbf{k}+\mathbf{G}')\mathbf{r}'}.$$

$$P^{\mathbf{R}}_{\mathbf{r}\mathbf{r}'}(\tau) = -\sum_{\alpha} G^{\alpha\mathbf{R}}_{\mathbf{r}\mathbf{r}'}(\tau) G^{\alpha\mathbf{R}}_{\mathbf{r}\mathbf{r}'}(\beta-\tau)$$

$$\widetilde{P}^{\mathbf{q}}_{\mathbf{G}\mathbf{G}'}(\tau) = \frac{1}{N_{\mathbf{r}}}\sum_{\mathbf{r}} e^{i(\mathbf{q}+\mathbf{G})\mathbf{r}} \frac{1}{N_{\mathbf{r}}}\sum_{\mathbf{r}'} e^{-i(\mathbf{q}+\mathbf{G}')\mathbf{r}'} \times \sum_{\mathbf{R}} e^{-i\mathbf{q}\mathbf{R}} P^{\mathbf{R}}_{\mathbf{r};\mathbf{r}'}(\tau).$$

$$P^{\mathbf{q}}_{K;K'}(\tau) = \sum_{\mathbf{G}\mathbf{G}'} \langle e^{i(\mathbf{q}+\mathbf{G})\mathbf{r}} | M^{\mathbf{q}}_{K} \rangle^{*}_{Int} \widetilde{P}^{\mathbf{q}}_{\mathbf{G}\mathbf{G}'}(\tau) \langle e^{i(\mathbf{q}+\mathbf{G}')\mathbf{r}'} | M^{\mathbf{q}}_{K'} \rangle_{Int}$$

Details of the GW implementation
Evaluation of the screened interaction W

$$W(12;\nu) = V(12) + \int d(34)V(13)P(34;\nu)W(42;\nu)$$

$$W^{\mathbf{q}}_{KK'}(\nu) = V^{\mathbf{q}}_{KK'} + \sum_{K''K'''} V^{\mathbf{q}}_{KK''}P^{\mathbf{q}}_{K''K'''}(\nu)W^{\mathbf{q}}_{K'''K'}(\nu)$$

For large unit cells (>10 atoms) this step becomes the most time consuming part of the GW algorithm. The interface with the SCALAPACK subroutines (PDGEMM/PZGEMM and PDGESV/PZGESV) was implemented (together with Anthony Ruth).

Details of the GW implementation
Evaluation of the self energy (Mt-Mt)

$$\Sigma(12;\tau) = -G(12;\tau)W(21;\tau)$$

$$\Sigma^{\mathbf{k}}_{\mathbf{t}L;\mathbf{t}'L'}(\tau) = \sum_{\mathbf{R}} e^{-i\mathbf{k}\mathbf{R}} \Sigma^{\mathbf{R}}_{\mathbf{t}L;\mathbf{t}'L'}(\tau)$$

$$\widetilde{W}^{\mathbf{R}}_{\mathbf{t}K;\mathbf{t}'K'}(\tau) = \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{q}} e^{i\mathbf{q}\mathbf{R}} \widetilde{W}^{\mathbf{q}}_{\mathbf{t}K;\mathbf{t}'K'}(\tau)$$

$$\begin{aligned}\Sigma^{\alpha\mathbf{R}}_{\mathbf{t}L;\mathbf{t}'L'}(\tau) = -\sum_{L''L'''}\sum_{KK'} &\langle \varphi^{\alpha\mathbf{t}}_{L} | \varphi^{\alpha\mathbf{t}}_{L''} M^{\mathbf{t}}_{K} \rangle \\ &\times G^{\alpha\mathbf{R}}_{\mathbf{t}L'';\mathbf{t}'L'''}(\tau) \widetilde{W}^{\mathbf{R}}_{\mathbf{t}K;\mathbf{t}'K'}(\beta-\tau) \\ &\times \langle \varphi^{\alpha\mathbf{t}'}_{L'} | \varphi^{\alpha\mathbf{t}'}_{L'''} M^{\mathbf{t}'}_{K'} \rangle,\end{aligned}$$

Details of the GW implementation
Evaluation of the self energy (Mt-Int)

$$\widetilde{W}^{\mathbf{R}}_{\mathbf{t}K;\mathbf{r}}(\tau) = \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{q}} e^{i\mathbf{q}\mathbf{R}} \sum_{\mathbf{G}} e^{-i(\mathbf{q}+\mathbf{G})\mathbf{r}} \widetilde{W}^{\mathbf{q}}_{\mathbf{t}K;\mathbf{G}}(\tau)$$

$$\Sigma^{\alpha\mathbf{R}}_{\mathbf{t}L;\mathbf{r}'}(\tau) = -\sum_{L'K} \langle \varphi^{\alpha\mathbf{t}}_{L} | \varphi^{\mathbf{t}}_{L'} M^{\mathbf{t}}_{K} \rangle G^{\alpha\mathbf{R}}_{\mathbf{t}L;\mathbf{r}'}(\tau) \widetilde{W}^{\mathbf{R}}_{\mathbf{t}K;\mathbf{r}'}(\beta - \tau)$$

$$\Sigma^{\alpha\mathbf{k}}_{\mathbf{t}L;\mathbf{r}'}(\tau) = \sum_{\mathbf{R}} e^{-i\mathbf{k}\mathbf{R}} \Sigma^{\alpha\mathbf{R}}_{\mathbf{t}L;\mathbf{r}'}(\tau)$$

$$\Sigma^{\alpha\mathbf{k}}_{\mathbf{t}L;\mathbf{r}'}(\tau) = \sum_{\mathbf{G}'} \tilde{\Sigma}^{\alpha\mathbf{k}}_{\mathbf{t}L;\mathbf{G}'} e^{-i(\mathbf{k}+\mathbf{G}')\mathbf{r}'}$$

$$\tilde{\Sigma}^{\alpha\mathbf{k}}_{\mathbf{t}L;\mathbf{G}'}(\tau) = \frac{1}{N_{\mathbf{r}}} \sum_{\mathbf{r}'} e^{i(\mathbf{k}+\mathbf{G}')\mathbf{r}'} \Sigma^{\alpha\mathbf{k}}_{\mathbf{t}L;\mathbf{r}'}(\tau)$$

$$\Sigma^{\alpha\mathbf{k}}_{\mathbf{t}L;\mathbf{G}'}(\tau) = \frac{1}{\sqrt{\Omega_0}} \sum_{\mathbf{G}''} \tilde{\Sigma}^{\alpha\mathbf{k}}_{\mathbf{t}L;\mathbf{G}''}(\tau) S^{\mathbf{k}}_{\mathbf{G}''\mathbf{G}'}$$

$$\Sigma^{\alpha\mathbf{k}}_{\lambda\lambda'}(\tau)|^{Mt}_{Int} = \sum_{\mathbf{t}L} \sum_{\mathbf{G}'} Z^{*\alpha\mathbf{k}\lambda}_{\mathbf{t}L} \Sigma^{\alpha\mathbf{k}}_{\mathbf{t}L;\mathbf{G}'}(\tau) A^{\alpha\mathbf{k}\lambda'}_{\mathbf{G}'} + H.C$$

Details of the GW implementation
Evaluation of the self energy (Int-Int)

$$\widetilde{W}^{\mathbf{R}}_{\mathbf{r};\mathbf{r}'}(\tau) = \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{q}} e^{i\mathbf{q}\mathbf{R}} \sum_{\mathbf{G}} e^{-i(\mathbf{q}+\mathbf{G})\mathbf{r}} \sum_{\mathbf{G}'} e^{i(\mathbf{q}+\mathbf{G}')\mathbf{r}'} \times \widetilde{W}^{\mathbf{q}}_{\mathbf{G}\mathbf{G}'}(\tau)$$

$$\Sigma^{\alpha\mathbf{R}}_{\mathbf{r}\mathbf{r}'} = -G^{\alpha\mathbf{R}}_{\mathbf{r}\mathbf{r}'}(\tau)\widetilde{W}^{\mathbf{R}}_{\mathbf{r}\mathbf{r}'}(\beta-\tau)$$

$$\Sigma^{\alpha\mathbf{k}}_{\mathbf{r}\mathbf{r}'}(\tau) = \sum_{\mathbf{R}} e^{-i\mathbf{k}\mathbf{R}} \Sigma^{\alpha\mathbf{R}}_{\mathbf{r}\mathbf{r}'}(\tau)$$

$$\Sigma^{\alpha\mathbf{k}}_{\mathbf{r}\mathbf{r}'}(\tau) = \sum_{\mathbf{G}} \sum_{\mathbf{G}'} e^{i(\mathbf{k}+\mathbf{G})\mathbf{r}} \tilde{\Sigma}^{\alpha\mathbf{k}}_{\mathbf{G};\mathbf{G}'}(\tau) e^{-i(\mathbf{k}+\mathbf{G}')\mathbf{r}'}$$

$$\tilde{\Sigma}^{\alpha\mathbf{k}}_{\mathbf{G};\mathbf{G}'}(\tau) = \frac{1}{N^2_{\mathbf{r}}} \sum_{\mathbf{r}\mathbf{r}'} e^{-i(\mathbf{k}+\mathbf{G})\mathbf{r}} e^{i(\mathbf{k}+\mathbf{G}')\mathbf{r}'} \Sigma^{\alpha\mathbf{k}}_{\mathbf{r}\mathbf{r}'}(\tau)$$

$$\Sigma^{\alpha\mathbf{k}}_{\mathbf{G};\mathbf{G}'}(\tau) = \frac{1}{\Omega_0} \sum_{\mathbf{G}''\mathbf{G}'''} S^{\mathbf{k}}_{\mathbf{G}\mathbf{G}''} \tilde{\Sigma}^{\alpha\mathbf{k}}_{\mathbf{G}'';\mathbf{G}'''}(\tau) S^{\mathbf{k}}_{\mathbf{G}'''\mathbf{G}'}$$

$$\Sigma^{\alpha\mathbf{k}}_{\lambda\lambda'}(\tau)\big|^{Int}_{Int} = \sum_{\mathbf{G}\mathbf{G}'} A^{*\alpha\mathbf{k}\lambda}_{\mathbf{G}} \Sigma^{\alpha\mathbf{k}}_{\mathbf{G};\mathbf{G}'}(\tau) A^{\alpha\mathbf{k}\lambda'}_{\mathbf{G}'}$$

Details of the GW implementation
Evaluation of updated Green's function

$$G(12;\omega) = G_0(12;\omega) + \int d(34) G_0(13;\omega)\Sigma(34;\omega)G(42;\omega)$$

$$\sum_{\lambda''}\{\delta_{\lambda\lambda''} - \mathcal{G}^{x,\alpha}_{\lambda}(\mathbf{k};\omega)\Sigma^{c,\alpha}_{\lambda\lambda''}(\mathbf{k};\omega)\}\mathcal{G}^{c,\alpha}_{\lambda''\lambda'}(\mathbf{k};\omega)$$

$$= \mathcal{G}^{x,\alpha}_{\lambda'}(\mathbf{k};\omega)\Sigma^{c,\alpha}_{\lambda\lambda''}(\mathbf{k};\omega)\mathcal{G}^{x,\alpha}_{\lambda'}(\mathbf{k};\omega),$$

The size of fermionic basis set (bands) usually is a few times smaller than the size of the bosonic basis set (product basis). Thus, the matrix equation for W is about 100 times more time consuming. However, we have to solve the Dyson's equation for G a few times during each sc iteration (chemical potential adjustment). SCALAPACK subroutines are planned to be used as well.

Details of the GW+Vertex implementation

(i) three-point vertex function from the Bethe-Salpeter equation

$$\Gamma^{\alpha}(123) = \delta(12)\delta(13) + \sum_{\beta} \frac{\delta\Sigma^{\alpha}(12)}{\delta G^{\beta}(45)} G^{\beta}(46)\Gamma^{\beta}(673)G^{\beta}(75), \quad (1)$$

where α and β are spin indexes, and the digits in the brackets represent space-Matsubara's time arguments;

(ii) polarizability

$$P(12) = \sum_{\alpha} G^{\alpha}(13)\Gamma^{\alpha}(342)G^{\alpha}(41); \quad (2)$$

(iii) screened interaction

$$W(12) = V(12) + V(13)P(34)W(42); \quad (3)$$

(iv) and the self-energy

$$\Sigma^{\alpha}(12) = -G^{\alpha}(14)\Gamma^{\alpha}(425)W(51). \quad (4)$$

In Eq. (3), V stands for the bare Coulomb interaction. The new approximation for the Green's function is obtained from Dyson's equation

$$G^{\alpha}(12) = G_0^{\alpha}(12) + G_0^{\alpha}(13)\Sigma^{\alpha}(34)G^{\alpha}(42), \quad (5)$$

where G_0 is the Green's function in Hartree approximation.

$$\frac{\delta\Sigma^{\alpha}(12)}{\delta G^{\beta}(34)} = -\delta_{\alpha\beta}\delta(13)\delta(24)W(21) - G^{\alpha}(12)G^{\beta}(43)[W(23)W(41) + W(24)W(31)]$$

$$\begin{aligned}\triangle\Gamma^{\alpha}(123) = &-W(2,1)G^{\alpha}(13)G^{\alpha}(32) \\ &- W(2,1)G^{\alpha}(14)\triangle\Gamma^{\alpha}(453)G^{\alpha}(52) \\ &- G^{\alpha}(12)\sum_{\beta} G^{\beta}(54)[W(24)W(51) \\ &+ W(25)W(41)][G^{\beta}(43)G^{\beta}(35) \\ &+ G^{\beta}(46)\triangle\Gamma^{\beta}(673)G^{\beta}(75)].\end{aligned}$$

Details of the GW+Vertex implementation (continuation)

$$K^{0\alpha}(123) = -G^{\alpha}(13)G^{\alpha}(32), \tag{9}$$

$$\triangle K^{\alpha}(123) = -G^{\alpha}(14)\triangle\Gamma^{\alpha}(453)G^{\alpha}(52), \tag{10}$$

$$K^{\alpha}(123) = K^{0\alpha}(123) + \triangle K^{\alpha}(123), \tag{11}$$

$$\begin{aligned}\triangle\Gamma_{\alpha}(123) = {} & W(21)K^{\alpha}(123) + G^{\alpha}(12) \\ & \times \sum_{\beta} W(24)\big[G^{\beta}(54)K^{\beta}(453) \\ & + G^{\beta}(45)K^{\beta}(543)\big]W(51).\end{aligned} \tag{12}$$

$$Q(123) = \sum_{\beta}\left[G^{\beta}(21)K^{\beta}(123) + G^{\beta}(12)K^{\beta}(213)\right] \tag{13}$$

$$T(213) = W(24)Q(453)W(51), \tag{14}$$

$$\triangle\Gamma_{\alpha}(123) = W(21)K^{\alpha}(123) + G^{\alpha}(12)T(213). \tag{15}$$

The iterations for the Γ_{GW} are performed as the following. One takes $K = K^0$ [Eq. (9)] as an initial approach, then calculates Q [Eq. (13)], T [Eq. (14)], and $\triangle\Gamma$ [Eq. (15)]. Then, a correction to K^0 [Eq. (10)] is evaluated and the process is repeated with a new $K = K^{\upsilon} + \triangle K$. The iterations for the Γ^0_{GW} are simpler. They follow the same scheme but without Q and T evaluation. Finally, the approximation Γ_1 is obtained with just one step: $\triangle\Gamma_1 = WK^0$.

