# GW approximation in exciting

**Manoar Hossain and team exciting**
Institut für Physik and IRIS Adlershof
Humboldt-Universität zu Berlin

HoW **exciting**! 2023

4th August

# Outline

- Introduction
  - Why GW (beyond DFT)
  - GW approximation
- Implementation in **`exciting`**
- How to use GW@**`exciting`**
  - Input file preparation
  - Output file inspection
  - Convergence test
- Summary

# Introduction

- Kohn-Sham equation

$$\left\{-\frac{1}{2}\nabla^2 + v_{\mathrm{ne}}(\mathbf{r}) + v_{\mathrm{H}}(\mathbf{r}) + v_{\mathrm{xc}}(\mathbf{r})\right\}\psi_i^{KS}(\mathbf{r}) = \epsilon_i^{KS}\psi_i^{KS}(\mathbf{r})$$

Physical review, 136, B864 (1964)
Physical review, 140, A1133 (1965)

# Introduction

- Kohn-Sham equation

$$\left\{-\frac{1}{2}\nabla^2 + v_{\mathrm{ne}}(\mathbf{r}) + v_{\mathrm{H}}(\mathbf{r}) + v_{\mathrm{xc}}(\mathbf{r})\right\}\psi_i^{KS}(\mathbf{r}) = \epsilon_i^{KS}\psi_i^{KS}(\mathbf{r})$$

- DFT does not give any recipe for **exchange-correlation** potential

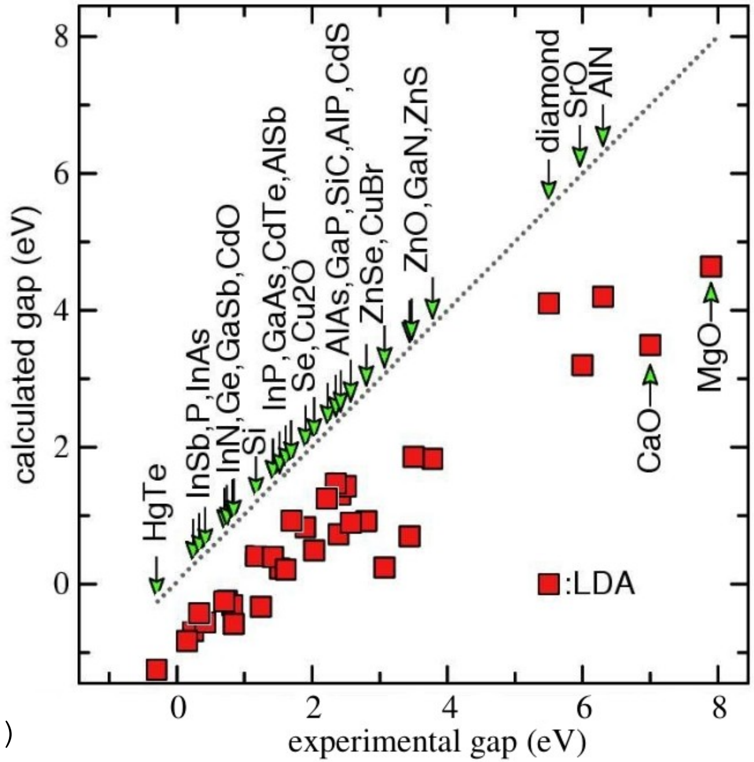
  (LDA, GGA, Hybrid ...)

# Introduction

- Kohn-Sham equation

$$\left\{-\frac{1}{2}\nabla^2 + v_{\mathrm{ne}}(\mathbf{r}) + v_{\mathrm{H}}(\mathbf{r}) + v_{\mathrm{xc}}(\mathbf{r})\right\}\psi_i^{KS}(\mathbf{r}) = \epsilon_i^{KS}\psi_i^{KS}(\mathbf{r})$$

- DFT does not give any recipe for **exchange-correlation** potential
  (LDA, GGA, Hybrid ...)




Schilfgaarde et al. PRL 96 226402(2006)

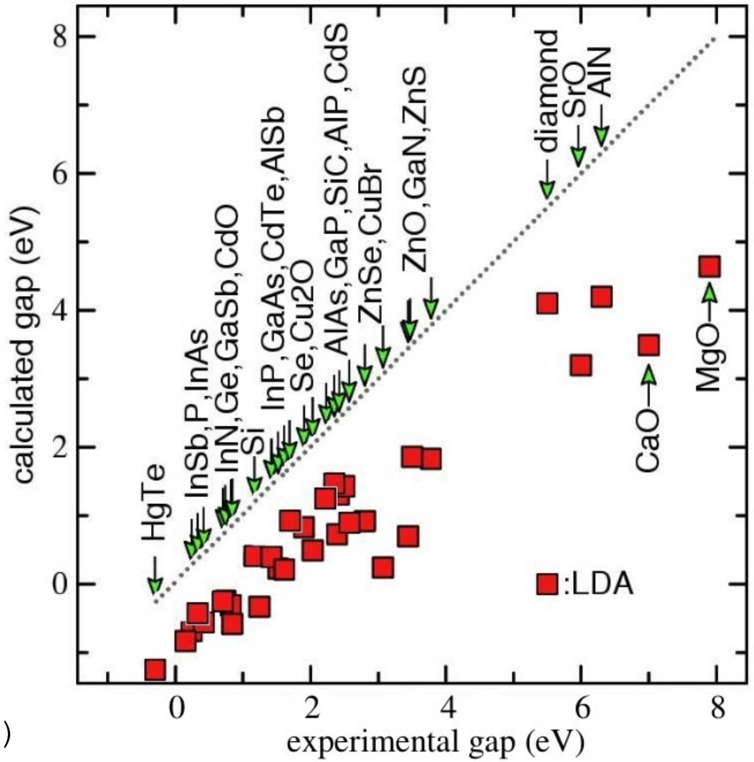
# Introduction

- Kohn-Sham equation

$$\left\{-\frac{1}{2}\nabla^2 + v_{\mathrm{ne}}(\mathbf{r}) + v_{\mathrm{H}}(\mathbf{r}) + v_{\mathrm{xc}}(\mathbf{r})\right\}\psi_i^{KS}(\mathbf{r}) = \epsilon_i^{KS}\psi_i^{KS}(\mathbf{r})$$

- DFT does not give any recipe for **exchange-correlation** potential
  (LDA, GGA, Hybrid ...)

- Ground-state formalism
- Predicts GS energy
- Inadequate description of quasi-particle nature of electron




Schilfgaarde et al. PRL 96 226402(2006)

# Introduction

- Kohn-Sham equation

$$\left\{-\frac{1}{2}\nabla^2 + v_{\mathrm{ne}}(\mathbf{r}) + v_{\mathrm{H}}(\mathbf{r}) + v_{\mathrm{xc}}(\mathbf{r})\right\}\psi_i^{KS}(\mathbf{r}) = \epsilon_i^{KS}\psi_i^{KS}(\mathbf{r})$$

- Quasi-particle equation

$$\left\{-\frac{1}{2}\nabla^2 + v_{\mathrm{ne}}(\mathbf{r}) + v_{\mathrm{H}}(\mathbf{r})\right\}\psi_i^{QP}(\mathbf{r}) +$$

$$\int d\mathbf{r}'\Sigma\left(\mathbf{r}, \mathbf{r}', \epsilon_i^{QP}\right)\psi_i^{QP}(\mathbf{r}') = \epsilon_i^{QP}\psi_i^{QP}(\mathbf{r})$$

# Introduction

- Kohn-Sham equation

$$\left\{ -\frac{1}{2}\nabla^2 + v_{\mathrm{ne}}(\mathbf{r}) + v_{\mathrm{H}}(\mathbf{r}) + v_{\mathrm{xc}}(\mathbf{r}) \right\} \psi_i^{KS}(\mathbf{r}) = \epsilon_i^{KS} \psi_i^{KS}(\mathbf{r})$$

- Quasi-particle equation

$$\left\{ -\frac{1}{2}\nabla^2 + v_{\mathrm{ne}}(\mathbf{r}) + v_{\mathrm{H}}(\mathbf{r}) \right\} \psi_i^{QP}(\mathbf{r}) +$$

$$\int d\mathbf{r}' \Sigma\left(\mathbf{r}, \mathbf{r}', \epsilon_i^{QP}\right) \psi_i^{QP}(\mathbf{r}') = \epsilon_i^{QP} \psi_i^{QP}(\mathbf{r})$$

# Introduction

- Kohn-Sham equation

$$\left\{-\frac{1}{2}\nabla^2 + v_{\mathrm{ne}}(\mathbf{r}) + v_{\mathrm{H}}(\mathbf{r}) + v_{\mathrm{xc}}(\mathbf{r})\right\}\psi_i^{KS}(\mathbf{r}) = \epsilon_i^{KS}\psi_i^{KS}(\mathbf{r})$$

- Quasi-particle equation

$$\left\{-\frac{1}{2}\nabla^2 + v_{\mathrm{ne}}(\mathbf{r}) + v_{\mathrm{H}}(\mathbf{r})\right\}\psi_i^{QP}(\mathbf{r}) +$$

$$\int d\mathbf{r}'\Sigma\left(\mathbf{r},\mathbf{r}',\epsilon_i^{QP}\right)\psi_i^{QP}(\mathbf{r}') = \epsilon_i^{QP}\psi_i^{QP}(\mathbf{r})$$

# Introduction

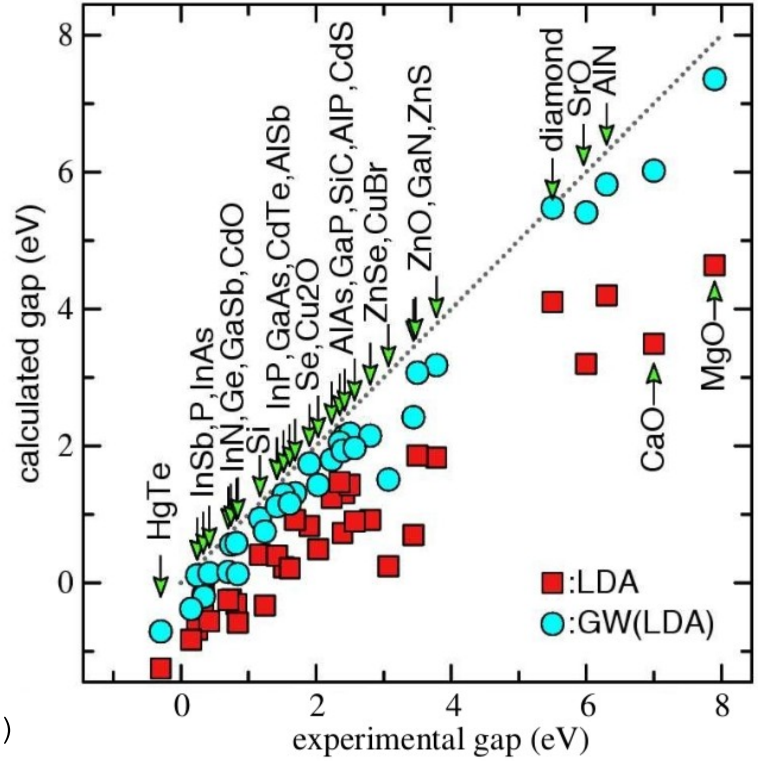
- Kohn-Sham equation

$$\left\{-\frac{1}{2}\nabla^2 + v_{\mathrm{ne}}(\mathbf{r}) + v_{\mathrm{H}}(\mathbf{r}) + v_{\mathrm{xc}}(\mathbf{r})\right\}\psi_i^{KS}(\mathbf{r}) = \epsilon_i^{KS}\psi_i^{KS}(\mathbf{r})$$