Details of the GW+Vertex implementation (K_0 calculation)

$$K^{0\alpha}(123) = -G^{\alpha}(13)G^{\alpha}(32).$$

$$K^{0\alpha\mathbf{k}}_{\lambda\lambda'}(s\mathbf{q};\omega;\nu) = -\sum_{\lambda''\lambda'''} G^{\alpha\mathbf{k}}_{\lambda\lambda''}(\omega)\left\langle \Psi^{\alpha\mathbf{k}}_{\lambda''} \middle| \Psi^{\alpha\mathbf{k}-\mathbf{q}}_{\lambda'''}\Pi^{\mathbf{q}}_{s}\right\rangle G^{\alpha,\mathbf{k}-\mathbf{q}}_{\lambda'''\lambda'}(\omega-\nu)$$

$$K^{0,HF,\alpha\mathbf{k}}_{\lambda\lambda'}(s\mathbf{q};\omega;\nu) = -\frac{\left\langle \Psi^{\alpha\mathbf{k}}_{\lambda} \middle| \Psi^{\alpha\mathbf{k}-\mathbf{q}}_{\lambda'}\Pi^{\mathbf{q}}_{s}\right\rangle}{\left(i\omega+\mu-\epsilon^{\alpha\mathbf{k}}_{\lambda}\right)\left[i(\omega-\nu)+\mu-\epsilon^{\alpha\mathbf{k}-\mathbf{q}}_{\lambda'}\right]}$$

$$K^{0,HF,\alpha\mathbf{k}}_{\lambda\lambda'}(s\mathbf{q};\tau;\nu) = \frac{\left\langle \Psi^{\alpha\mathbf{k}}_{\lambda} \middle| \Psi^{\alpha\mathbf{k}-\mathbf{q}}_{\lambda'}\Pi^{\mathbf{q}}_{s}\right\rangle}{i\nu+\epsilon^{\alpha\mathbf{k}-\mathbf{q}}_{\lambda'}-\epsilon^{\alpha\mathbf{k}}_{\lambda}} \times\left\{G^{HF,\alpha,\mathbf{k}}_{\lambda}(\tau)-e^{-i\nu\tau}G^{HF,\alpha,\mathbf{k}-\mathbf{q}}_{\lambda'}(\tau)\right\}. \tag{A9}$$

In case $\nu = 0$ and $\epsilon^{\alpha\mathbf{k}-\mathbf{q}}_{\lambda'} = \epsilon^{\alpha\mathbf{k}}_{\lambda}$ the expression is different:

$$K^{0,HF,\alpha\mathbf{k}}_{\lambda\lambda'}(s\mathbf{q};\tau;\nu) = \left\langle \Psi^{\alpha\mathbf{k}}_{\lambda} \middle| \Psi^{\alpha\mathbf{k}-\mathbf{q}}_{\lambda'}\Pi^{\mathbf{q}}_{s}\right\rangle G^{HF,\alpha,\mathbf{k}}_{\lambda}(\tau)$$

$$K^{0\alpha\mathbf{k}}_{\lambda\lambda'}(s\mathbf{q};\tau;\nu) = \frac{1}{\beta}\sum_{\omega\leqslant\nu/2} e^{-i\omega\tau}\underbrace{K^{0\alpha\mathbf{k}}_{\lambda\lambda'}(s\mathbf{q};\omega;\nu)}_{\text{large at }\omega=0} + \frac{1}{\beta}\sum_{\omega\geqslant\nu/2} e^{-i\omega\tau}\underbrace{K^{0\alpha\mathbf{k}}_{\lambda\lambda'}(s\mathbf{q};\omega;\nu)}_{\text{large at }\omega=\nu}$$

$$= \underbrace{\frac{1}{\beta}\sum_{\omega\leqslant\nu/2} e^{-i\omega\tau}K^{0\alpha\mathbf{k}}_{\lambda\lambda'}(s\mathbf{q};\omega;\nu)}_{\text{smooth function of }\tau} + e^{-i\nu\tau}\underbrace{\frac{1}{\beta}\sum_{\omega\geqslant\nu/2} e^{-i(\omega-\nu)\tau}K^{0\alpha\mathbf{k}}_{\lambda\lambda'}(s\mathbf{q};\omega;\nu)}_{\text{smooth function of }\tau}.$$

Details of the GW+Vertex implementation (*K* function in real space)

MT-MT:

$$K^{\alpha\mathbf{R}}_{\mathbf{t}L;\mathbf{t}'L'}(s\mathbf{q};\tau;\nu) = \frac{1}{N_\mathbf{k}}\sum_\mathbf{k} e^{i\mathbf{k}\mathbf{R}} \sum_{\lambda\lambda'} Z^{\alpha\mathbf{k}}_{\mathbf{t}L;\lambda} K^{\alpha\mathbf{k}}_{\lambda\lambda'}(s\mathbf{q};\tau;\nu) Z^{*\alpha\mathbf{k}-\mathbf{q}}_{\mathbf{t}'L';\lambda'}$$

Int-MT:

$$K^{\alpha\mathbf{R}}_{\mathbf{r};\mathbf{t}'L'}(s\mathbf{q};\tau;\nu) = \frac{1}{N_\mathbf{k}}\sum_\mathbf{k} e^{i\mathbf{k}\mathbf{R}} \sum_{\lambda\lambda'} A^{\alpha\mathbf{k}}_{\mathbf{r};\lambda} K^{\alpha\mathbf{k}}_{\lambda\lambda'}(s\mathbf{q};\tau;\nu) Z^{*\alpha\mathbf{k}-\mathbf{q}}_{\mathbf{t}'L';\lambda'}$$

MT-Int:

$$K^{\alpha\mathbf{R}}_{\mathbf{t}L;\mathbf{r}'}(s\mathbf{q};\tau;\nu) = \frac{1}{N_\mathbf{k}}\sum_\mathbf{k} e^{i\mathbf{k}\mathbf{R}} \sum_{\lambda\lambda'} Z^{\alpha\mathbf{k}}_{\mathbf{t}L;\lambda} K^{\alpha\mathbf{k}}_{\lambda\lambda'}(s\mathbf{q};\tau;\nu) A^{*\alpha\mathbf{k}-\mathbf{q}}_{\mathbf{r}';\lambda'}$$

Int-Int:

$$K^{\alpha\mathbf{R}}_{\mathbf{r};\mathbf{r}'}(s\mathbf{q};\tau;\nu) = \frac{1}{N_\mathbf{k}}\sum_\mathbf{k} e^{i\mathbf{k}\mathbf{R}} \sum_{\lambda\lambda'} A^{\alpha\mathbf{k}}_{\mathbf{r};\lambda} K^{\alpha\mathbf{k}}_{\lambda\lambda'}(s\mathbf{q};\tau;\nu) A^{*\alpha\mathbf{k}-\mathbf{q}}_{\mathbf{r}';\lambda'}$$

with

$$A^{\alpha\mathbf{k}}_{\mathbf{r};\lambda} = \frac{1}{\sqrt{\Omega_0}}\sum_\mathbf{G} e^{i(\mathbf{k}+\mathbf{G})\mathbf{r}} A^{\alpha\mathbf{k}}_{\mathbf{G};\lambda}.$$

The coefficients $A^{\alpha\mathbf{k}}_{\mathbf{G};\lambda}$ represent the expansion of band states in plane waves in the interstitial region $\Psi^{\alpha\mathbf{k}}_\lambda(\mathbf{r}) = \frac{1}{\Omega_0}\sum_\mathbf{G} A^{\alpha\mathbf{k}}_{\mathbf{G};\lambda} e^{i(\mathbf{k}+\mathbf{G})\mathbf{r}}$, and the coefficients $Z^{\alpha\mathbf{k}}_{\mathbf{t}L;\lambda}$ represent the expansion of the band states in the orbital basis inside MT spheres $\Psi^{\alpha\mathbf{k}}_\lambda(\mathbf{r})|_\mathbf{t} = \sum_L Z^{\alpha\mathbf{k}}_{\mathbf{t}L;\lambda}\phi^{\alpha\mathbf{t}}_L(\mathbf{r})$.

Details of the GW+Vertex implementation (evaluation of W(21)K(123))

$$\Delta\Gamma^{\alpha}(123;\tau;\nu) = W(12;\tau)K^{\alpha}(123;\tau;\nu)$$

MT-MT:

$$\Delta\Gamma^{\alpha\mathbf{R}}_{\mathbf{t}L;\mathbf{t}'L'}(s\mathbf{q};\tau;\nu) = \sum_{s'L''}\sum_{s''}\sum_{L'''} K^{\alpha\mathbf{R}}_{\mathbf{t}L'';\mathbf{t}'L'''}(s\mathbf{q};\tau;\nu)\left\langle\phi^{\alpha\mathbf{t}'}_{L'}\middle|\phi^{\alpha\mathbf{t}'}_{L'''}\Pi^{\mathbf{t}'}_{s''}\right\rangle^{*} \times W^{\mathbf{R}}_{\mathbf{t}s';\mathbf{t}'s''}(\tau)\left\langle\phi^{\alpha\mathbf{t}}_{L}\middle|\phi^{\alpha\mathbf{t}}_{L''}\Pi^{\mathbf{t}}_{s'}\right\rangle; \quad \text{(A17)}$$

Int-MT:

$$\Delta\Gamma^{\alpha\mathbf{R}}_{\mathbf{r};\mathbf{t}'L'}(s\mathbf{q};\tau;\nu) = \sum_{L'''}\sum_{s''}\left\langle\phi^{\alpha\mathbf{t}'}_{L'}\middle|\phi^{\alpha\mathbf{t}'}_{L'''}\Pi^{\mathbf{t}'}_{s''}\right\rangle^{*} \times W^{\mathbf{R}}_{\mathbf{r};\mathbf{t}'s''}(\tau)K^{\alpha\mathbf{R}}_{\mathbf{r};\mathbf{t}'L'''}(s\mathbf{q};\tau;\nu); \quad \text{(A18)}$$

MT-Int:

$$\Delta\Gamma^{\alpha\mathbf{R}}_{\mathbf{t}L;\mathbf{r}'}(s\mathbf{q};\tau;\nu) = \sum_{L''}\sum_{s'}\left\langle\phi^{\alpha\mathbf{t}}_{L}\middle|\phi^{\alpha\mathbf{t}}_{L''}\Pi^{\mathbf{t}}_{s'}\right\rangle W^{\mathbf{R}}_{\mathbf{t}s';\mathbf{r}'}(\tau) \times K^{\alpha\mathbf{R}}_{\mathbf{t}L'';\mathbf{r}'}(s\mathbf{q};\tau;\nu); \quad \text{(A19)}$$

Int-Int:

$$\Delta\Gamma^{\alpha\mathbf{R}}_{\mathbf{r};\mathbf{r}'}(s\mathbf{q};\tau;\nu) = W^{\mathbf{R}}_{\mathbf{r};\mathbf{r}'}(\tau)K^{\alpha\mathbf{R}}_{\mathbf{r};\mathbf{r}'}(s\mathbf{q};\tau;\nu). \quad \text{(A20)}$$

Details of the GW+Vertex implementation (transformation of vertex to band representation)

$$\begin{aligned}\triangle\Gamma^{\alpha\mathbf{k}}_{\lambda\lambda'}(s\mathbf{q};\tau;\nu) = &\sum_{\mathbf{t}L}\sum_{\mathbf{t}'L'} Z^{*\alpha\mathbf{k}\lambda}_{\mathbf{t}L}\sum_{\mathbf{R}} e^{-i\mathbf{k}\mathbf{R}}\triangle\Gamma^{\alpha\mathbf{R}}_{\mathbf{t}L;\mathbf{t}'L'}(s\mathbf{q};\tau;\nu)Z^{\alpha\mathbf{k}-\mathbf{q}\lambda'}_{\mathbf{t}'L'} + \sum_{\mathbf{r}}\sum_{\mathbf{t}'L'} X^{*\alpha\mathbf{k}}_{\mathbf{r}\lambda}\sum_{\mathbf{R}} e^{-i\mathbf{k}\mathbf{R}}\triangle\Gamma^{\alpha\mathbf{R}}_{\mathbf{r};\mathbf{t}'L'}(s\mathbf{q};\tau;\nu)Z^{\alpha\mathbf{k}-\mathbf{q}\lambda'}_{\mathbf{t}'L'} \\ &+ \sum_{\mathbf{t}L}\sum_{\mathbf{r}'} Z^{*\alpha\mathbf{k}\lambda}_{\mathbf{t}L}\sum_{\mathbf{R}} e^{-i\mathbf{k}\mathbf{R}}\triangle\Gamma^{\alpha\mathbf{R}}_{\mathbf{t}L;\mathbf{r}'}(s\mathbf{q};\tau;\nu)X^{\alpha\mathbf{k}-\mathbf{q}}_{\mathbf{r}'\lambda'} + \sum_{\mathbf{r}}\sum_{\mathbf{r}'} X^{*\alpha\mathbf{k}}_{\mathbf{r}\lambda}\sum_{\mathbf{R}} e^{-i\mathbf{k}\mathbf{R}}\triangle\Gamma^{\alpha\mathbf{R}}_{\mathbf{r};\mathbf{r}'}(s\mathbf{q};\tau;\nu)X^{\alpha\mathbf{k}-\mathbf{q}}_{\mathbf{r}'\lambda'},\end{aligned}$$

$$X^{\alpha\mathbf{k}}_{\mathbf{r}\lambda} = \frac{1}{N_{\mathbf{r}}}\sum_{\mathbf{G}} e^{i(\mathbf{k}+\mathbf{G})\mathbf{r}}\left\{\int_{\Omega_{Int}} d\mathbf{r}\,\Psi^{*\alpha\mathbf{k}}_{\lambda}(\mathbf{r})e^{i(\mathbf{k}+\mathbf{G})\mathbf{r}}\right\}^*$$

Details of the GW+Vertex implementation (ΔK evaluation)

$$\triangle K^{\alpha}(123;\omega;\nu) = -\iint d(45) G^{\alpha}(14;\omega)\triangle\Gamma^{\alpha}(453;\omega;\nu)G^{\alpha}(52;\omega-\nu)$$

$$\triangle K^{0\alpha\mathbf{k}}_{\lambda\lambda'}(s\mathbf{q};\omega;\nu) = -\sum_{\lambda''\lambda'''} G^{\alpha\mathbf{k}}_{\lambda\lambda''}(\omega)\triangle\Gamma^{\alpha\mathbf{k}}_{\lambda''\lambda'''}(s\mathbf{q};\omega;\nu)G^{\alpha,\mathbf{k}-\mathbf{q}}_{\lambda'''\lambda'}(\omega-\nu)$$

Details of the GW+Vertex implementation (correction to polarizability)

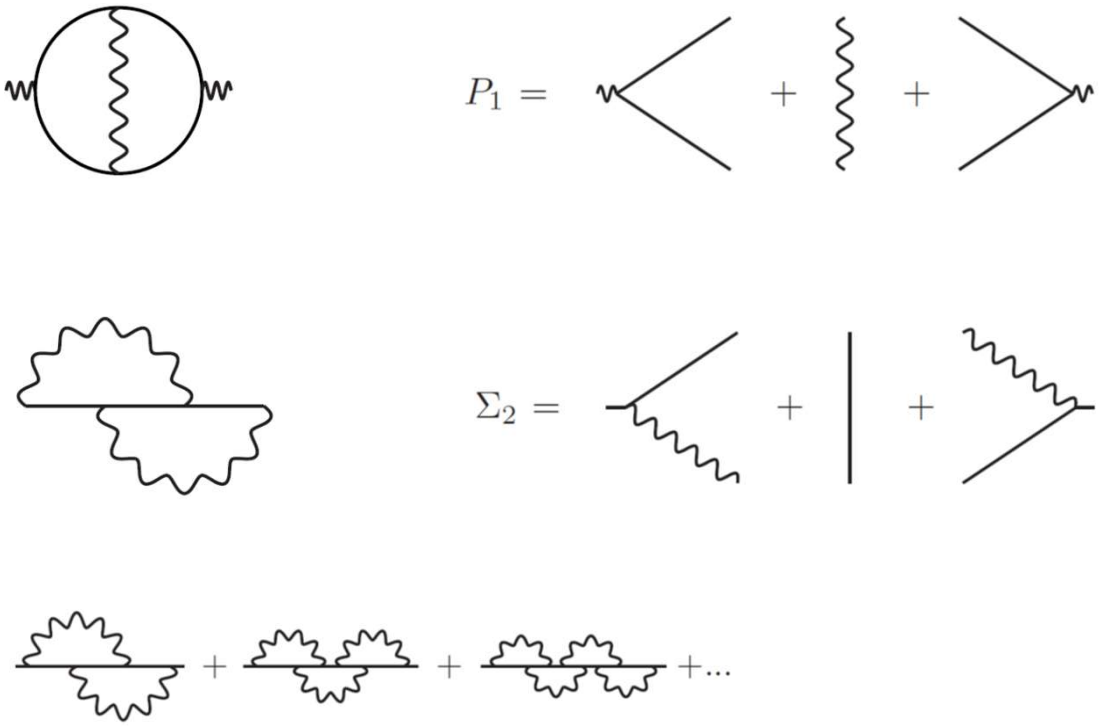
$$\Delta P(12) = \sum_{\alpha} G^{\alpha}(13)\Delta\Gamma^{\alpha}(342)G^{\alpha}(41)$$

$$= -\sum_{\alpha} \Delta K^{\alpha}(112).$$

$$\Delta P^{\mathbf{q}}_{ss'}(\nu) = -\frac{1}{N_{\mathbf{k}}} \sum_{\alpha\mathbf{k}} \sum_{\lambda\lambda'} \left\langle \Psi^{\alpha\mathbf{k}}_{\lambda} | \Psi^{\alpha\mathbf{k}-\mathbf{q}}_{\lambda'} \Pi^{\mathbf{q}}_{s} \right\rangle^{*}$$

$$\times \Delta K^{\alpha\mathbf{k}}_{\lambda\lambda'}(s'\mathbf{q}; \tau = 0; \nu).$$

Details of the GW+Vertex implementation (correction to the self-energy)



scGW, QSGW: combination with DFT kernel

$$P_0 = GG$$

$$P = P_0 + P_0 \frac{\delta V_{xc}}{\delta \rho} P$$

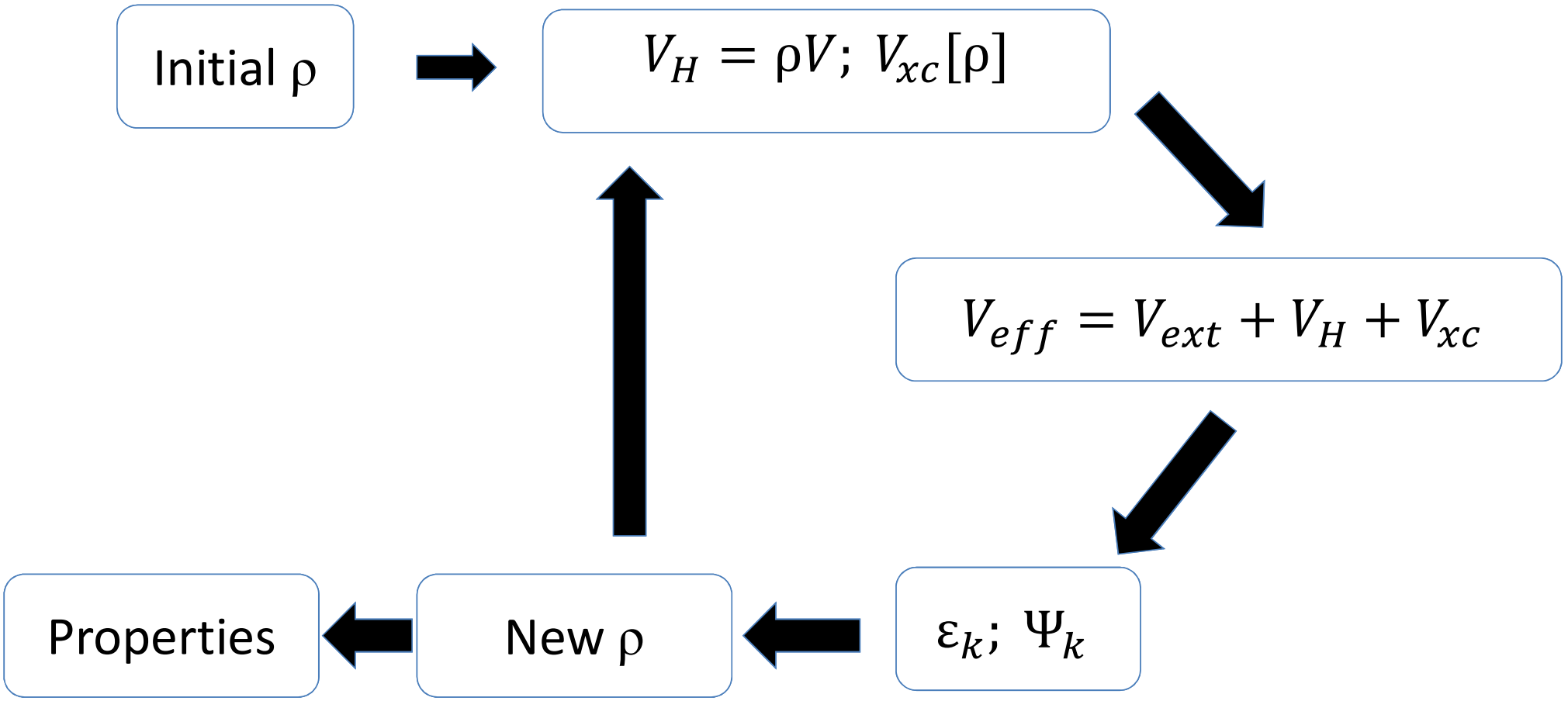
$$W = V + VPW$$

$$\Sigma = GW$$

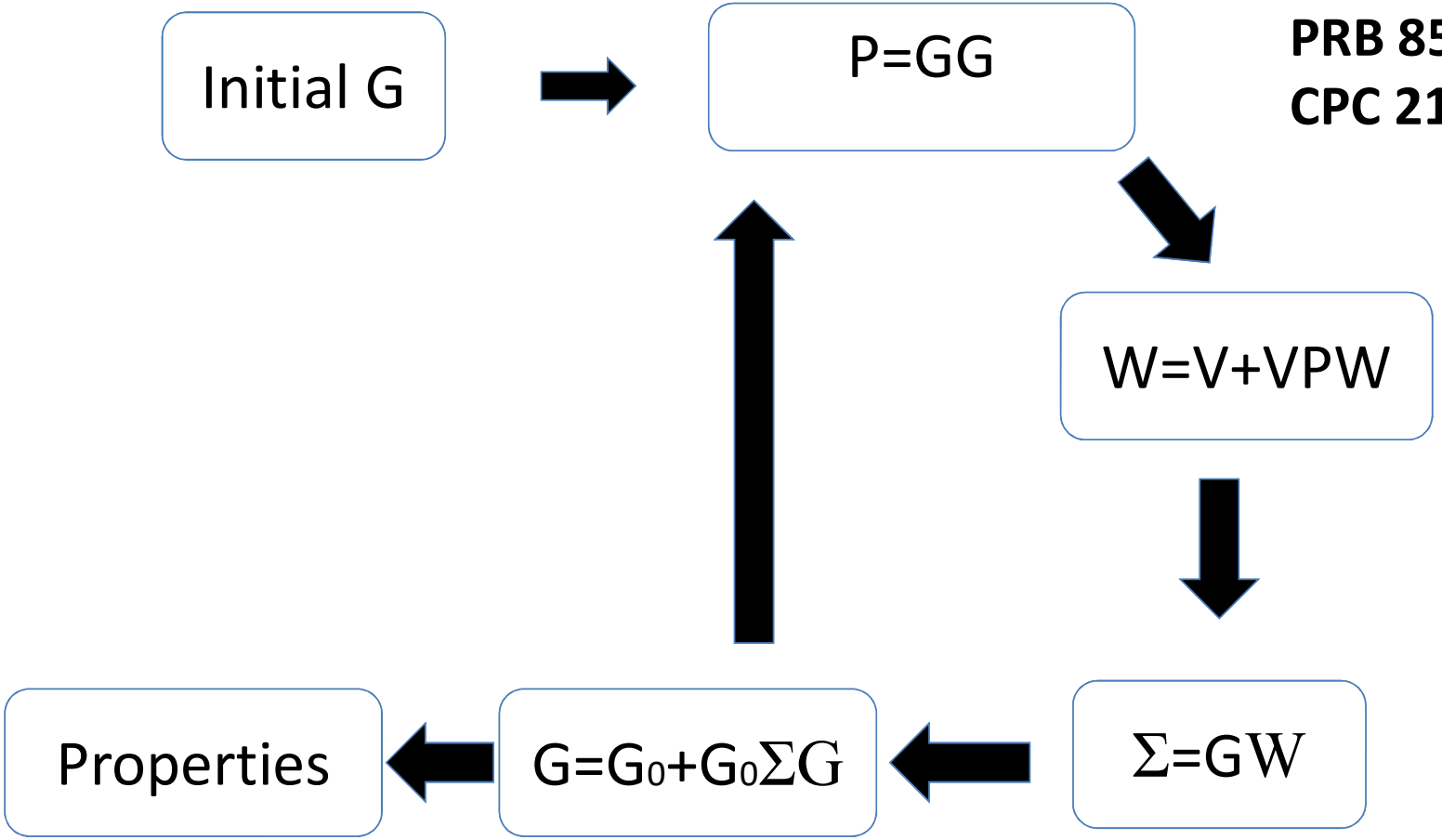
$$G = G_0 + G_0 \Sigma G$$

Good reference:
R. Del Sole et al., Phys. Rev. B 49, 8024 (1994)