- Quasi-particle equation

$$\left\{-\frac{1}{2}\nabla^2 + v_{\mathrm{ne}}(\mathbf{r}) + v_{\mathrm{H}}(\mathbf{r})\right\}\psi_i^{QP}(\mathbf{r}) +$$

$$\int d\mathbf{r}'\Sigma\left(\mathbf{r},\mathbf{r}',\epsilon_i^{QP}\right)\psi_i^{QP}(\mathbf{r}') = \epsilon_i^{QP}\psi_i^{QP}(\mathbf{r})$$




Schilfgaarde et al. PRL 96 226402(2006)

# Introduction

- Kohn-Sham equation

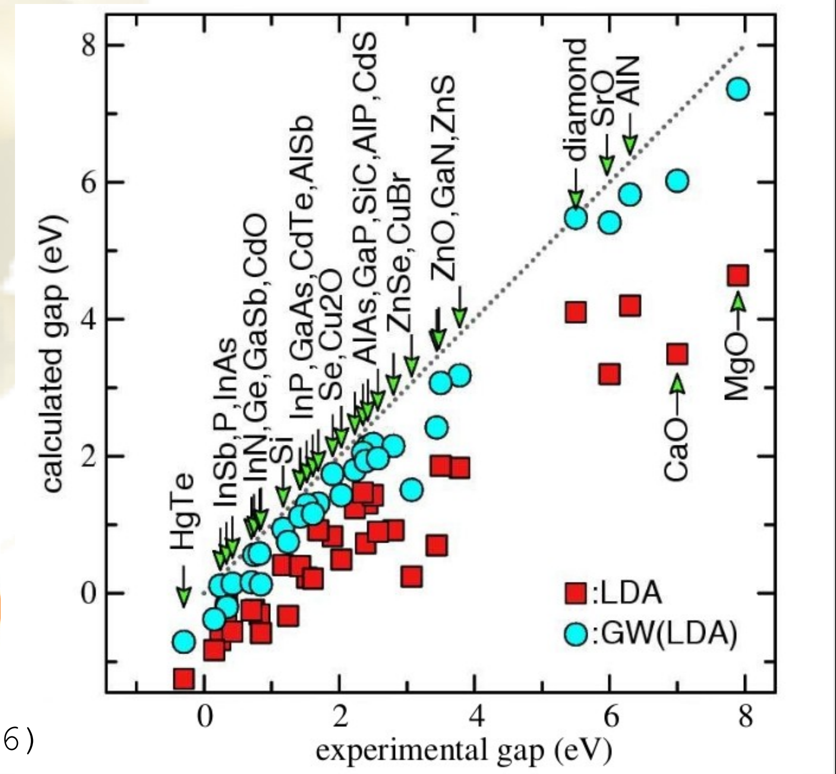
$$\left\{-\frac{1}{2}\nabla^2 + v_{\text{ne}}(\mathbf{r}) + v_{\text{H}}(\mathbf{r}) + v_{\text{xc}}(\mathbf{r})\right\}\psi_i^{KS}(\mathbf{r}) = \epsilon_i^{KS}\psi_i^{KS}(\mathbf{r})$$

- Quasi-particle equation

$$\left\{-\frac{1}{2}\nabla^2 + v_{\text{ne}}(\mathbf{r}) + v_{\text{H}}(\mathbf{r})\right\}\psi_i^{QP}(\mathbf{r}) +$$

$$\int d\mathbf{r}'\,\Sigma\left(\mathbf{r},\mathbf{r}',\epsilon_i^{QP}\right)\psi_i^{QP}(\mathbf{r}') = \epsilon_i^{QP}\psi_i^{QP}(\mathbf{r})$$

- How to calculate the **self-energy**?




Schilfgaarde et al. PRL 96 226402(2006)

# Introduction

- Kohn-Sham equation

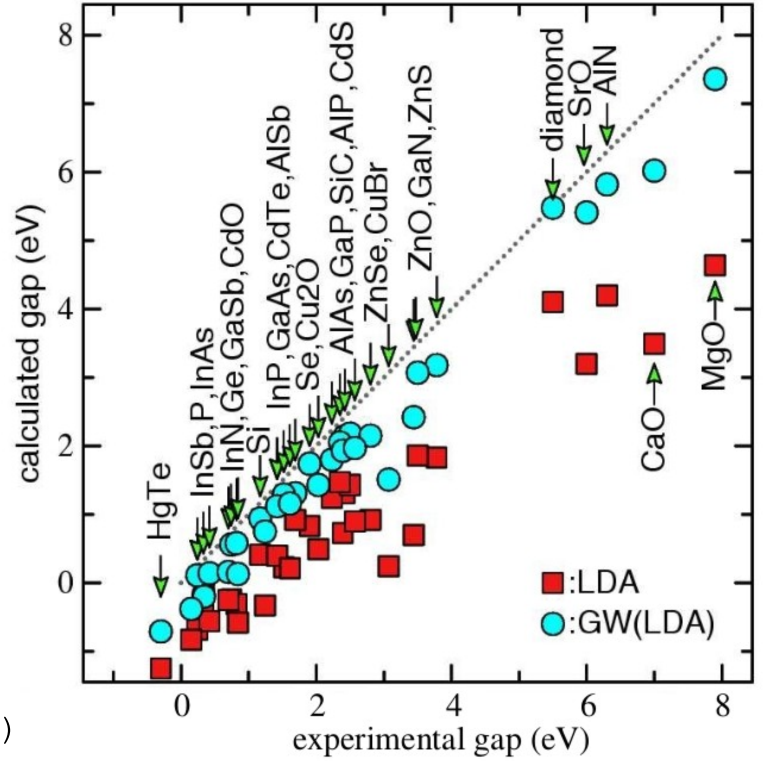
$$\left\{-\frac{1}{2}\nabla^2 + v_{\mathrm{ne}}(\mathbf{r}) + v_{\mathrm{H}}(\mathbf{r}) + v_{\mathrm{xc}}(\mathbf{r})\right\}\psi_i^{KS}(\mathbf{r}) = \epsilon_i^{KS}\psi_i^{KS}(\mathbf{r})$$

- Quasi-particle equation

$$\left\{-\frac{1}{2}\nabla^2 + v_{\mathrm{ne}}(\mathbf{r}) + v_{\mathrm{H}}(\mathbf{r})\right\}\psi_i^{QP}(\mathbf{r}) +$$

$$\int d\mathbf{r}'\Sigma\left(\mathbf{r},\mathbf{r}',\epsilon_i^{QP}\right)\psi_i^{QP}(\mathbf{r}') = \epsilon_i^{QP}\psi_i^{QP}(\mathbf{r})$$

- How to calculate the **self-energy**?
- Hedin's equations $\Sigma = GW$




Schilfgaarde et al. PRL 96 226402(2006)

# GW approximation

- Self-energy

$$\Sigma\left(\mathbf{r},\mathbf{r}',\omega\right)=\frac{i}{2\pi}\int G\left(\mathbf{r},\mathbf{r}',\omega-\omega'\right)W\left(\mathbf{r},\mathbf{r}',\omega'\right)e^{-i\delta\omega'}d\omega'$$

# GW approximation

- Self-energy

$$\Sigma\left(\mathbf{r},\mathbf{r}',\omega\right) = \frac{i}{2\pi}\int G\left(\mathbf{r},\mathbf{r}',\omega-\omega'\right) W\left(\mathbf{r},\mathbf{r}',\omega'\right) e^{-i\delta\omega'}\,d\omega'$$

- Screened Coulomb interaction

$$W\left(\mathbf{r},\mathbf{r}',\omega\right) = \int \epsilon^{-1}\left(\mathbf{r},\mathbf{r}'',\omega\right) v\left(\mathbf{r}'',\mathbf{r}'\right) d\mathbf{r}''$$

# GW approximation

- Self-energy

$$\Sigma(\mathbf{r},\mathbf{r}',\omega) = \frac{i}{2\pi}\int G(\mathbf{r},\mathbf{r}',\omega-\omega')\,W(\mathbf{r},\mathbf{r}',\omega')\,e^{-i\delta\omega'}\,d\omega'$$

- Screened Coulomb interaction

$$W(\mathbf{r},\mathbf{r}',\omega) = \int \epsilon^{-1}(\mathbf{r},\mathbf{r}'',\omega)\,v(\mathbf{r}'',\mathbf{r}')\,d\mathbf{r}''$$

- Dielectric function

$$\epsilon(\mathbf{r},\mathbf{r}',\omega) = \delta(\mathbf{r}-\mathbf{r}') - \int v(\mathbf{r},\mathbf{r}'')\,P(\mathbf{r}'',\mathbf{r}',\omega)\,d\mathbf{r}''$$

# GW approximation

- Self-energy

$$\Sigma(\mathbf{r},\mathbf{r}',\omega) = \frac{i}{2\pi}\int G(\mathbf{r},\mathbf{r}',\omega-\omega')\,W(\mathbf{r},\mathbf{r}',\omega')\,e^{-i\delta\omega'}\,d\omega'$$

- Screened Coulomb interaction

$$W(\mathbf{r},\mathbf{r}',\omega) = \int \epsilon^{-1}(\mathbf{r},\mathbf{r}'',\omega)\,v(\mathbf{r}'',\mathbf{r}')\,d\mathbf{r}''$$

- Dielectric function

$$\epsilon(\mathbf{r},\mathbf{r}',\omega) = \delta(\mathbf{r}-\mathbf{r}') - \int v(\mathbf{r},\mathbf{r}'')\,P(\mathbf{r}'',\mathbf{r}',\omega)\,d\mathbf{r}''$$

- Polarizability function

$$P(\mathbf{r},\mathbf{r}',\omega) = -\frac{i}{2\pi}\int G(\mathbf{r}',\mathbf{r},\omega-\omega')\,G(\mathbf{r},\mathbf{r}',\omega')\,e^{-i\delta\omega'}\,d\omega'$$