DFT

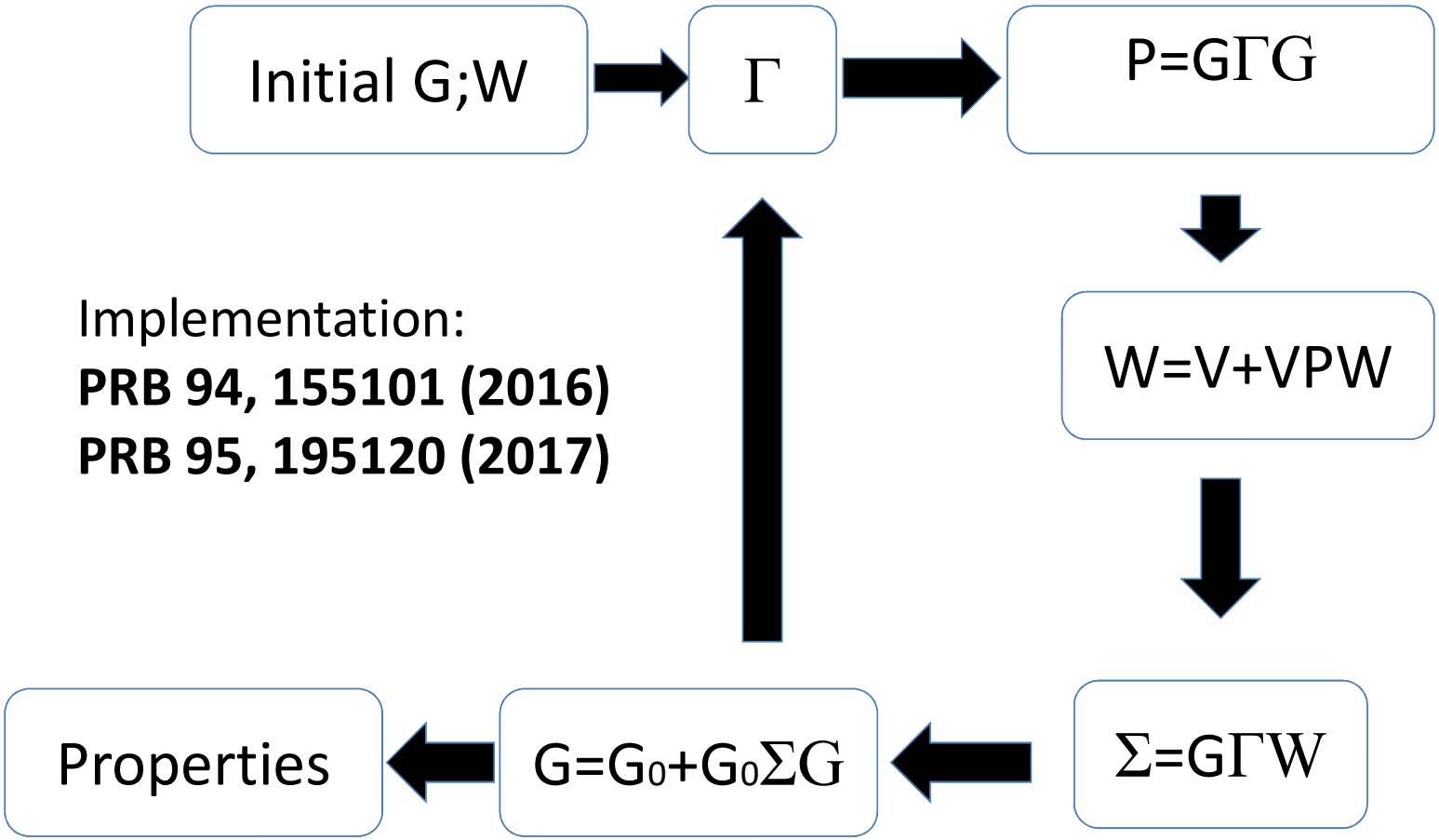

Initial ρ
$V_H = \rho V;\ V_{xc}[\rho]$
$V_{eff} = V_{ext} + V_H + V_{xc}$
$\varepsilon_k;\ \Psi_k$
New ρ
Properties

GW



Implementation:
PRB 85, 155129 (2012)
CPC 219, 407 (2017)

Vertex corrected GW

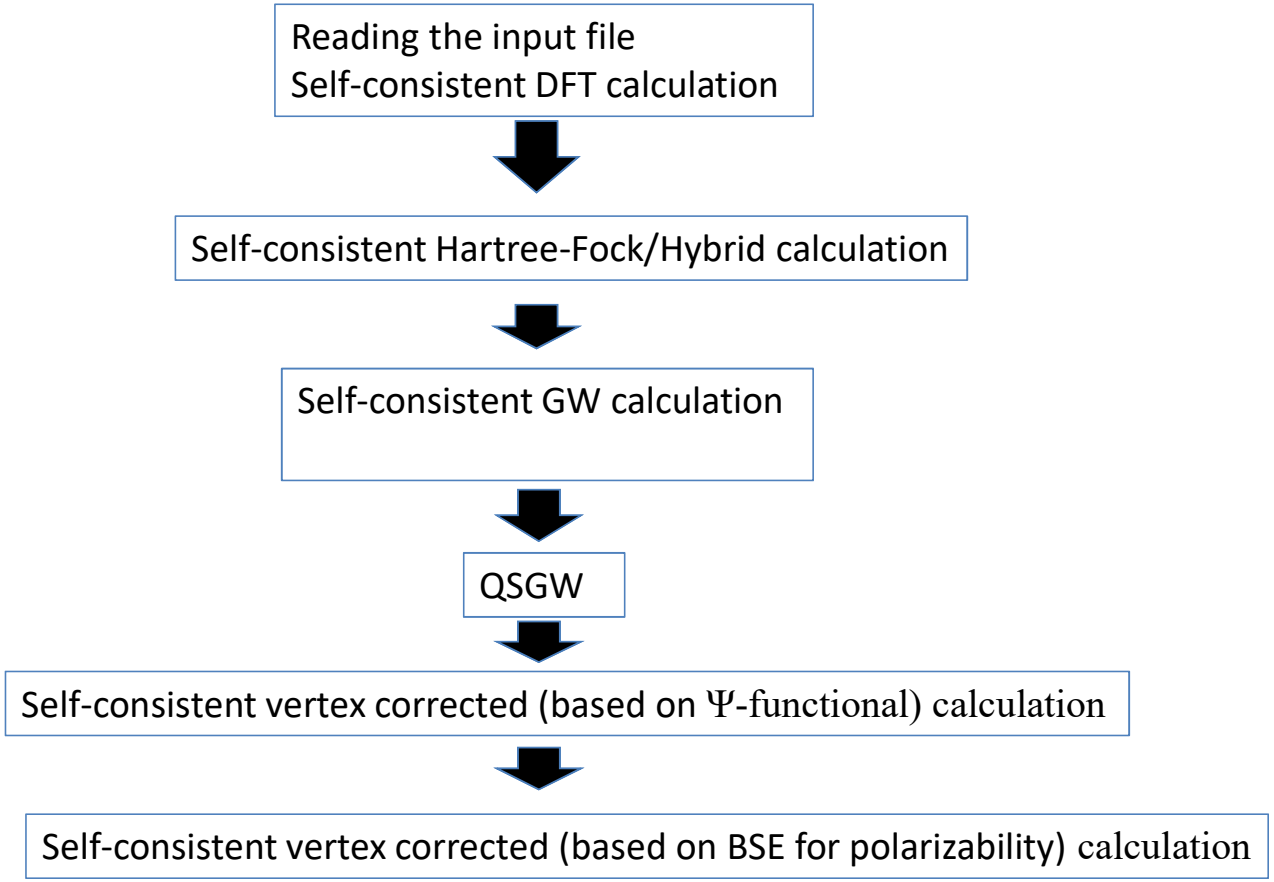


Implementation:
PRB 94, 155101 (2016)
PRB 95, 195120 (2017)

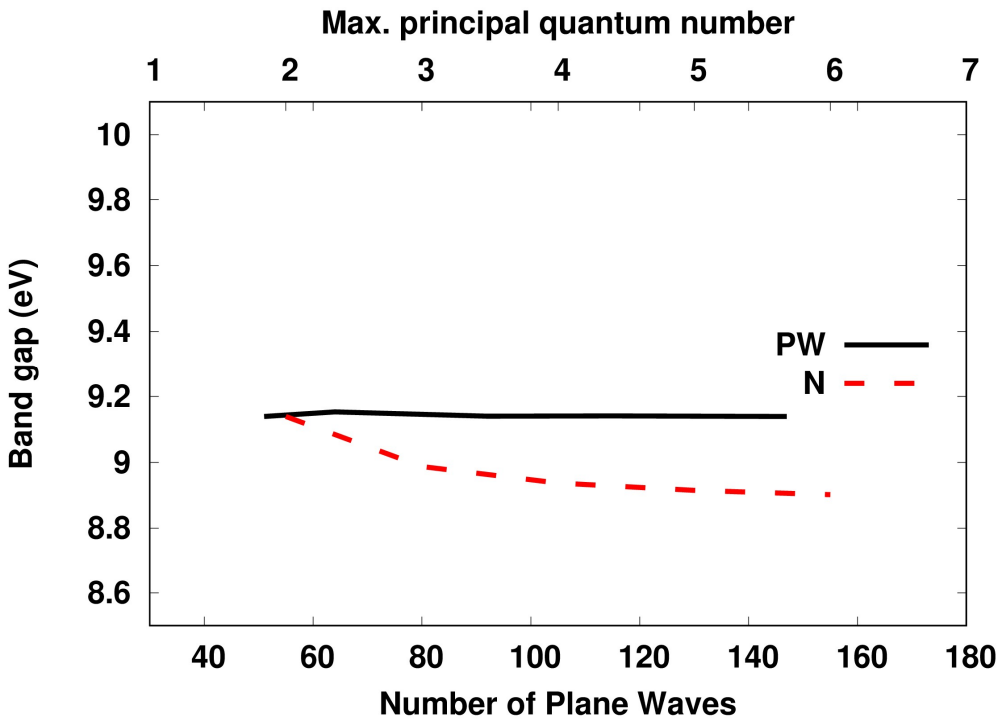
General information about FlapwMBPT

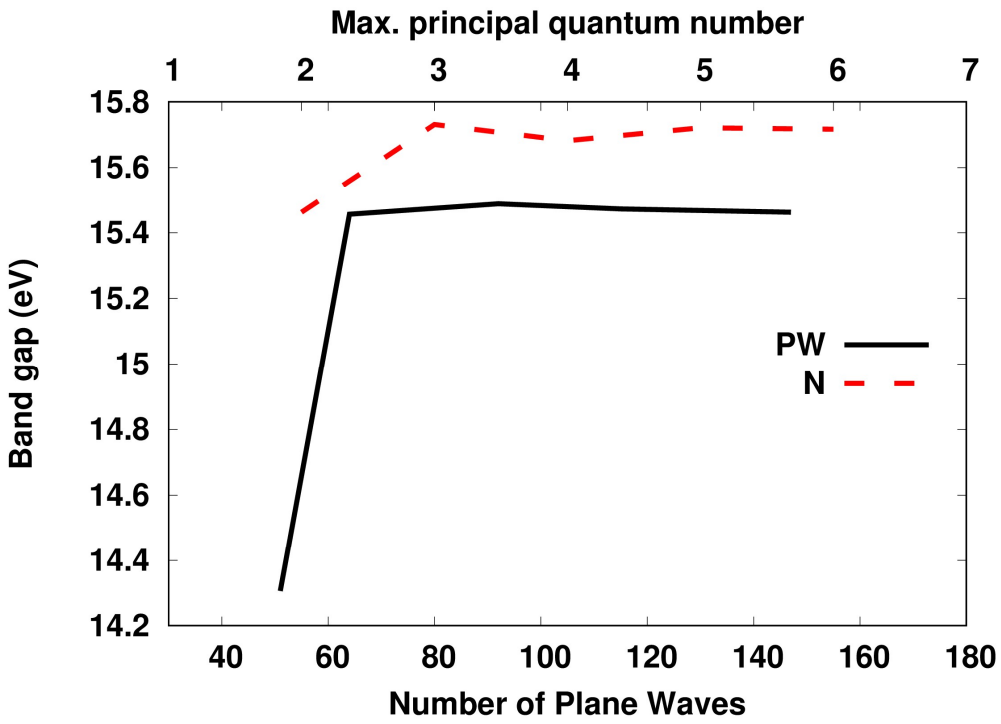
- Solid or electron gas (this talk is about solids only)
- Flexible FLAPW+LO/APW+lo all-electron basis set
- Non-relativistic, scalar-relativistic, or Dirac fully relativistic treatment of relativity
- Spin-polarized calculations
- MPI for parallelization
- Language: Fortran