# GW approximation

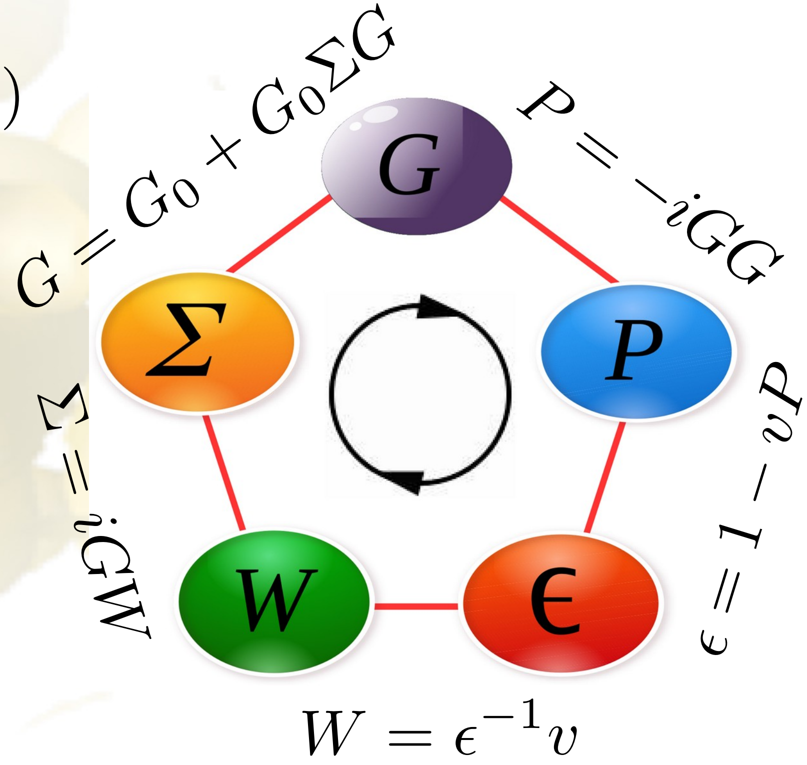
- Green's function (updated)

$$G^{-1}\left(\mathbf{r},\mathbf{r}',\omega\right) = G_0^{-1}\left(\mathbf{r},\mathbf{r}',\omega\right) - \Sigma\left(\mathbf{r},\mathbf{r}',\omega\right)$$

# GW approximation

- Green's function (updated)

$$G^{-1}(\mathbf{r},\mathbf{r}',\omega) = G_0^{-1}(\mathbf{r},\mathbf{r}',\omega) - \Sigma(\mathbf{r},\mathbf{r}',\omega)$$



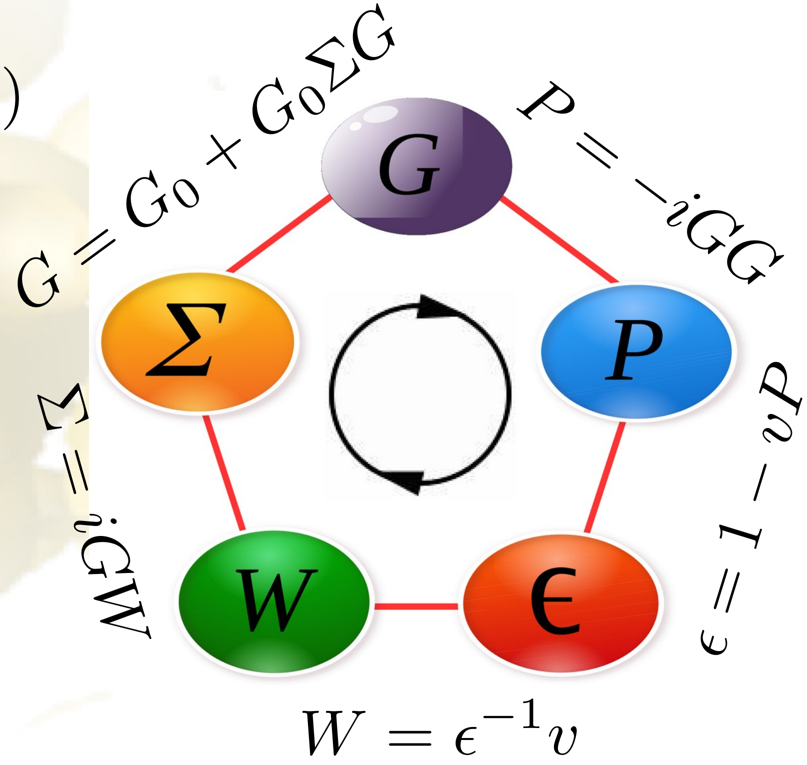
# GW approximation

- Green's function (updated)

$$G^{-1}(\mathbf{r},\mathbf{r}',\omega) = G_0^{-1}(\mathbf{r},\mathbf{r}',\omega) - \Sigma(\mathbf{r},\mathbf{r}',\omega)$$

- Quasi-particle energies

$$\epsilon_{n\mathbf{k}}^{QP} = \epsilon_{n\mathbf{k}}^{KS} + \langle \psi_{n\mathbf{k}}^{KS} \mid \Sigma - V_{xc}^{KS} \mid \psi_{n\mathbf{k}}^{KS} \rangle$$



# GW approximation

- Green's function (updated)

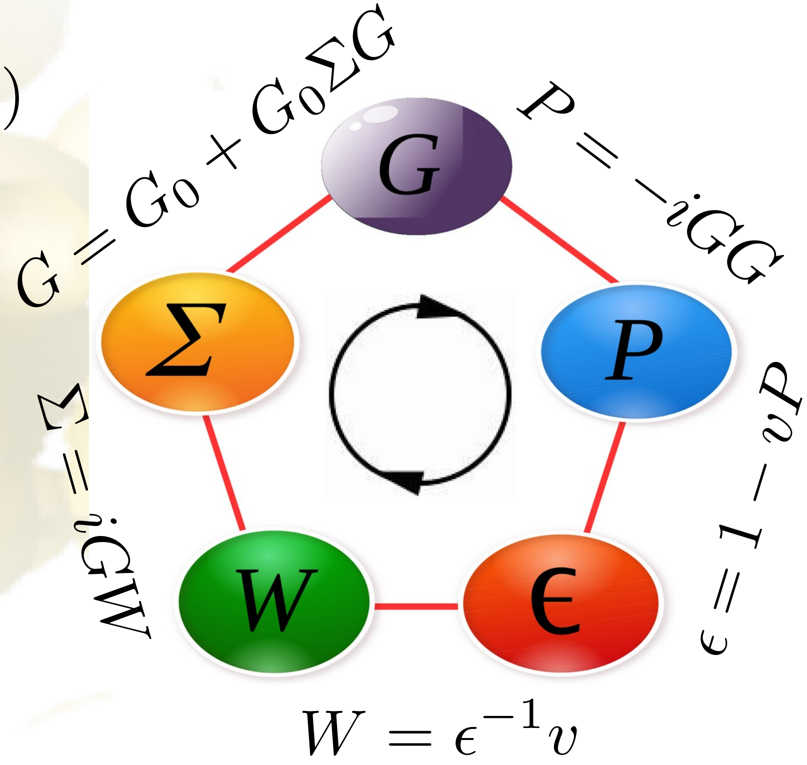
$$G^{-1}(\mathbf{r},\mathbf{r}',\omega) = G_0^{-1}(\mathbf{r},\mathbf{r}',\omega) - \Sigma(\mathbf{r},\mathbf{r}',\omega)$$

- Quasi-particle energies

$$\epsilon_{n\mathbf{k}}^{QP} = \epsilon_{n\mathbf{k}}^{KS} + \langle \psi_{n\mathbf{k}}^{KS} \mid \Sigma - V_{xc}^{KS} \mid \psi_{n\mathbf{k}}^{KS} \rangle$$

- Green's function from KS states

$$G_0(\mathbf{r},\mathbf{r}',\omega) = \sum_{n\mathbf{k}} \frac{\psi_{n\mathbf{k}}^{KS}(\mathbf{r})\psi_{n\mathbf{k}}^{KS^*}(\mathbf{r}')}{\omega - \epsilon_{n\mathbf{k}}^{KS} \pm i\eta}$$



# GW approximation

- Green's function (updated)

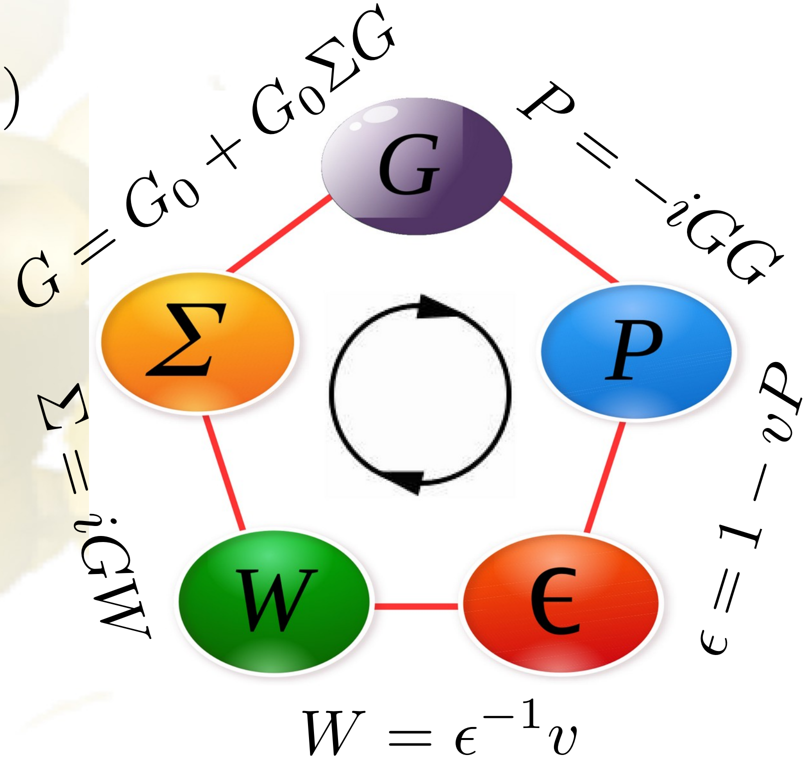
$$G^{-1}(\mathbf{r},\mathbf{r}',\omega) = G_0^{-1}(\mathbf{r},\mathbf{r}',\omega) - \Sigma(\mathbf{r},\mathbf{r}',\omega)$$

- Quasi-particle energies

$$\epsilon_{n\mathbf{k}}^{QP} = \epsilon_{n\mathbf{k}}^{KS} + \langle\psi_{n\mathbf{k}}^{KS} \mid \Sigma - V_{xc}^{KS} \mid \psi_{n\mathbf{k}}^{KS}\rangle$$

- Green's function from KS states

$$G_0(\mathbf{r},\mathbf{r}',\omega) = \sum_{n\mathbf{k}} \frac{\psi_{n\mathbf{k}}^{KS}(\mathbf{r})\psi_{n\mathbf{k}}^{KS^*}(\mathbf{r}')}{\omega - \epsilon_{n\mathbf{k}}^{KS} \pm i\eta}$$




exciting


L. Hedin, Phys. Rev. 139, A796 (1965)
L. Hedin and B. I. Lundqvist, Solid State Phys. 23, 1 (1969)
M. Hybertsen and S. Louie, PRB 34, 5390 (1986)