How different methods are combined in one code

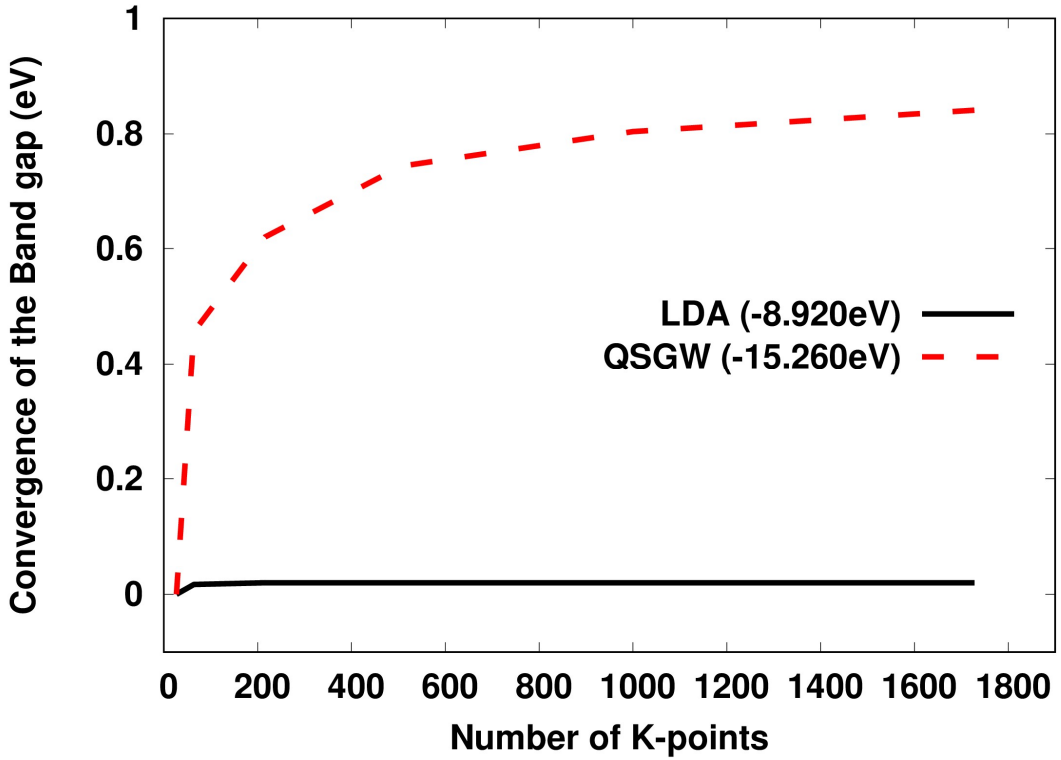


Convergence wrt the basis set (LiF)





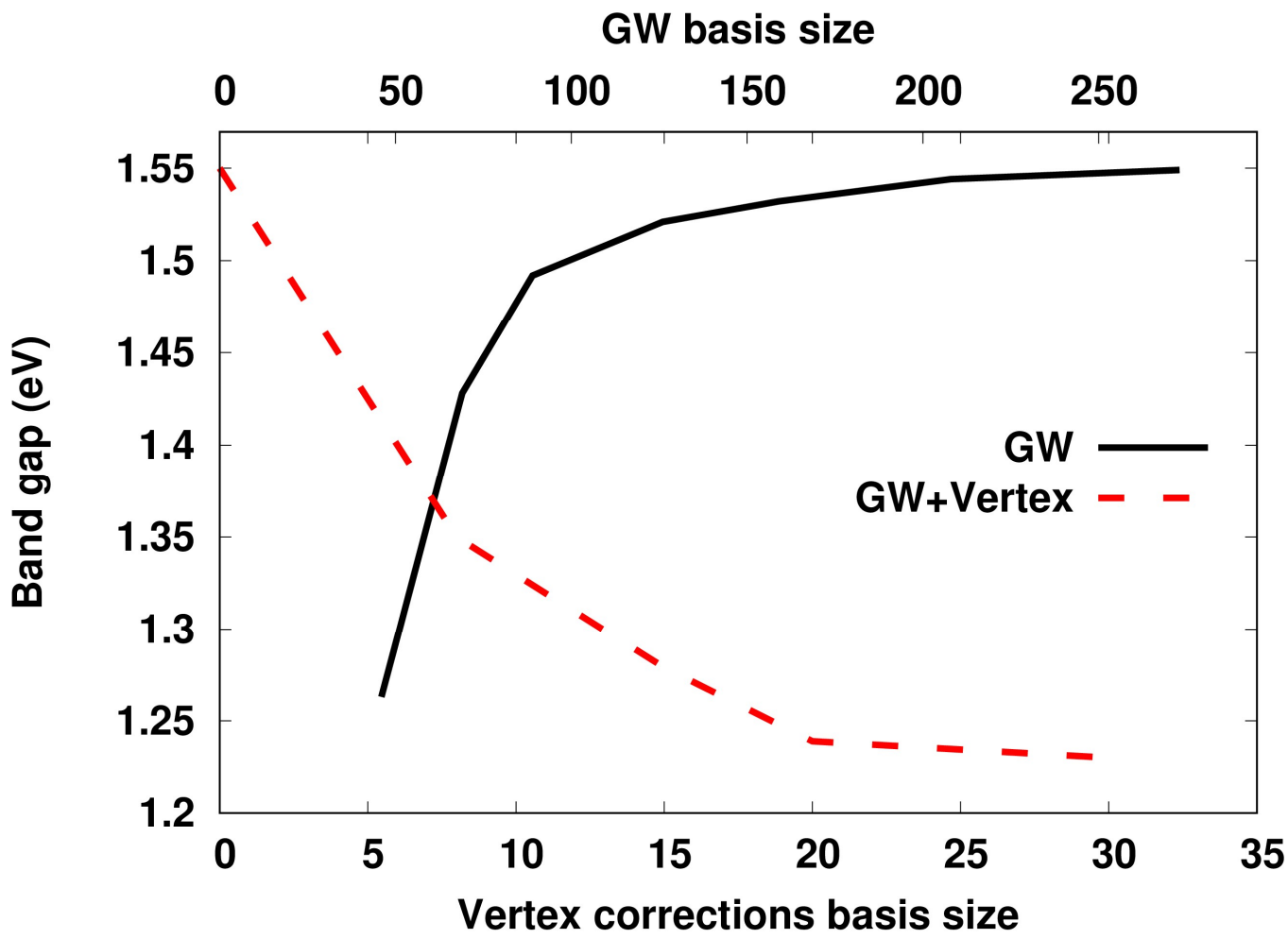
Convergence wrt the number of k-points (LiF)



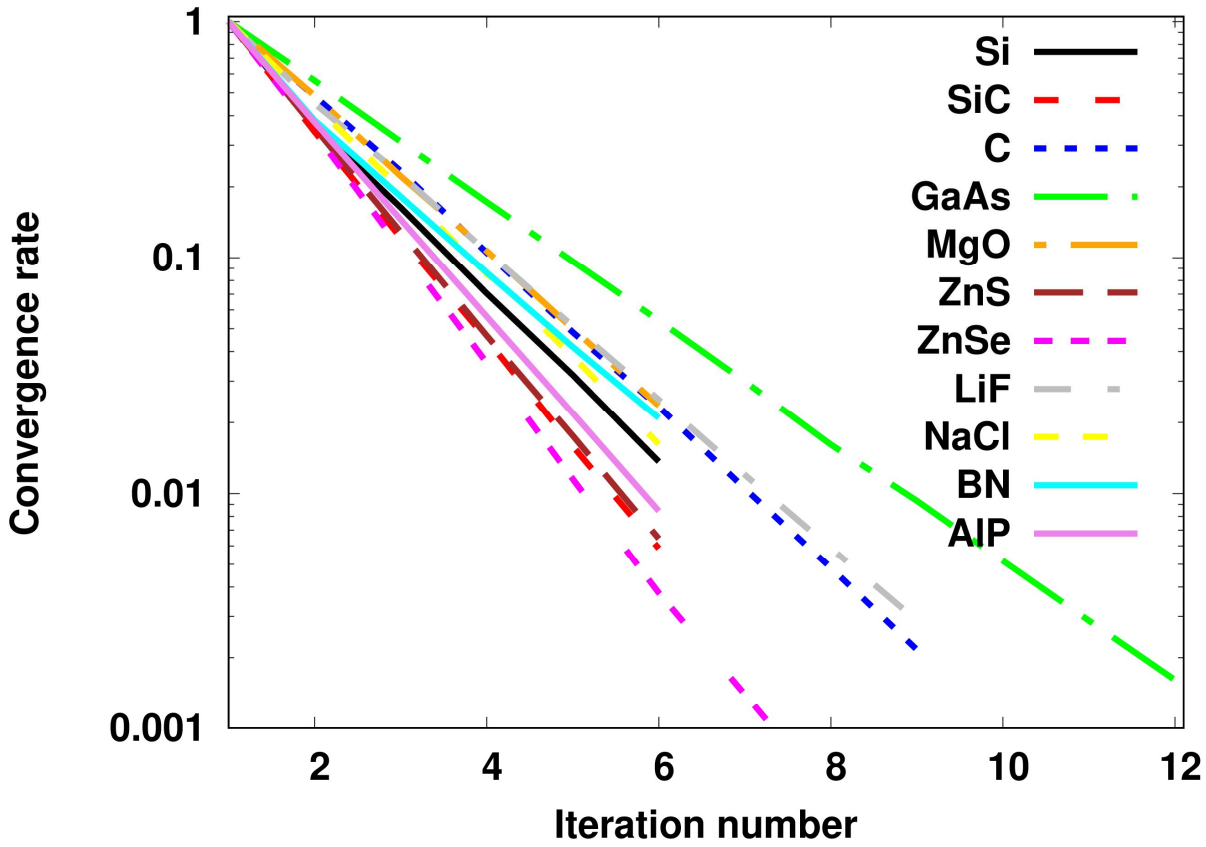
Convergence of MgO band gap (GW+Vertex)

Parameter	Setup	Band gap
N_{bnd}	0	9.31
	5	8.81
	10	8.40
	20	8.28
	30	8.29
ϕ_{nl}	3s(Mg)/2p(O)	8.56
	3s3p(Mg)/3s2p(O)	8.40
	3s3p3d(Mg)/3s2p3d(O)	8.28
	3s3p3d4f(Mg)/3s2p3d4f(O)	8.27
$N_{\mathbf{G}}$	26	8.19
	59	8.25
	92	8.28
$N_{\mathbf{k}}$	2^3	8.28
	3^3	8.24
	4^3	8.27
n_τ, n_ω, n_v	46	8.28
	62	8.29
	94	8.29

Convergence with respect to the basis size (Si)

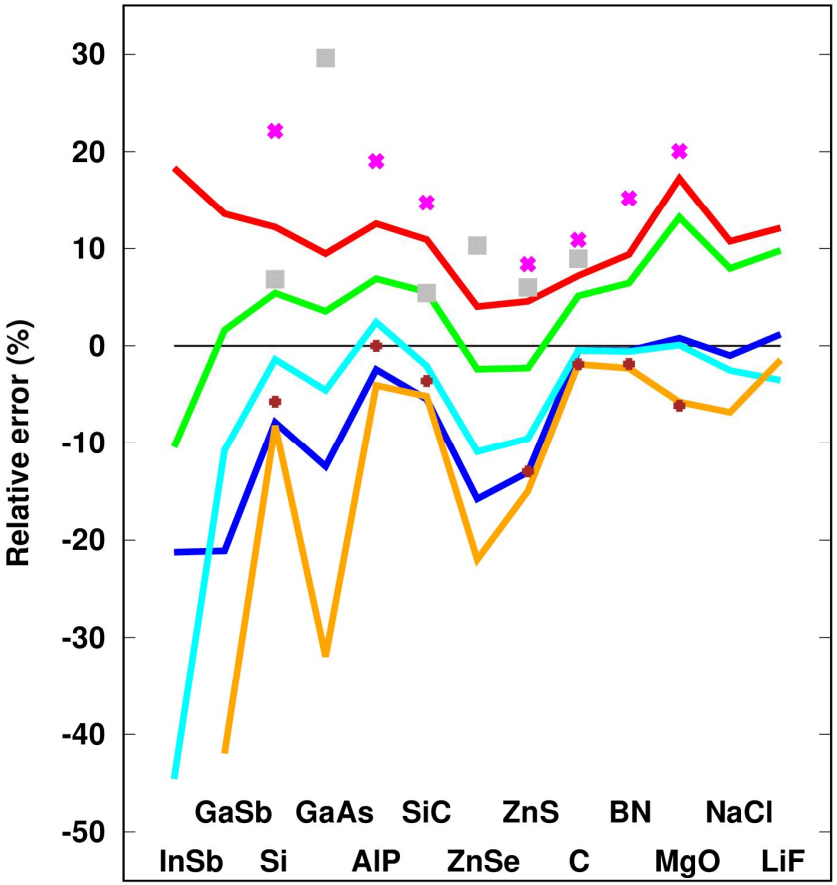


Convergence of the ladder sums



$$\Gamma = \mathbf{1} + \boldsymbol{WGG} + (\boldsymbol{WGG})^{2} + (\boldsymbol{WGG})^{3} + \cdots$$

Easy ways to improve QSGW results



Exp - E-ph
LQSGW
$LQSGW_{LDA}$
$LQSGW\Gamma_{LDA}$
$LQSGW_{BTS}$
G_0W_0(Wien-2k)
G_0W_0(VASP)
QSGW(VASP)
QSGW(Kotani et al.)