# Implementation in `exciting`

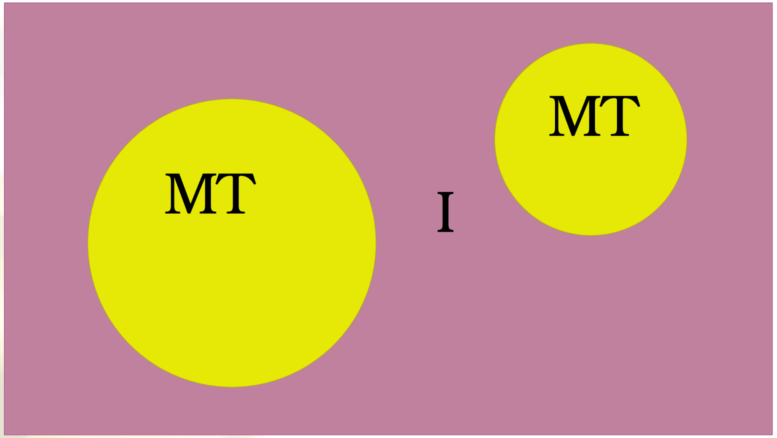
# Implementation in `exciting`

# Implementation in `exciting`

exciting

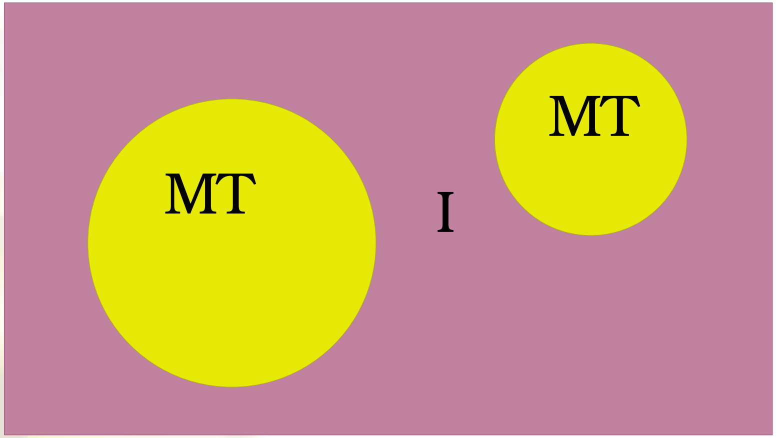
- All electron DFT code
- Employs LAPW and LO
- Treats core electron with radial Dirac eq.
- DFT, TDDFT (RTD), GW, BSE ...

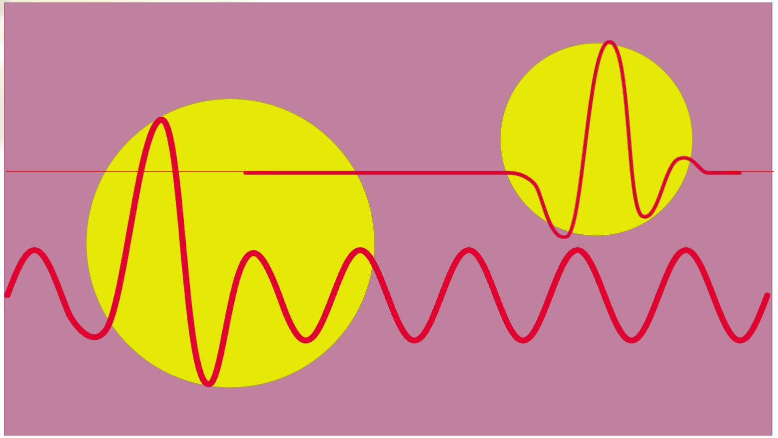
# Implementation in `exciting`




- All electron DFT code
- Employs LAPW and LO
- Treats core electron with radial Dirac eq.
- DFT, TDDFT (RTD), GW, BSE ...

# Implementation in `exciting`



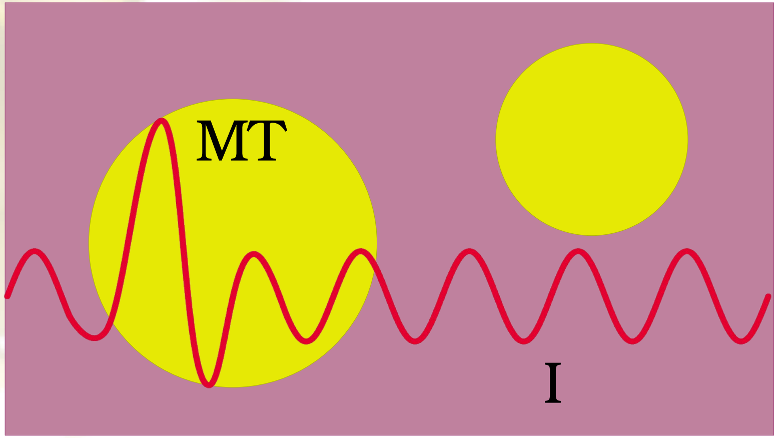
- All electron DFT code
- Employs LAPW and LO
- Treats core electron with radial Dirac eq.
- DFT, TDDFT (RTD), GW, BSE ...

https://exciting-code.org/

# Implementation in `exciting`

- Linearized augmented plane wave (LAPW) basis

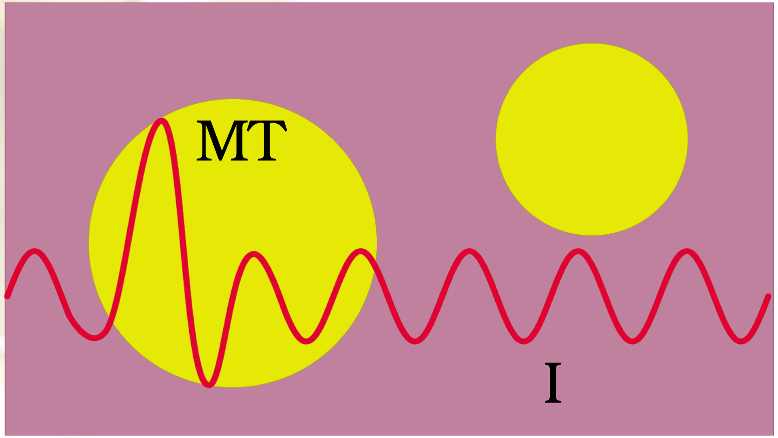
$$\phi_{\mathbf{G}}^{\mathbf{k}}(\mathbf{r}) = \begin{cases} \sum_{lm} \left[A_{\alpha lm}(\mathbf{k}+\mathbf{G}) u_{\alpha l}\left(r^\alpha, E_l\right) + \ldots\right] Y_{lm}\left(\hat{\mathbf{r}}^\alpha\right) & r^\alpha < R_{\mathrm{MT}}^\alpha \\ \frac{1}{\sqrt{\Omega}} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} & \mathbf{r} \in I \end{cases}$$



# Implementation in `exciting`

- Linearized augmented plane wave (LAPW) basis

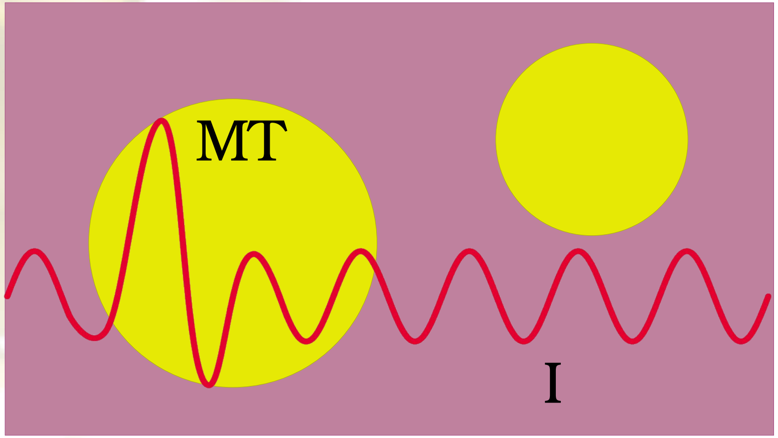
$$\phi_{\mathbf{G}}^{\mathbf{k}}(\mathbf{r}) = \begin{cases} \sum_{lm} \left[A_{\alpha lm}(\mathbf{k}+\mathbf{G}) u_{\alpha l}\left(r^{\alpha}, E_l\right) + \ldots\right] Y_{lm}\left(\hat{\mathbf{r}}^{\alpha}\right) & r^{\alpha} < R_{\mathrm{MT}}^{\alpha} \\ \frac{1}{\sqrt{\Omega}} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} & \mathbf{r} \in I \end{cases}$$



# Implementation in `exciting`

- Linearized augmented plane wave (LAPW) basis

$$\phi_{\mathbf{G}}^{\mathbf{k}}(\mathbf{r}) = \begin{cases} \sum_{lm} \left[ A_{\alpha lm}(\mathbf{k}+\mathbf{G}) u_{\alpha l}(r^{\alpha}, E_l) + \ldots \right] Y_{lm}(\hat{\mathbf{r}}^{\alpha}) & r^{\alpha} < R_{\mathrm{MT}}^{\alpha} \\ \frac{1}{\sqrt{\Omega}} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} & \mathbf{r} \in I \end{cases}$$



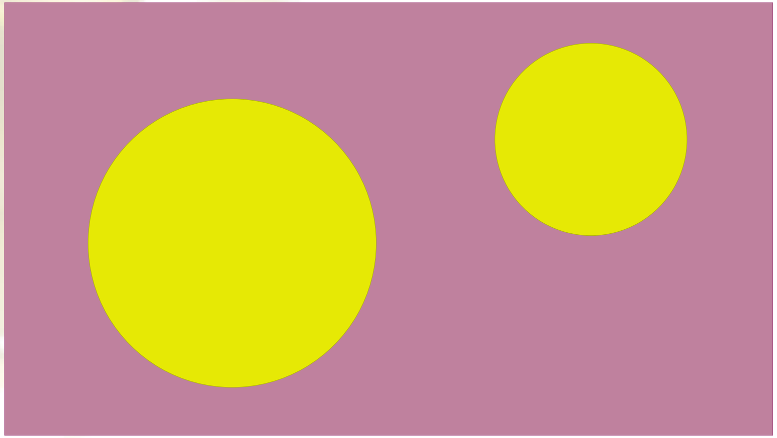
# Implementation in `exciting`

- Linearized augmented plane wave (LAPW) basis

$$\phi_{\mathbf{G}}^{\mathbf{k}}(\mathbf{r}) = \begin{cases} \sum_{lm} \left[ A_{\alpha lm}(\mathbf{k}+\mathbf{G}) u_{\alpha l}\left(r^{\alpha}, E_l\right) + \ldots \right] Y_{lm}\left(\hat{\mathbf{r}}^{\alpha}\right) & r^{\alpha} < R_{\mathrm{MT}}^{\alpha} \\ \frac{1}{\sqrt{\Omega}} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} & \mathbf{r} \in I \end{cases}$$

- Kohn-Sham wave function

$$\psi_{n\mathbf{k}}^{KS}(\mathbf{r}) = \sum_{\mathbf{G}} C_{n\mathbf{k},\mathbf{G}} \phi_{\mathbf{G}}^{\mathbf{k}}(\mathbf{r})$$



A. Gulans et al. J. Phys. Cond. Mat. 26(36), 363202 (2014)

# Implementation in `exciting`

- Mixed basis in MT region
  - We only consider $u_{\alpha l}(r^{\alpha})$ with $l \leq l_{max}^{MB}$