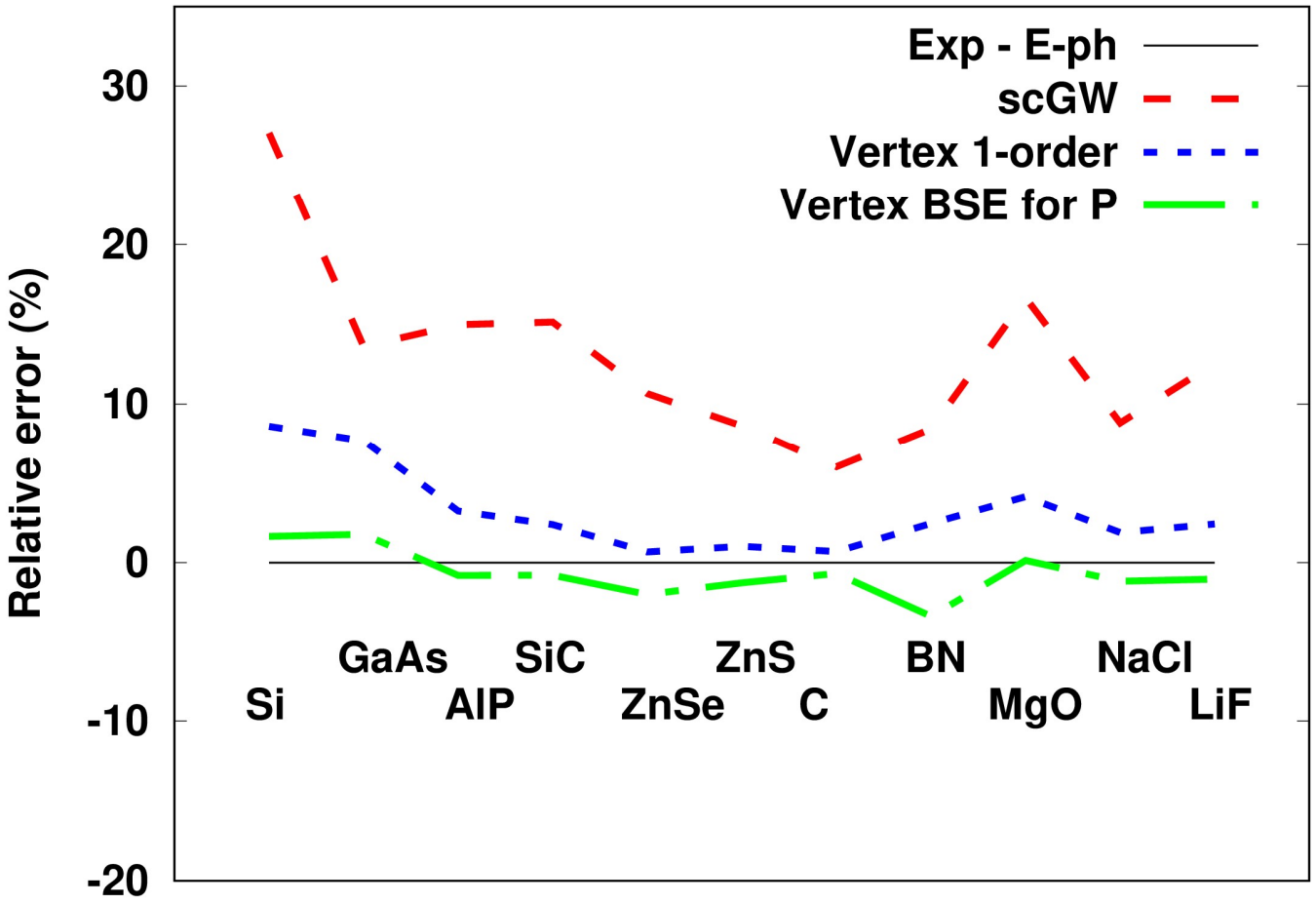
Exp:
PRB 20, 624(1979)
PRB 35, 9174(1987)
PRB 53, 16283(1996)

E-ph corr-n:
PRB 89, 214304(2014)
PRL 112, 215501(2014)
RMP 77, 1173(2005)
PRB 93, 100301(2016)

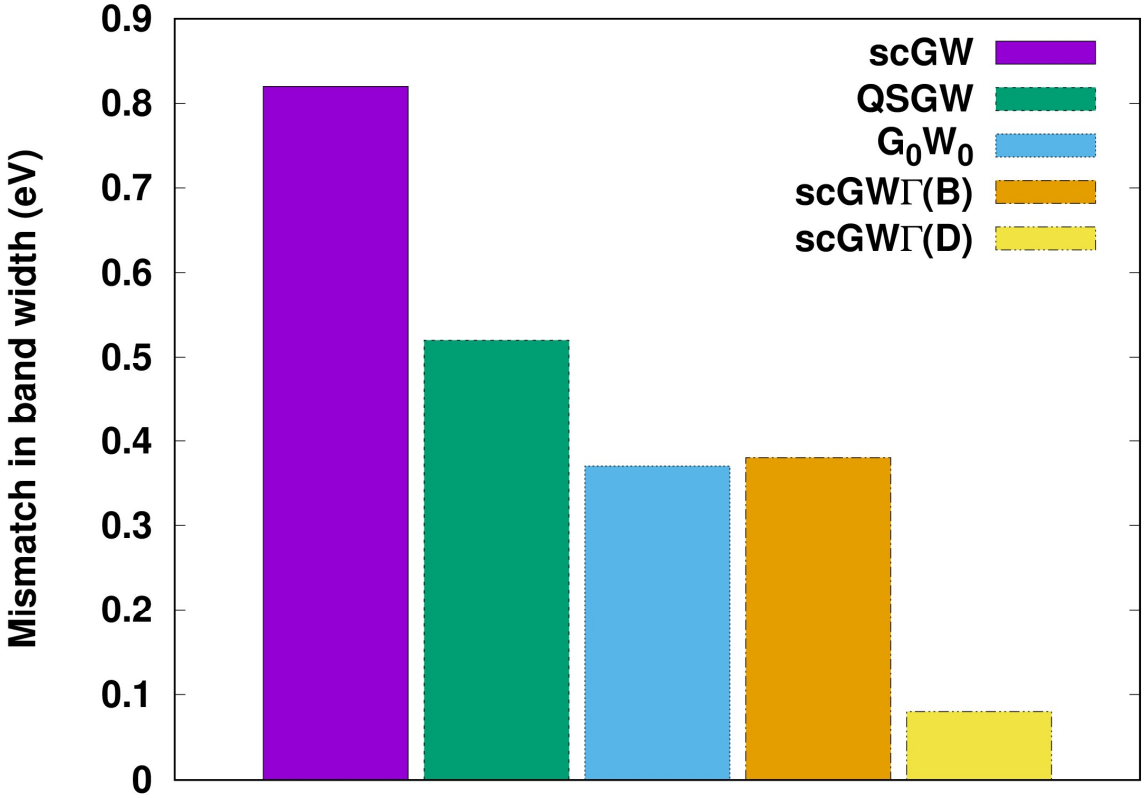
Bootstrap approach:

S. Sharma et al., Phys. Rev. Lett. 107, 186401 (2011)

Self consistent GWΓ: Band gaps



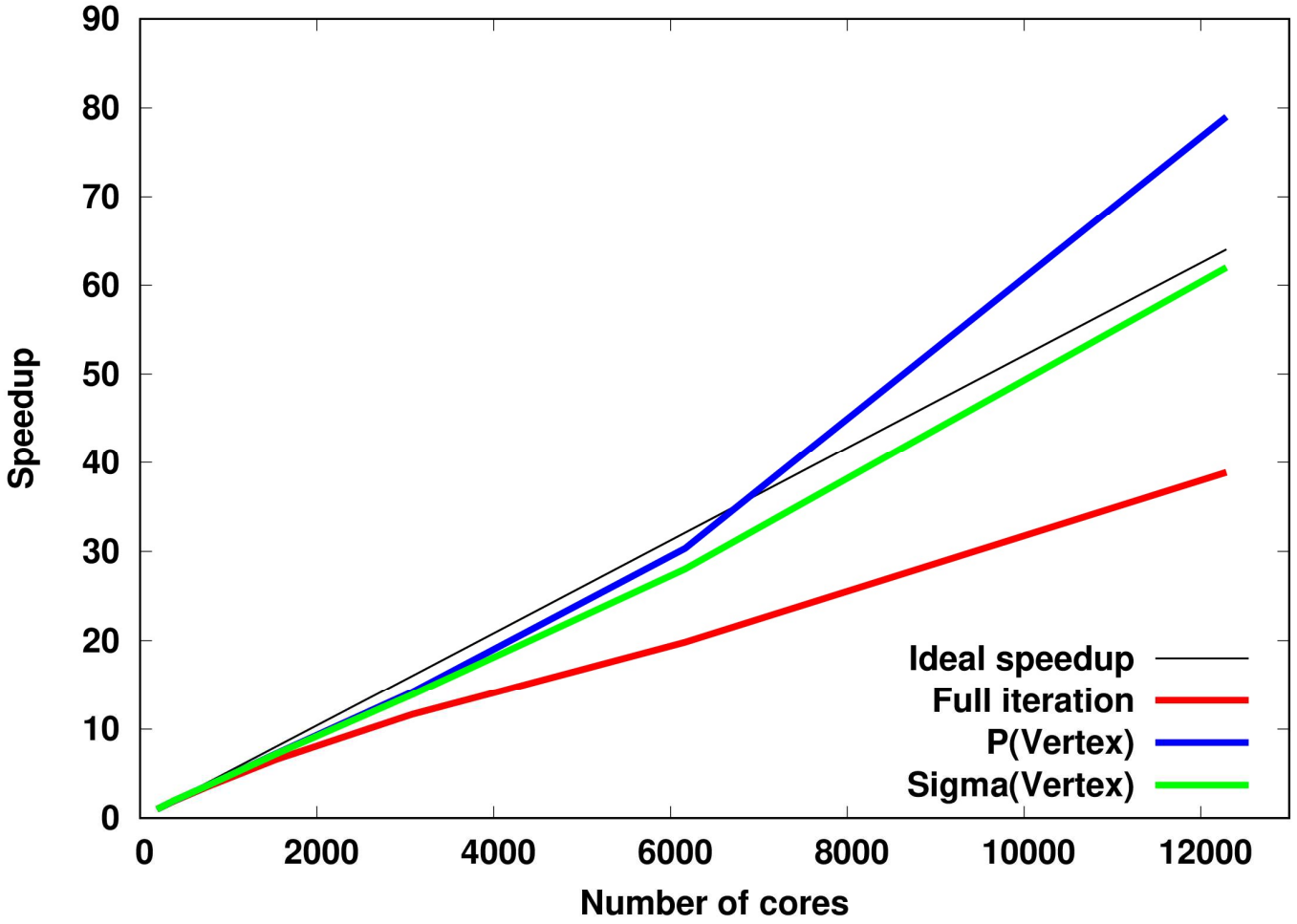
Band width of Na



Details:
PRB 94, 155101 (2016)

Relative to the experimental band width 2.65 eV from:
PRL 60, 1558 (1988),
PRB 41, 8075 (1990)

Scalability (PbTe)



Future plans for development

- Inclusion of more diagrams in the vertex part + optimization
- Optimization of DFT, Hartree-Fock, and GW parts
- Standard implementation of BSE (frequency-independent W, based on DFT or QSGW)
- Non-collinear magnetism implementation
- Linear response for phonons, electron-phonon interaction (DFT)

Hands on training (Plan)

- Basic DFT run – LiF
- QSGW - LiF
- QSGW+LDA_Vertex (one shot) – LiF
- QSGW+LDA_Vertex – LiF
- scGWΓ_1 – LiF
- scGWΓ_{GW} – LiF
- Homework

Details about the variables in input file
/home/akutepov/EXAMPLES/FlapwMBPT_Input.pdf

How to run the code

- copy **/home/akutepov/EXAMPLES** to your working directory

- In order to run the code, go in any of the subdirectories and perform:
- **qsub sub.pbs (please, replace e-mail with your e-mail before submitting!!!)**
- The results will go in the same subdirectory.