# Implementation in `exciting`

- Mixed basis in MT region
  - We only consider $u_{\alpha l}(r^{\alpha})$ with $l \leq l_{max}^{MB}$ `lmaxmb`

# Implementation in `exciting`

- Mixed basis in MT region
  - We only consider $u_{\alpha l}(r^\alpha)$ with $l \leq l_{max}^{MB}$ **`lmaxmb`**
  - We take $u_{\alpha l}(r^\alpha)u_{\alpha l'}(r^\alpha) = v_{\alpha NL}(r^\alpha)$ with $|l - l'| \leq L \leq |l + l'|$

# Implementation in `exciting`

- Mixed basis in MT region
  - We only consider $u_{\alpha l}(r^{\alpha})$ with $l \leq l_{max}^{MB}$ **`lmaxmb`**
  - We take $u_{\alpha l}(r^{\alpha})u_{\alpha l'}(r^{\alpha}) = v_{\alpha NL}(r^{\alpha})$ with $|l - l'| \leq L \leq |l + l'|$
  - Overlap matrix, diagonalize and eliminate linearly dependent ones

# Implementation in `exciting`

- Mixed basis in MT region
  - We only consider $u_{\alpha l}(r^{\alpha})$ with $l \leq l_{max}^{MB}$ **`lmaxmb`**
  - We take $u_{\alpha l}(r^{\alpha})u_{\alpha l'}(r^{\alpha}) = v_{\alpha NL}(r^{\alpha})$ with $|l - l'| \leq L \leq |l + l'|$
  - Overlap matrix, diagonalize and eliminate linearly dependent ones **`epsmb`**

# Implementation in `exciting`

- Mixed basis in MT region
  - We only consider $u_{\alpha l}(r^\alpha)$ with $l \leq l_{max}^{MB}$ **`lmaxmb`**
  - We take $u_{\alpha l}(r^\alpha) u_{\alpha l'}(r^\alpha) = v_{\alpha NL}(r^\alpha)$ with $|l - l'| \leq L \leq |l + l'|$
  - Overlap matrix, diagonalize and eliminate linearly dependent ones **`epsmb`**
  - Product basis with translational symmetry

$$\gamma_{\alpha NLM}^{\mathbf{q}}(\mathbf{r}) = \frac{1}{\sqrt{N_c}} \sum_{\mathbf{R}} e^{i\mathbf{q}\cdot(\mathbf{r}_\alpha + \mathbf{R})} v_{\alpha NL}(r^\alpha) Y_{LM}(\hat{\mathbf{r}}^\alpha)$$


F. Aryasetiawan and O. Gunnarsson, Phys. Rev. B 49, 16214 (1994)
T. Kotani and M. van Schilfgaarde, Solid State Comm. 121, 461 (2002)

# Implementation in `exciting`

- Mixed basis in Interstitial region
  - Overlap matrix

$$\mathbb{O}_{\mathbf{G}\mathbf{G}'} = \frac{1}{\Omega}\int_{\Omega} \theta_I(\mathbf{r}) e^{i(\mathbf{G}-\mathbf{G}')\cdot\mathbf{r}} d^3r$$

# Implementation in `exciting`

- Mixed basis in Interstitial region
  - Overlap matrix
    $$\mathbb{O}_{\mathbf{G}\mathbf{G}'} = \frac{1}{\Omega}\int_{\Omega} \theta_I(\mathbf{r}) e^{i(\mathbf{G}-\mathbf{G}')\cdot\mathbf{r}} d^3r$$
  - Diagonalize the overlap matrix
    $$\sum_{\mathbf{G}'} \mathbb{O}_{\mathbf{G}\mathbf{G}'} S_{\mathbf{G}'i} = \lambda_i S_{\mathbf{G}i}$$

# Implementation in `exciting`

- Mixed basis in Interstitial region
  - Overlap matrix

$$\mathbb{O}_{\mathbf{G}\mathbf{G}'} = \frac{1}{\Omega}\int_{\Omega} \theta_I(\mathbf{r}) e^{i(\mathbf{G}-\mathbf{G}')\cdot\mathbf{r}} d^3r$$

  - Diagonalize the overlap matrix

$$\sum_{\mathbf{G}'} \mathbb{O}_{\mathbf{G}\mathbf{G}'} S_{\mathbf{G}'i} = \lambda_i S_{\mathbf{G}i}$$

  - Orthonormal basis set

$$P_i^{\mathbf{q}}(\mathbf{r}) \equiv \frac{1}{\sqrt{\Omega}} \sum_{\mathbf{G}}^{G_{max}^{MB}} \tilde{S}_{\mathbf{G}i} e^{i(\mathbf{G}+\mathbf{q})\cdot\mathbf{r}} \theta_I(\mathbf{r})$$

# Implementation in `exciting`

- Mixed basis in Interstitial region
  - Overlap matrix

$$\mathbb{O}_{\mathbf{G}\mathbf{G}'} = \frac{1}{\Omega}\int_{\Omega} \theta_I(\mathbf{r}) e^{i(\mathbf{G}-\mathbf{G}')\cdot\mathbf{r}} d^3r$$

  - Diagonalize the overlap matrix

$$\sum_{\mathbf{G}'} \mathbb{O}_{\mathbf{G}\mathbf{G}'} S_{\mathbf{G}'i} = \lambda_i S_{\mathbf{G}i}$$

  - Orthonormal basis set

$G_{max}^{MB}$ gmb

$$P_i^{\mathbf{q}}(\mathbf{r}) \equiv \frac{1}{\sqrt{\Omega}} \sum_{\mathbf{G}}^{G_{max}^{MB}} \tilde{S}_{\mathbf{G}i} e^{i(\mathbf{G}+\mathbf{q})\cdot\mathbf{r}} \theta_I(\mathbf{r})$$

# Implementation in `exciting`

- Orthonormal mixed basis set

$$\{\chi_j^{\mathbf{q}}(\mathbf{r})\} \equiv \{\gamma_{\alpha NLM}^{\mathbf{q}}(\mathbf{r}), P_i^{\mathbf{q}}(\mathbf{r})\}$$

# Implementation in `exciting`

- Orthonormal mixed basis set

$$\{\chi_j^{\mathbf{q}}(\mathbf{r})\} \equiv \{\gamma_{\alpha NLM}^{\mathbf{q}}(\mathbf{r}), P_i^{\mathbf{q}}(\mathbf{r})\}$$

- Polarizability

$$P_0(\mathbf{r},\mathbf{r}',\omega) = \sum_{n,m}\sum_{\mathbf{k},\mathbf{q}} F_{nm}(\mathbf{k},\mathbf{q};\omega)\psi_{n\mathbf{k}}(\mathbf{r})\psi^*_{m\mathbf{k}-\mathbf{q}}(\mathbf{r})\psi^*_{n\mathbf{k}}(\mathbf{r}')\,\psi_{m\mathbf{k}-\mathbf{q}}(\mathbf{r}')$$

# Implementation in `exciting`

- Orthonormal mixed basis set

$$\{\chi_j^{\mathbf{q}}(\mathbf{r})\} = \{\gamma_{\alpha NLM}^{\mathbf{q}}(\mathbf{r}), P_i^{\mathbf{q}}(\mathbf{r})\}$$

- Polarizability

$$P_0(\mathbf{r},\mathbf{r}',\omega) = \sum_{n,m}\sum_{\mathbf{k},\mathbf{q}} F_{nm}(\mathbf{k},\mathbf{q};\omega)\psi_{n\mathbf{k}}(\mathbf{r})\psi^*_{m\mathbf{k}-\mathbf{q}}(\mathbf{r})\psi^*_{n\mathbf{k}}(\mathbf{r}')\psi_{m\mathbf{k}-\mathbf{q}}(\mathbf{r}')$$

# Implementation in `exciting`

- Orthonormal mixed basis set

$$\{\chi_j^{\mathbf{q}}(\mathbf{r})\} \equiv \{\gamma_{\alpha NLM}^{\mathbf{q}}(\mathbf{r}), P_i^{\mathbf{q}}(\mathbf{r})\}$$

- Polarizability

$$P_0(\mathbf{r},\mathbf{r}',\omega) = \sum_{n,m}\sum_{\mathbf{k},\mathbf{q}} F_{nm}(\mathbf{k},\mathbf{q};\omega)\psi_{n\mathbf{k}}(\mathbf{r})\psi^*_{m\mathbf{k}-\mathbf{q}}(\mathbf{r})\psi^*_{n\mathbf{k}}(\mathbf{r}')\psi_{m\mathbf{k}-\mathbf{q}}(\mathbf{r}')$$

$$\psi_{n\mathbf{k}}(\mathbf{r})\psi^*_{m\mathbf{k}-\mathbf{q}}(\mathbf{r}) = \sum_i M^i_{nm}(\mathbf{k},\mathbf{q})\chi_i^{\mathbf{q}}(\mathbf{r})$$

# Implementation in exciting

- Orthonormal mixed basis set

$$\{\chi_j^{\mathbf{q}}(\mathbf{r})\} = \{\gamma_{\alpha NLM}^{\mathbf{q}}(\mathbf{r}), P_i^{\mathbf{q}}(\mathbf{r})\}$$

- Polarizability

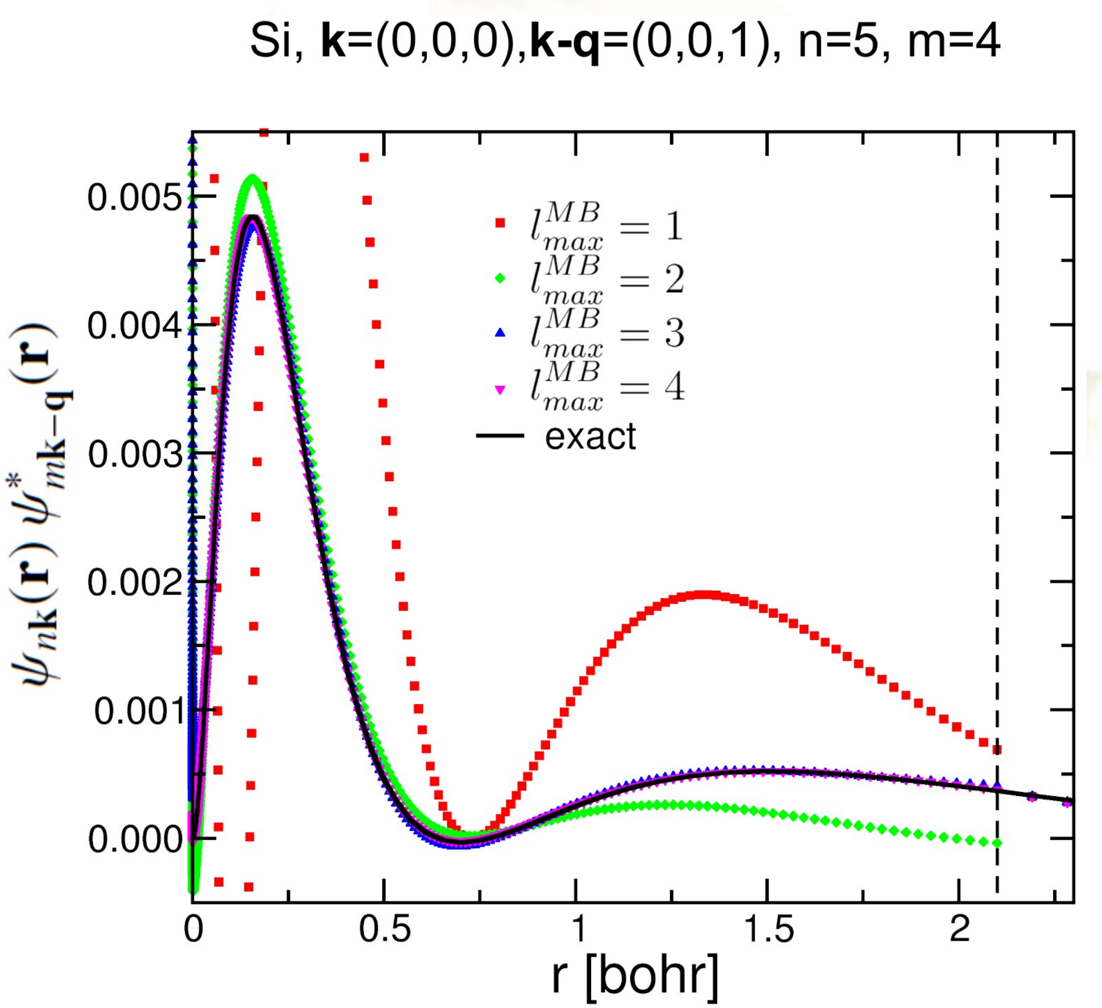
$$P_0(\mathbf{r},\mathbf{r}',\omega) = \sum_{n,m}\sum_{\mathbf{k},\mathbf{q}} F_{nm}(\mathbf{k},\mathbf{q};\omega)\psi_{n\mathbf{k}}(\mathbf{r})\psi^*_{m\mathbf{k}-\mathbf{q}}(\mathbf{r})\psi^*_{n\mathbf{k}}(\mathbf{r}')\psi_{m\mathbf{k}-\mathbf{q}}(\mathbf{r}')$$

$$\psi_{n\mathbf{k}}(\mathbf{r})\psi^*_{m\mathbf{k}-\mathbf{q}}(\mathbf{r}) = \sum_i M^i_{nm}(\mathbf{k},\mathbf{q})\chi_i^{\mathbf{q}}(\mathbf{r})$$

$$M^i_{nm}(\mathbf{k},\mathbf{q}) \equiv \int_\Omega [\chi_i^{\mathbf{q}}(\mathbf{r})\psi_{m\mathbf{k}-\mathbf{q}}(\mathbf{r})]^*\,\psi_{n\mathbf{k}}(\mathbf{r})dr$$

# Implementation in `exciting`

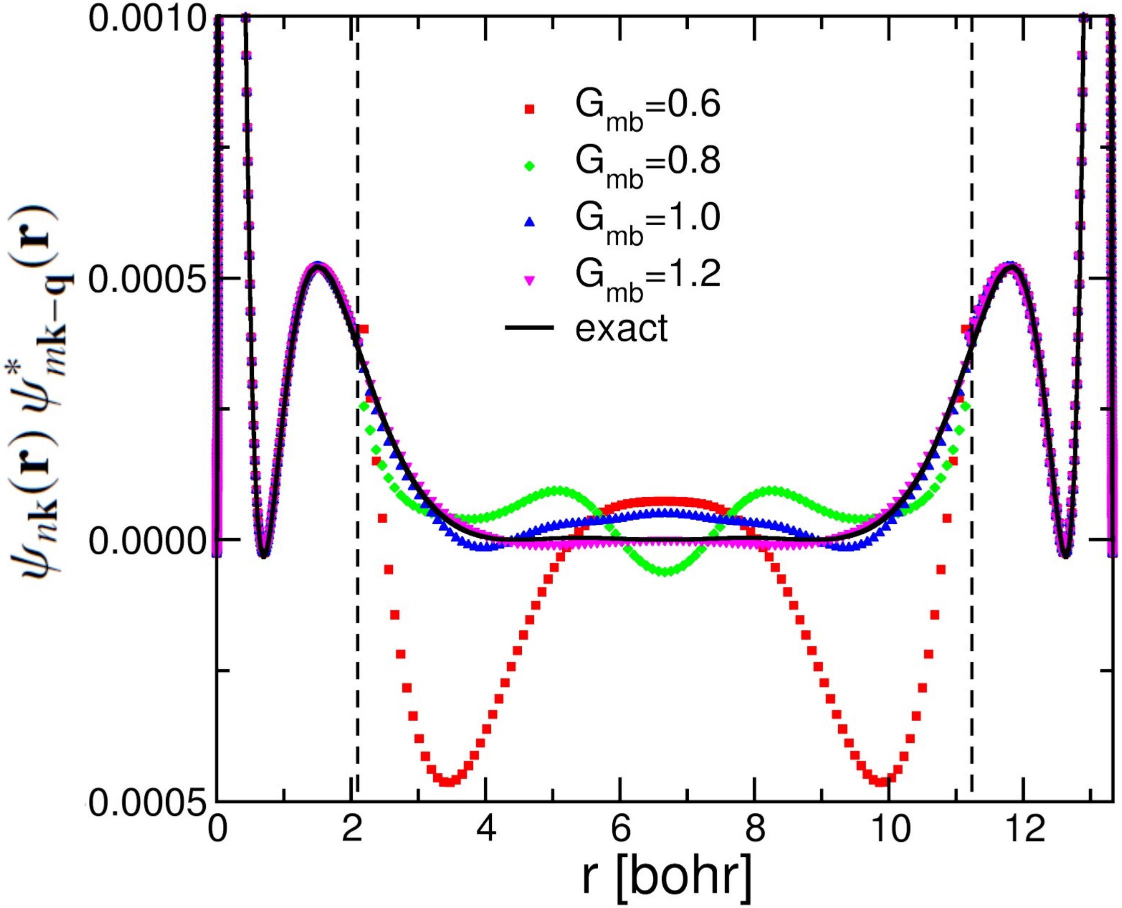
`lmaxmb`



# Implementation in `exciting`

gmb

Si, **k**=(0,0,0),**k-q**=(0,0,1), n=5, m=4



# Implementation in `exciting`

- Self-energy can be split into two parts

$$\Sigma\left(\mathbf{r},\mathbf{r}',\omega\right)=\Sigma^{x}\left(\mathbf{r},\mathbf{r}'\right)+\Sigma^{c}\left(\mathbf{r},\mathbf{r}',\omega\right)$$

# Implementation in `exciting`

- Self-energy can be split into two parts

$$\Sigma\left(\mathbf{r},\mathbf{r}',\omega\right)=\Sigma^{x}\left(\mathbf{r},\mathbf{r}'\right)+\Sigma^{c}\left(\mathbf{r},\mathbf{r}',\omega\right)$$

- Exchange part of the self-energy

$$\Sigma^{x}_{n\mathbf{k}}=-\frac{1}{N_c}\sum_{\mathbf{q}}^{BZ}\sum_{i,j}v_{ij}(\mathbf{q})\sum_{m}^{occ}\left[M^{i}_{nm}(\mathbf{k},\mathbf{q})\right]^{*}M^{j}_{nm}(\mathbf{k},\mathbf{q})$$

# Implementation in `exciting`

- Self-energy can be split into two parts

$$\Sigma\left(\mathbf{r},\mathbf{r}',\omega\right)=\Sigma^{x}\left(\mathbf{r},\mathbf{r}'\right)+\Sigma^{c}\left(\mathbf{r},\mathbf{r}',\omega\right)$$

- Exchange part of the self-energy

$$\Sigma^{x}_{n\mathbf{k}}=-\frac{1}{N_c}\sum_{\mathbf{q}}^{BZ}\sum_{i,j}v_{ij}(\mathbf{q})\sum_{m}^{occ}\left[M^{i}_{nm}(\mathbf{k},\mathbf{q})\right]^{*}M^{j}_{nm}(\mathbf{k},\mathbf{q})$$

- Coulomb potential in the product basis

$$v_{ij}(\mathbf{q})=\int_{\Omega}\int_{\Omega}[\chi^{\mathbf{q}}_{i}(\mathbf{r})]^{*}\,v(\mathbf{r},\mathbf{r}')\chi^{\mathbf{q}}_{j}(\mathbf{r}')d\mathbf{r}d\mathbf{r}'$$

# Implementation in `exciting`

- Polarizability in mixed basis

$$P_{ij}(\mathbf{q},\omega) = \frac{1}{N_c} \sum_{\mathbf{k}}^{BZ} \sum_{n}^{occ} \sum_{m}^{empty} F_{nm}(\mathbf{k},\mathbf{q};\omega) M^{i}_{nm}(\mathbf{k},\mathbf{q}) \left[ M^{j}_{nm}(\mathbf{k},\mathbf{q}) \right]^*$$

# Implementation in `exciting`

- Polarizability in mixed basis

$$P_{ij}(\mathbf{q},\omega) = \frac{1}{N_c}\sum_{\mathbf{k}}^{BZ}\sum_{n}^{occ}\sum_{m}^{empty} F_{nm}(\mathbf{k},\mathbf{q};\omega)M^{i}_{nm}(\mathbf{k},\mathbf{q})\left[M^{j}_{nm}(\mathbf{k},\mathbf{q})\right]^*$$

`ngridq`

# Implementation in `exciting`

- Polarizability in mixed basis

$$P_{ij}(\mathbf{q},\omega) = \frac{1}{N_c}\sum_{\mathbf{k}}^{BZ}\sum_{n}^{occ}\sum_{m}^{empty} F_{nm}(\mathbf{k},\mathbf{q};\omega) M^{i}_{nm}(\mathbf{k},\mathbf{q}) \left[M^{j}_{nm}(\mathbf{k},\mathbf{q})\right]^{*}$$

`nempty`

# Implementation in `exciting`

- Polarizability in mixed basis

$$P_{ij}(\mathbf{q},\omega) = \frac{1}{N_c}\sum_{\mathbf{k}}^{BZ}\sum_{n}^{occ}\sum_{m}^{empty} F_{nm}(\mathbf{k},\mathbf{q};\omega)M^{i}_{nm}(\mathbf{k},\mathbf{q})\left[M^{j}_{nm}(\mathbf{k},\mathbf{q})\right]^{*}$$

`nomeg`

# Implementation in `exciting`

- Polarizability in mixed basis

$$P_{ij}(\mathbf{q},\omega) = \frac{1}{N_c}\sum_{\mathbf{k}}^{BZ}\sum_{n}^{occ}\sum_{m}^{empty} F_{nm}(\mathbf{k},\mathbf{q};\omega) M^{i}_{nm}(\mathbf{k},\mathbf{q}) \left[M^{j}_{nm}(\mathbf{k},\mathbf{q})\right]^{*}$$

`ngridq`

`nempty`

`nomeg`

- Dielectric function

$$\epsilon_{ij}\left(\mathbf{q},\omega\right) = \delta_{ij} - \sum_{i'j'} v^{\frac{1}{2}}_{ii'}\left(\mathbf{q}\right) P_{i'j'}\left(\mathbf{q},\omega\right) v^{\frac{1}{2}}_{j'j}\left(\mathbf{q}\right)$$