Input file (ini) - LiF

```
TEXT    *** band structure calculation of LiF (B1)  ***
CONTROL  iter_dft 20  iter_hf  0  iter_gw 16 iter_qp  0
       iter_psi 0  iter_bsp  16
       restart_begin  0 restart_end   0
       admix 0.3  adspin 0.7 adm_gw 0.3 acc_it_gw 0.3
       iexch 5 scal_spin 1.0 psi_fncl_use  0
       irel 0 clight 274.074 rel_interst F
       temperature  300.0
MPI mpi_pref ktb
  nproc_t 16 nproc_k 1 nproc_b 1
FILES
 allfile 'lif'
 tmpfile 'lif'
SYM symgen 'I_R4Z_R3D_'
STRUCTURE  par  7.60804  nsort  2  istruc  3
    b_a 1.0  c_a 1.0
    a   '0.0,0.5,0.5'
    b   '0.5,0.0,0.5'
    c   '0.5,0.5,0.0'
  tau   '0.0,0.0,0.0'
       '0.5,0.5,.5'
REAL SPACE MESHES mdiv  16  16  16
           nrdiv  10  10  10
         nrdiv_red   3   3   3
BASIS  cut_gw_ratio 0.6 cut_vrt_ratio 1.0
    eps_pb 0.001 eps_pb_vrt 0.01
ZONES nbndf 80 nbndf_bnd  1  6
BND_PLOT n_k_div 18
DOS   emindos -1.0  emaxdos  1.0   ndos 600
    e_small 0.005 e_small_bos 0.04
K_POINT  ndiv   4   4   4  k_line 001
    ndiv_c   2   2   2
    k_integral FD n_k_int 1 1 1
```

```
MULTI_SCF vv0  1.0
MAGNET  b_extval   0.0 iter_h_ext 00000
      b_ext  0.0  0.0  1.0
COULOMB eps_coul 0.0001
W   w_sc_gw scf w_sc_qp scf w_sc_psi scf w_sc_bsp non
HARTREE-FOCK alpha_hbr 0.25 omega_hse 0.165
hybrid_type 0
VERTEX_P psi_p 60000 bse_kernel_p 6000
      iter_ladder_p  6 nu_w_stat 0
VERTEX_S psi_sig 60000 psi2_sig 60000
      iter_sigma_gwg  1
VERTEX_XI iter_ladder_xi 0 q_suscept  2
       chi_cmp 000 vrt_x_appr 000
       nrax_chi 100 freq_chi  1.0
       theta_bse GW0
OPTICS opt_mode 000000 opt_loc_fld F
TAU MESH n_tau  62  exp_tau_gw  4.0
OMEGA MESH n_omega_exa 10 n_omega_geom  46
n_omega_asy 6
        omega_geom  500.0 omega_max 1900.0
NU MESH n_nu_exa 10 n_nu_geom 46  n_nu_asy  6
      nu_geom  300.0  nu_max 900.0
HEG rs  -4.0  k_inf  5.0  n_k_heg  50
ATOMIC DATA ----------------------------------------------------------
 txtel Li   z  3.0 magn_shift 0.0 z_dop 0.0
 smt 1.9 h 1.d-6 nrad  600
 lmb 6  lmpb 4
 lim_pb_mt= 12 10 10 10 10 10 10
 lim_pb_mt_red 4 2 2 0 0 0 0
 ntle  4  3  2  1  1  1  1
```

```
l  augm  atocc   ptnl  corr idmd
0  LOC  2.0  1.9    N   0
0  AWL  1.0  2.9    L   0
0  LOC  0.0  3.9    N   1
0  LOC  0.0  4.9    N   1
1  AWL  0.0  2.9    L   0
1  LOC  0.0  3.9    N   1
1  LOC  0.0  4.9    N   1
2  AWL  0.0  3.9    N   0
2  LOC  0.0  4.9    N   1
3  APW  0.0  4.9    N   0
4  APW  0.0  5.9    N   0
5  APW  0.0  6.9    N   0
6  APW  0.0  7.9    N   0
txtel _F    z  9.0 magn_shift 0.0 z_dop 0.0
smt 1.9 h 1.d-6 nrad  600
lmb 6  lmpb 4
lim_pb_mt= 12 10 10 10 10 10 10
lim_pb_mt_red 4 2 2 0 0 0 0
ntle=  3  3  2  1  1  1  1
l  augm  atocc   ptnl  corr idmd
0  AWL  2.0  2.9    L   0
0  LOC  0.0  3.9    N   1
0  LOC  0.0  4.9    N   1
1  AWL  5.0  2.9    L   0
1  LOC  0.0  3.9    N   1
1  LOC  0.0  4.9    N   1
2  AWL  0.0  3.9    N   0
2  LOC  0.0  4.9    N   1
3  APW  0.0  4.9    N   0
4  APW  0.0  5.9    N   0
5  APW  0.0  6.9    N   0
6  APW  0.0  7.9    N   0
```

Basic DFT – output files

- **LiF_LDA.o611874** – monitoring total energy/density convergence
- **lif.out** – general output (basis set sizes, timings,…)
- **lif_dft.dos** - DOS
- **lif_dn_dft.dosk** – k-resolved DOS
- **lifLi___sum_dft.pdos** – PDOS for Li
- **Lif_F___sum_dft.pdos** – PDOS for F
- **lif_dft_band_LAPW.dat** – data file for band plotting
- **lif_dft_band_LAPW.gnu** – GNUPLOT file for band plotting

QSGW example – output files

- **……..**
- **lif_qp.dos** – DOS for QSGW
- **lif_dn_qp.dosk** – k-resolved DOS for QSGW
- **lifLi___sum_qp.pdos** – QSGW PDOS for Li
- **lif_F___sum_qp.pdos** – QSGW PDOS for F
- **lif_Nu_Q____P_Re.qp** – P as a function of Matsubara freq-cy
- **lif_Im_sigc_w_band_k.qp** – Im part of Sigma_corr
- **lif_Re_sigc_w_band_k.qp** – Re part of Sigma_corr
- **lif__qp_x.eig** – QSGW one electron energies
- **lif_Z_factor_band_k_x.qp** – Renorm Z-factor

scGWΓ example – output files

- **…….**
- **lif_psi.dos** – Spectral function (SF) for scGWΓ
- **lif_dn_psi.dosk** – k-resolved SF for scGWΓ
- **lifLi__Chain_psi.pdos** – scGWΓ PSF for Li
- **lif_F__Chain_psi.pdos** – scGWΓ PSF for F
- **lif_Nu_Q____P_Re.psi** – P as a function of Matsubara freq-cy
- **lif_Im_sigc_w_band_k.psi** – Im part of Sigma_corr
- **lif_Re_sigc_w_band_k.psi** – Re part of Sigma_corr

  lif_Z_factor_band_k_x.psi – Renorm Z-factor

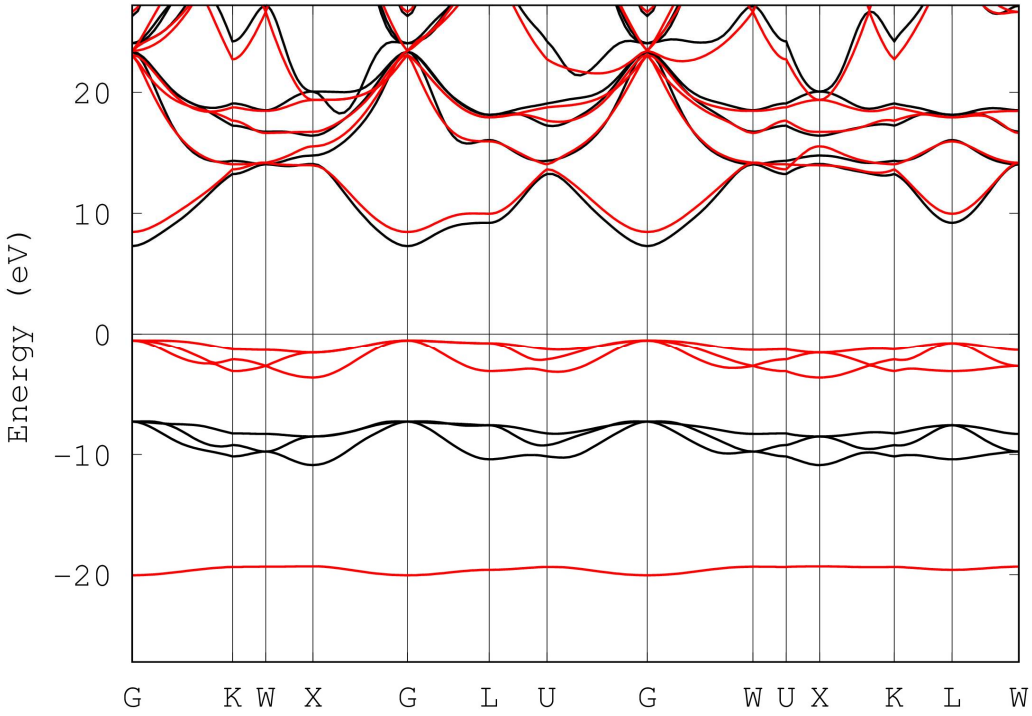
For Bethe-Salpeter based calculations “psi” is replaced with “bsp”

File **lif_bsp_qp.eig**

QP Eigen states relative to the Chemical Potential (eV)

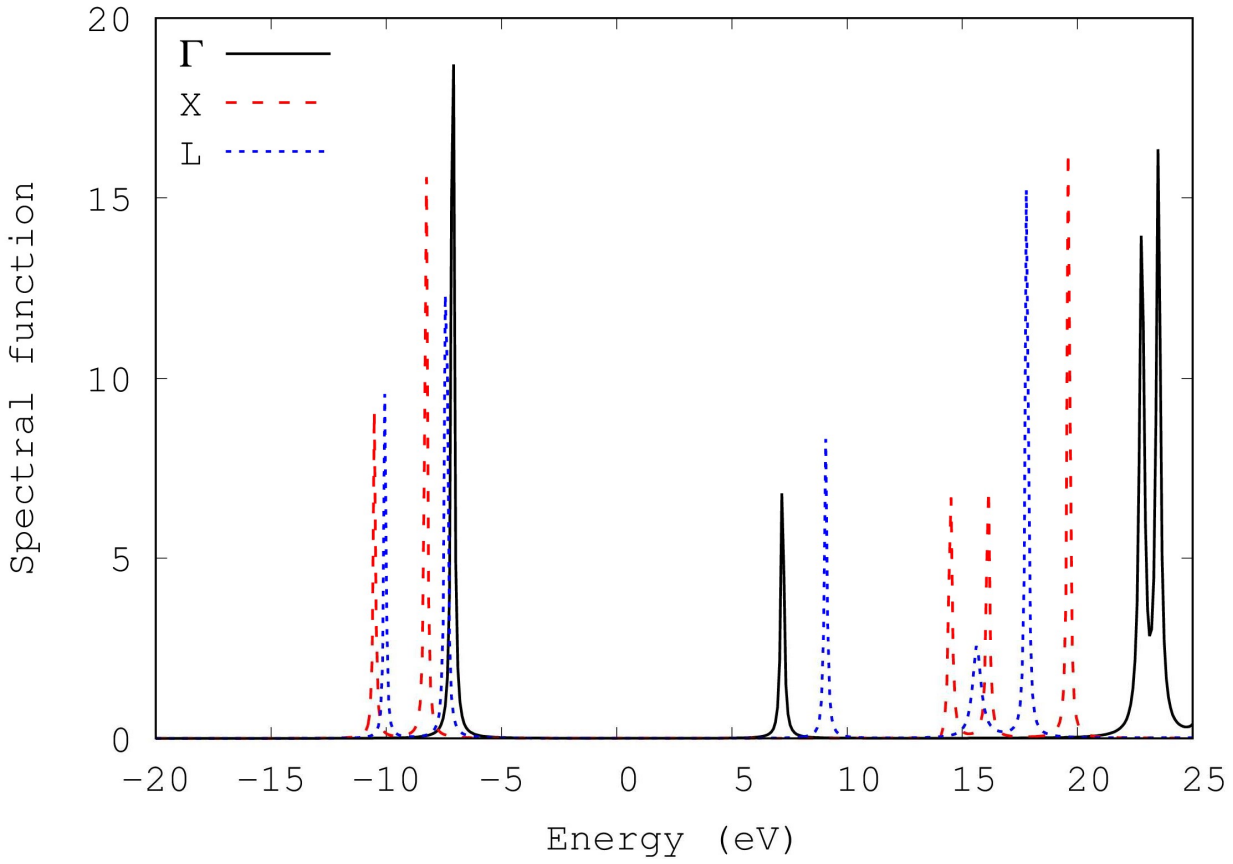
K\Band	1	2	3	4	5	6	7	8	9
1	-57.0698	-31.4757	-7.2689	-7.2689	-7.2689	7.2688	23.2200	23.2200	23.2200
2	-57.0409	-31.1694	-8.9305	-7.4340	-7.4340	8.6936	16.7809	19.8054	19.8054
3	-57.0149	-30.9087	-10.3690	-7.5677	-7.5677	9.0583	15.8777	17.9970	17.9970
4	-57.0332	-31.0488	-8.9646	-7.8999	-7.8999	9.9236	17.1144	18.8727	20.0458
5	-57.0063	-30.7120	-10.1212	-8.6751	-8.0528	11.5622	14.6430	17.8156	18.9570
6	-57.0146	-30.8479	-9.5330	-8.8664	-7.5983	10.6295	14.5394	18.7095	18.7164
7	-56.9999	-30.5803	-10.8597	-8.4868	-8.4868	13.8695	14.6428	16.3576	19.8552
8	-56.9980	-30.5772	-9.7477	-9.7477	-8.2816	13.8594	13.8594	16.5586	18.4393