- Correlation part of the screened Coulomb interaction

$$W^{c}_{ij}\left(\mathbf{q},\omega\right) = \sum_{i'j'} v^{\frac{1}{2}}_{ii'}\left(\mathbf{q}\right)\left[\epsilon^{-1}_{i'j'}\left(\mathbf{q},\omega\right) - \delta_{i'j'}\right] v^{\frac{1}{2}}_{j'j}\left(\mathbf{q}\right)$$

# Implementation in `exciting`

- Correlation part of the self-energy

$$\Sigma^c_{n\mathbf{k}}(\omega) = \sum_{\mathbf{q}}^{BZ} \sum_{m}^{occ+empty} \int d\omega' \frac{\sum_{ij} \left[M^i_{nm}(\mathbf{k},\mathbf{q})\right]^* W^c_{ij}(\mathbf{q},\omega') M^j_{nm}(\mathbf{k},\mathbf{q})}{\omega + \omega' - \tilde{\epsilon}_{m\mathbf{k}-\mathbf{q}}}$$

# Implementation in `exciting`

- Correlation part of the self-energy

$$\Sigma^c_{n\mathbf{k}}(\omega) = \sum_{\mathbf{q}}^{BZ} \sum_{m}^{occ+empty} \int d\omega' \frac{\sum_{ij} \left[M^i_{nm}(\mathbf{k},\mathbf{q})\right]^* W^c_{ij}(\mathbf{q},\omega') M^j_{nm}(\mathbf{k},\mathbf{q})}{\omega + \omega' - \tilde{\epsilon}_{m\mathbf{k}-\mathbf{q}}}$$

`ngridq`

`nempty`

`nomeg`

# Implementation in `exciting`

- Correlation part of the self-energy

$$\Sigma^c_{n\mathbf{k}}(\omega) = \sum_{\mathbf{q}}^{BZ} \sum_{m}^{occ+empty} \int d\omega' \frac{\sum_{ij} \left[M^i_{nm}(\mathbf{k},\mathbf{q})\right]^* W^c_{ij}(\mathbf{q},\omega') M^j_{nm}(\mathbf{k},\mathbf{q})}{\omega + \omega' - \tilde{\epsilon}_{m\mathbf{k}-\mathbf{q}}}$$

`ngridq`

`nempty`

`nomeg`

# Implementation in `exciting`

- Correlation part of the self-energy

$$\Sigma^c_{n\mathbf{k}}(\omega) = \sum_{\mathbf{q}}^{BZ} \sum_{m}^{occ+empty} \int d\omega' \frac{\sum_{ij} \left[M^i_{nm}(\mathbf{k},\mathbf{q})\right]^* W^c_{ij}(\mathbf{q},\omega') M^j_{nm}(\mathbf{k},\mathbf{q})}{\omega + \omega' - \tilde{\epsilon}_{m\mathbf{k}-\mathbf{q}}}$$

- Perform in imaginary frequency

$$\Sigma^c_{n\mathbf{k}}(iu) = \sum_{\mathbf{q}}^{BZ} \sum_{m}^{occ+empty} \int du' X_{nm}(\mathbf{k},\mathbf{q};\omega') \frac{2(\tilde{\epsilon}_{m\mathbf{k}-\mathbf{q}} - iu)}{u'^2 + (\tilde{\epsilon}_{m\mathbf{k}-\mathbf{q}} - iu)}$$

`ngridq`

`nempty`

`nomeg`

# Implementation in `exciting`

- Correlation part of the self-energy

$$\Sigma^c_{n\mathbf{k}}(\omega) = \sum_{\mathbf{q}}^{BZ} \sum_{m}^{occ+empty} \int d\omega' \frac{\sum_{ij} \left[M^i_{nm}(\mathbf{k},\mathbf{q})\right]^* W^c_{ij}(\mathbf{q},\omega') M^j_{nm}(\mathbf{k},\mathbf{q})}{\omega + \omega' - \tilde{\epsilon}_{m\mathbf{k}-\mathbf{q}}}$$

`ngridq`

- Perform in imaginary frequency

$$\Sigma^c_{n\mathbf{k}}(iu) = \sum_{\mathbf{q}}^{BZ} \sum_{m}^{occ+empty} \int du' X_{nm}(\mathbf{k},\mathbf{q};\omega') \frac{2(\tilde{\epsilon}_{m\mathbf{k}-\mathbf{q}} - iu)}{u'^2 + (\tilde{\epsilon}_{m\mathbf{k}-\mathbf{q}} - iu)}$$

`nempty`

`nomeg`

Analytic continuation onto real frequency

# Implementation in `exciting`

- Correlation part of the self-energy

$$\Sigma^c_{n\mathbf{k}}(\omega) = \sum_{\mathbf{q}}^{BZ} \sum_{m}^{occ+empty} \int d\omega' \frac{\sum_{ij} \left[M^i_{nm}(\mathbf{k},\mathbf{q})\right]^* W^c_{ij}(\mathbf{q},\omega') M^j_{nm}(\mathbf{k},\mathbf{q})}{\omega + \omega' - \tilde{\epsilon}_{m\mathbf{k}-\mathbf{q}}}$$

`ngridq`

- Perform in imaginary frequency

`nempty`

$$\Sigma^c_{n\mathbf{k}}(iu) = \sum_{\mathbf{q}}^{BZ} \sum_{m}^{occ+empty} \int du' X_{nm}(\mathbf{k},\mathbf{q};\omega') \frac{2(\tilde{\epsilon}_{m\mathbf{k}-\mathbf{q}} - iu)}{u'^2 + (\tilde{\epsilon}_{m\mathbf{k}-\mathbf{q}} - iu)}$$

`nomeg`

Analytic continuation onto real frequency

- Quasi-particle energies

$$\epsilon^{QP}_{n\mathbf{k}} = \epsilon^{KS}_{n\mathbf{k}} + Z_{n\mathbf{k}} \left[\mathcal{R}\Sigma^c_{n\mathbf{k}}(\epsilon^{KS}_{n\mathbf{k}}) + \Sigma^x_{n\mathbf{k}} - V^{KS}_{xc}\right]$$

H. Jiang et al., Comput. Phys. Commun. 184, 348 (2013)

# exciting Usage

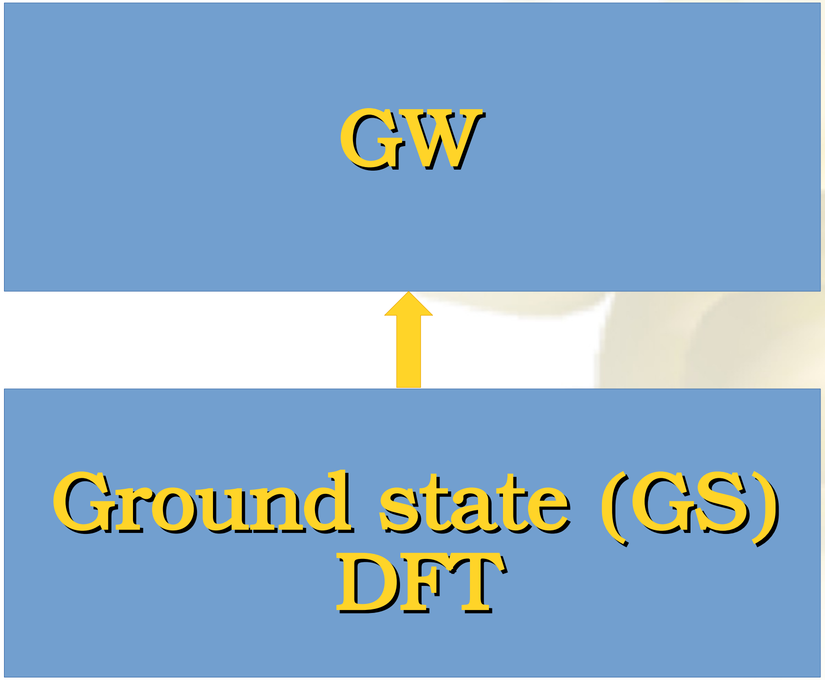
Ground state (GS)
DFT

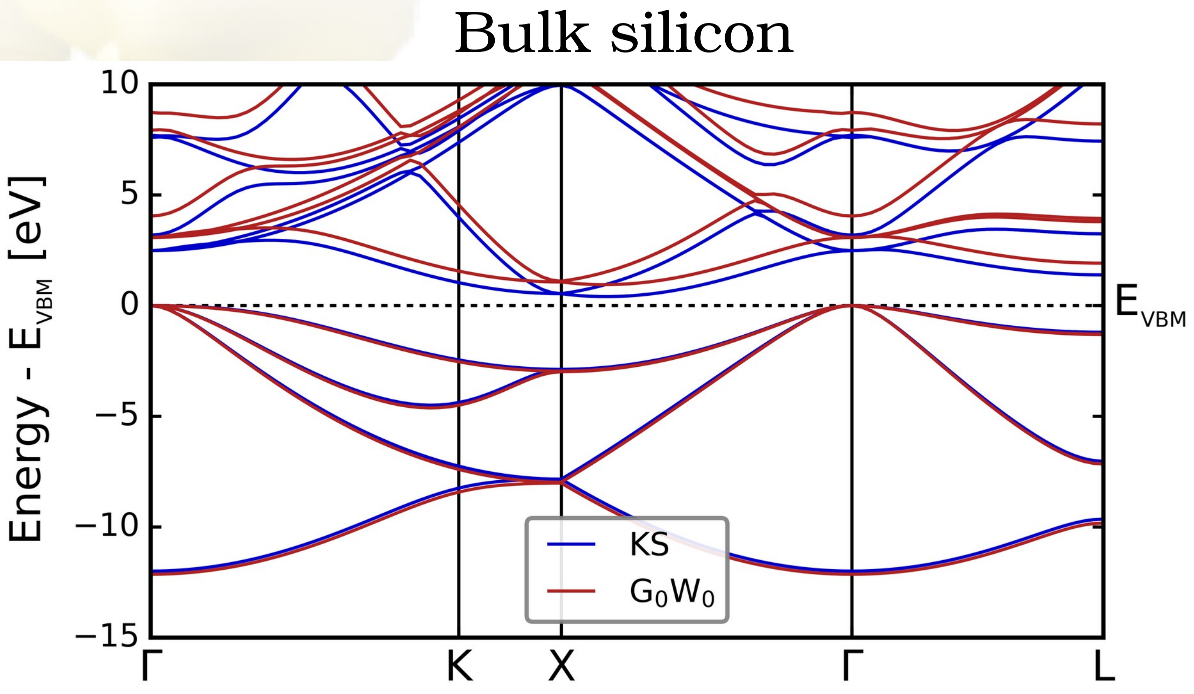
# exciting Usage

GW

Ground state (GS)
DFT

# exciting Usage



# **exciting** Usage

- GS input file

# exciting Usage

- GS input file

```
<input>

   <title>Silicon-GW</title>

   <structure
      speciespath="/users/sol/manoarphy/neon/species">
      <crystal>
         <basevect>5.13 5.13 0.00</basevect>
         <basevect>5.13 0.00 5.13</basevect>
         <basevect>0.00 5.13 5.13</basevect>
      </crystal>
      <species speciesfile="Si.xml" rmt="2.1">
         <atom coord="0.00 0.00 0.00"></atom>
         <atom coord="0.25 0.25 0.25"></atom>
      </species>
   </structure>

   <groundstate
      do="fromscratch"
      rgkmax="7.0"
      ngridk="3 3 3"
      xctype="LDA_PW"
   ></groundstate>

</input>
```