LDA band structure vs GW+Vertex



Lifbsp_band.gnu
Lif_bsp_band.dat
Lif_dft_band_LAPW.dat

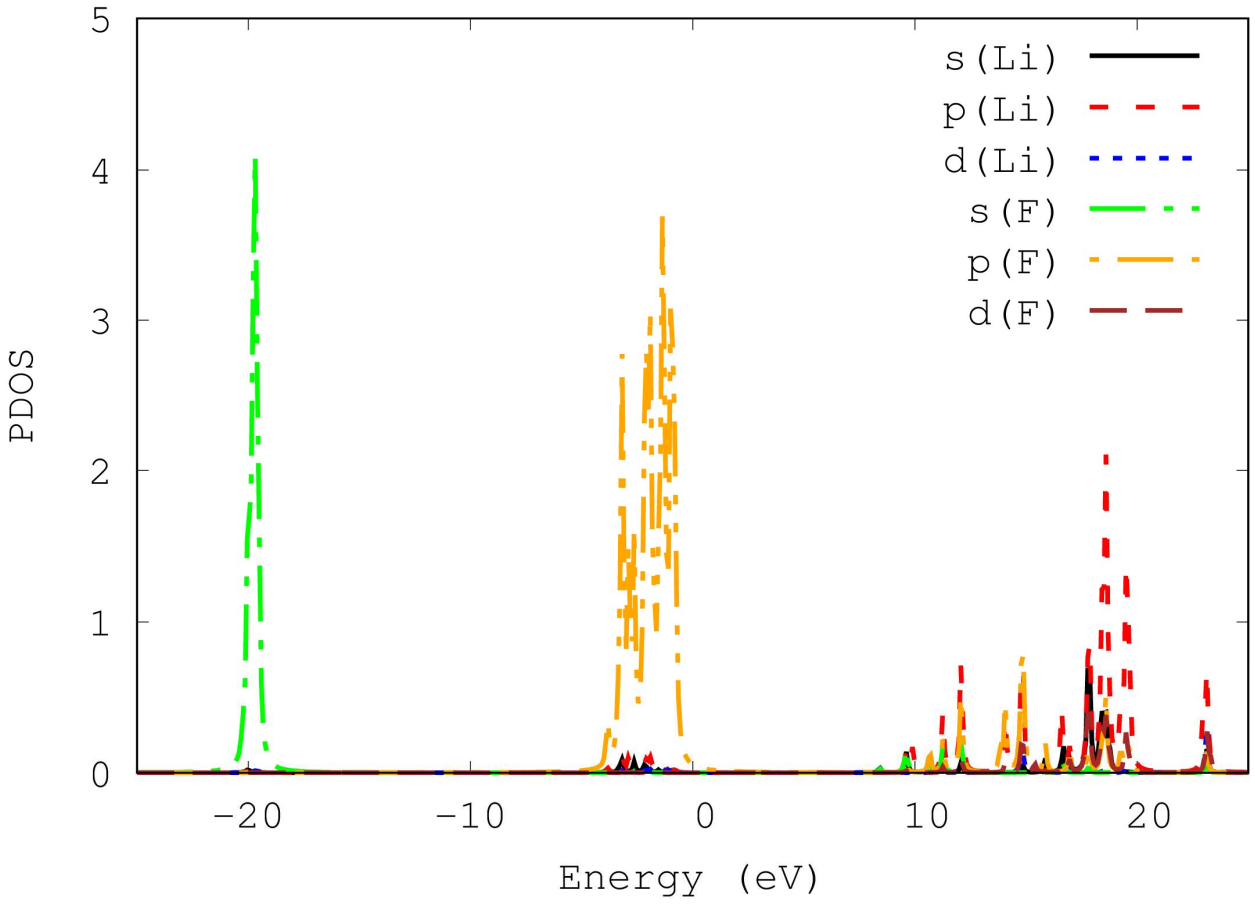
K-resolved spectral function



Lif_dn_bsp.dosk

	G	X	W	L
-27.21070	0.03560	0.03753	0.06087	0.03409
-27.12000	0.03354	0.03467	0.05648	0.03177
-27.02930	0.03163	0.03211	0.05254	0.02966
-26.93859	0.02988	0.02982	0.04900	0.02774
-26.84789	0.02825	0.02775	0.04580	0.02598
-26.75719	0.02674	0.02588	0.04290	0.02437
-26.66649	0.02533	0.02419	0.04026	0.02289
-26.57578	0.02402	0.02264	0.03785	0.02153
-26.48508	0.02280	0.02123	0.03565	0.02027
-26.39438	0.02166	0.01993	0.03362	0.01910
-26.30368	0.02060	0.01874	0.03176	0.01802
-26.21297	0.01960	0.01765	0.03004	0.01702
-26.12227	0.01866	0.01664	0.02844	0.01609
-26.03157	0.01778	0.01570	0.02697	0.01522
-25.94087	0.01695	0.01484	0.02560	0.01440
-25.85016	0.01617	0.01403	0.02432	0.01364
-25.75946	0.01544	0.01328	0.02314	0.01293
-25.66876	0.01475	0.01258	0.02203	0.01227
-25.57806	0.01410	0.01193	0.02099	0.01164
-25.48736	0.01348	0.01132	0.02002	0.01105
-25.39665	0.01290	0.01075	0.01911	0.01050
-25.30595	0.01235	0.01022	0.01825	0.00998
-25.21525	0.01183	0.00972	0.01744	0.00948
-25.12455	0.01133	0.00924	0.01669	0.00902
-25.03384	0.01086	0.00880	0.01597	0.00858
-24.94314	0.01042	0.00838	0.01530	0.00817
-24.85244	0.01000	0.00799	0.01466	0.00777
-24.76174	0.00959	0.00761	0.01406	0.00740
-24.67103	0.00921	0.00726	0.01349	0.00705
-24.58033	0.00885	0.00693	0.01295	0.00671
-24.48963	0.00850	0.00662	0.01244	0.00640
-24.39893	0.00818	0.00632	0.01196	0.00609

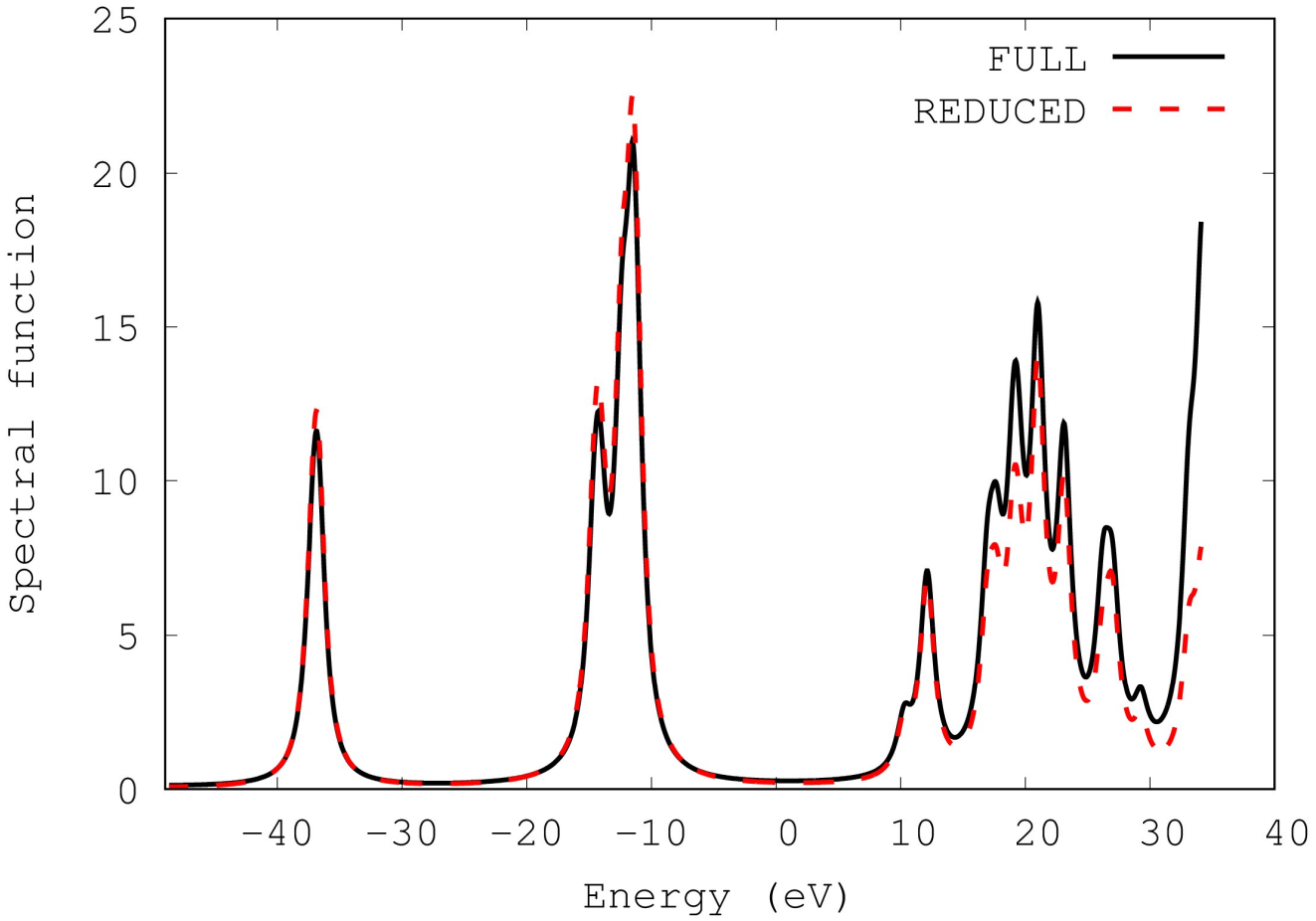
Assessing the quality of the reduced basis set



Lif_F___sum_dft.pdos
lifLi___sum_dft.pdos

-20.771	0.043	0.000	0.000	0.000
-20.680	0.053	0.000	0.000	0.000
-20.589	0.068	0.000	0.000	0.000
-20.499	0.091	0.000	0.000	0.000
-20.408	0.132	0.000	0.000	0.000
-20.317	0.231	0.000	0.000	0.000
-20.227	0.389	0.000	0.000	0.000
-20.136	0.620	0.001	0.000	0.000
-20.045	1.550	0.001	0.000	0.000
-19.955	1.690	0.001	0.000	0.000
-19.864	1.865	0.001	0.000	0.000
-19.773	3.293	0.001	0.000	0.000
-19.682	4.099	0.001	0.000	0.000
-19.592	2.622	0.001	0.000	0.000
-19.501	1.583	0.001	0.000	0.000
-19.410	0.594	0.000	0.000	0.000
-19.320	0.299	0.000	0.000	0.000
-19.229	0.184	0.000	0.000	0.000
-19.138	0.125	0.000	0.000	0.000
-19.047	0.092	0.000	0.000	0.000
-18.957	0.070	0.000	0.000	0.000
-18.866	0.055	0.000	0.000	0.000
-18.775	0.045	0.000	0.000	0.000
-18.685	0.037	0.000	0.000	0.000
-18.594	0.031	0.000	0.000	0.000

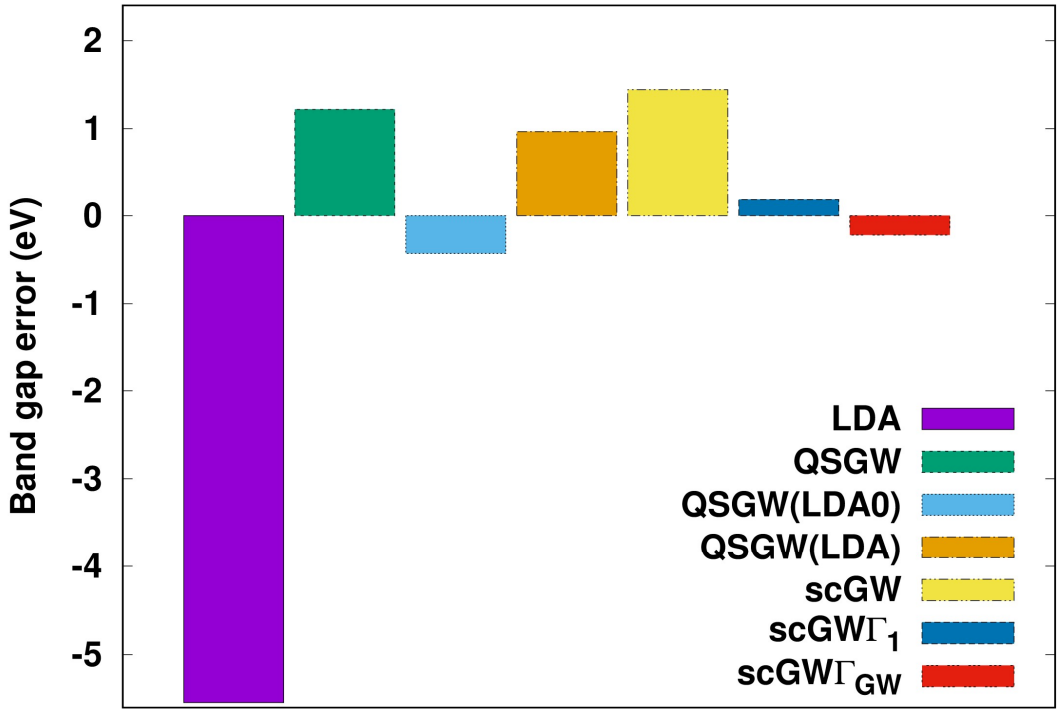
Assessing the quality of the reduced basis set



lifX_FULL_RED.dos

-16.73566	1.49960	1.58143
-16.64486	1.58879	1.67938
-16.55406	1.68721	1.78747
-16.46326	1.79620	1.90719
-16.37246	1.91734	2.04029
-16.28166	2.05252	2.18885
-16.19086	2.20400	2.35536
-16.10006	2.37448	2.54278
-16.00926	2.56718	2.75468
-15.91846	2.78598	2.99534
-15.82766	3.03551	3.26987
-15.73686	3.32131	3.58436
-15.64606	3.64988	3.94600
-15.55526	4.02874	4.36307
-15.46446	4.46631	4.84486
-15.37366	4.97147	5.40113
-15.28286	5.55254	6.04101
-15.19206	6.21542	6.77093
-15.10126	6.96050	7.59116
-15.01046	7.77840	8.49109
-14.91966	8.64545	9.44427
-14.82886	9.52160	10.40605
-14.73806	10.35398	11.31764
-14.64726	11.08721	12.11773
-14.55646	11.67552	12.75601
-14.46566	12.08762	13.19876
-14.37486	12.30271	13.42425
-14.28406	12.30718	13.41886
-14.19326	12.10181	13.18445
-14.10246	11.71431	12.75190
-14.01166	11.20228	12.18434

Summary of the calculated band gap (LiF)



Homework

- Try to apply the same approaches to Si:

- Copy “ini” file in another directory and edit it:
- New crystal structure (a=10.26)
- New symmetry operations
- New kind of atomic data

Thank you!