# exciting Usage

- GS input file

```
<input>

   <title>Silicon-GW</title>

   <structure
      speciespath="/users/sol/manoarphy/neon/species">
      <crystal>
         <basevect>5.13 5.13 0.00</basevect>
         <basevect>5.13 0.00 5.13</basevect>
         <basevect>0.00 5.13 5.13</basevect>
      </crystal>
      <species speciesfile="Si.xml" rmt="2.1">
         <atom coord="0.00 0.00 0.00"></atom>
         <atom coord="0.25 0.25 0.25"></atom>
      </species>
   </structure>

   <groundstate
      do="fromscratch"
      rgkmax="7.0"
      ngridk="3 3 3"
      xctype="LDA_PW"
   ></groundstate>

</input>
```

# exciting Usage

- GS input file

```
<input>

   <title>Silicon-GW</title>

   <structure
      speciespath="/users/sol/manoarphy/neon/species">
      <crystal>
         <basevect>5.13 5.13 0.00</basevect>
         <basevect>5.13 0.00 5.13</basevect>
         <basevect>0.00 5.13 5.13</basevect>
      </crystal>
      <species speciesfile="Si.xml" rmt="2.1">
         <atom coord="0.00 0.00 0.00"></atom>
         <atom coord="0.25 0.25 0.25"></atom>
      </species>
   </structure>

   <groundstate
      do="fromscratch"
      rgkmax="7.0"
      ngridk="3 3 3"
      xctype="LDA_PW"
   ></groundstate>

</input>
```

# exciting Usage

- GS input file

```
<input>

   <title>Silicon-GW</title>

   <structure
      speciespath="/users/sol/manoarphy/neon/species">
      <crystal>
         <basevect>5.13 5.13 0.00</basevect>
         <basevect>5.13 0.00 5.13</basevect>
         <basevect>0.00 5.13 5.13</basevect>
      </crystal>
      <species speciesfile="Si.xml" rmt="2.1">
         <atom coord="0.00 0.00 0.00"></atom>
         <atom coord="0.25 0.25 0.25"></atom>
      </species>
   </structure>

   <groundstate
      do="fromscratch"
      rgkmax="7.0"
      ngridk="3 3 3"
      xctype="LDA_PW"
   ></groundstate>

</input>
```

# exciting Usage

- GS input file

```
<input>

   <title>Silicon-GW</title>

   <structure
      speciespath="/users/sol/manoarphy/neon/species">
      <crystal>
         <basevect>5.13 5.13 0.00</basevect>
         <basevect>5.13 0.00 5.13</basevect>
         <basevect>0.00 5.13 5.13</basevect>
      </crystal>
      <species speciesfile="Si.xml" rmt="2.1">
         <atom coord="0.00 0.00 0.00"></atom>
         <atom coord="0.25 0.25 0.25"></atom>
      </species>
   </structure>

   <groundstate
      do="fromscratch"
      rgkmax="7.0"
      ngridk="3 3 3"
      xctype="LDA_PW"
   ></groundstate>

</input>
```

# exciting Usage

- GS input file

```
<input>

   <title>Silicon-GW</title>

   <structure
      speciespath="/users/sol/manoarphy/neon/species">
      <crystal>
         <basevect>5.13 5.13 0.00</basevect>
         <basevect>5.13 0.00 5.13</basevect>
         <basevect>0.00 5.13 5.13</basevect>
      </crystal>
      <species speciesfile="Si.xml" rmt="2.1">
         <atom coord="0.00 0.00 0.00"></atom>
         <atom coord="0.25 0.25 0.25"></atom>
      </species>
   </structure>

   <groundstate
      do="fromscratch"
      rgkmax="7.0"
      ngridk="3 3 3"
      xctype="LDA_PW"
   ></groundstate>

</input>
```

# exciting Usage

- GS input file

```
<input>

   <title>Silicon-GW</title>

   <structure
      speciespath="/users/sol/manoarphy/neon/species">
      <crystal>
         <basevect>5.13 5.13 0.00</basevect>
         <basevect>5.13 0.00 5.13</basevect>
         <basevect>0.00 5.13 5.13</basevect>
      </crystal>
      <species speciesfile="Si.xml" rmt="2.1">
         <atom coord="0.00 0.00 0.00"></atom>
         <atom coord="0.25 0.25 0.25"></atom>
      </species>
   </structure>

   <groundstate
      do="fromscratch"
      rgkmax="7.0"
      ngridk="3 3 3"
      xctype="LDA_PW"
   ></groundstate>

</input>
```

# exciting Usage

- GS input file

```
<input>

  <title>Silicon-GW</title>

  <structure
     speciespath="/users/sol/manoarphy/neon/species">
     <crystal>
        <basevect>5.13 5.13 0.00</basevect>
        <basevect>5.13 0.00 5.13</basevect>
        <basevect>0.00 5.13 5.13</basevect>
     </crystal>
     <species speciesfile="Si.xml" rmt="2.1">
        <atom coord="0.00 0.00 0.00"></atom>
        <atom coord="0.25 0.25 0.25"></atom>
     </species>
  </structure>

  <groundstate
     do="fromscratch"
     rgkmax="7.0"
     ngridk="3 3 3"
     xctype="LDA_PW"
  ></groundstate>

</input>
```

# exciting Usage

- GS input file

```
<input>

   <title>Silicon-GW</title>

   <structure
      speciespath="/users/sol/manoarphy/neon/species">
      <crystal>
         <basevect>5.13 5.13 0.00</basevect>
         <basevect>5.13 0.00 5.13</basevect>
         <basevect>0.00 5.13 5.13</basevect>
      </crystal>
      <species speciesfile="Si.xml" rmt="2.1">
         <atom coord="0.00 0.00 0.00"></atom>
         <atom coord="0.25 0.25 0.25"></atom>
      </species>
   </structure>

   <groundstate
      do="fromscratch"
      rgkmax="7.0"
      ngridk="3 3 3"
      xctype="LDA_PW"
   ></groundstate>

</input>
```

# exciting Usage

- GW input file

# exciting Usage

- GW input file

```
<input>
  ...
  <groundstate
     do="skip"
     ...

</input>
```

# exciting Usage

- GW input file

```
<input>
   ...
   <groundstate
     do="skip"
     ...

</input>
```

# exciting Usage

- GW input file

```
<input>
   ...
   <groundstate
      do="skip"
      ...
   ><gw
      taskname="g0w0"
      ngridq="3 3 3"
      nempty="22"
      ibgw="1"
      nbgw="10"
      coreflag="xal"
      ><mixbasis
         lmaxmb="3"
         epsmb="1.d-4"
         gmb="1.0"
      ></mixbasis>
      <freqgrid
         nomeg="12"
      ></freqgrid>
   </gw>

</input>
```

# exciting Usage

- GW input file

```
<input>
   ...
   <groundstate
     do="skip"
     ...
   ><gw
     taskname="g0w0"
     ngridq="3 3 3"
     nempty="22"
     ibgw="1"
     nbgw="10"
     coreflag="xal"
     ><mixbasis
        lmaxmb="3"
        epsmb="1.d-4"
        gmb="1.0"
     ></mixbasis>
     <freqgrid
        nomeg="12"
     ></freqgrid>
   </gw>

</input>
```

taskname="band"

taskname="dos"

# `exciting` Usage

- GW input file

$$\Sigma^c_{n\mathbf{k}}(\omega) = \sum_{\mathbf{q}}^{BZ} \sum_{m}^{occ+empty} \cdots$$

```
<input>
   ...
   <groundstate
     do="skip"
     ...
  ><gw
     taskname="g0w0"
     ngridq="3 3 3"
     nempty="22"
     ibgw="1"
     nbgw="10"
     coreflag="xal"
     ><mixbasis
        lmaxmb="3"
        epsmb="1.d-4"
        gmb="1.0"
     ></mixbasis>
     <freqgrid
        nomeg="12"
     ></freqgrid>
  </gw>

</input>
```

# exciting Usage

- GW input file

$$\Sigma^c_{n\mathbf{k}}(\omega) = \sum_{\mathbf{q}}^{BZ} \sum_{m}^{occ+empty} \cdots$$

```
<input>
   ...
   <groundstate
      do="skip"
      ...
   ><gw
      taskname="g0w0"
      ngridq="3 3 3"
      nempty="22"
      ibgw="1"
      nbgw="10"
      coreflag="xal"
      ><mixbasis
         lmaxmb="3"
         epsmb="1.d-4"
         gmb="1.0"
      ></mixbasis>
      <freqgrid
         nomeg="12"
      ></freqgrid>
   </gw>

</input>
```

# exciting Usage

- GW input file

$$\Sigma^c_{n\mathbf{k}}(\omega) = \sum_{\mathbf{q}}^{BZ} \sum_{m}^{occ+empty} \cdots$$

```
<input>
   ...
   <groundstate
      do="skip"
      ...
   ><gw
      taskname="g0w0"
      ngridq="3 3 3"
      nempty="22"
      ibgw="1"
      nbgw="10"
      coreflag="xal"
      ><mixbasis
         lmaxmb="3"
         epsmb="1.d-4"
         gmb="1.0"
      ></mixbasis>
      <freqgrid
         nomeg="12"
      ></freqgrid>
   </gw>

</input>
```

# exciting Usage

- GW input file

$$\Sigma^c_{n\mathbf{k}}(\omega) = \sum_{\mathbf{q}}^{BZ} \sum_{m}^{occ+empty} \cdots$$

```
<input>
   ...
   <groundstate
     do="skip"
     ...
   ><gw
     taskname="g0w0"
     ngridq="3 3 3"
     nempty="22"
     ibgw="1"
     nbgw="10"
     coreflag="xal"
     ><mixbasis
       lmaxmb="3"
       epsmb="1.d-4"
       gmb="1.0"
     ></mixbasis>
     <freqgrid
       nomeg="12"
     ></freqgrid>
   </gw>

</input>
```

# `exciting` Usage

- GW input file

$$\Sigma^c_{n\mathbf{k}}(\omega) = \sum_{\mathbf{q}}^{BZ} \sum_{m}^{occ+empty} \cdots$$

```
<input>
   ...
   <groundstate
     do="skip"
     ...
   ><gw
      taskname="g0w0"
      ngridq="3 3 3"
      nempty="22"
      ibgw="1"
      nbgw="10"
      coreflag="xal"
      ><mixbasis
         lmaxmb="3"
         epsmb="1.d-4"
         gmb="1.0"
      ></mixbasis>
      <freqgrid
         nomeg="12"
      ></freqgrid>
   </gw>

</input>
```

# exciting Usage

```
.
..
atoms.xml
BANDLINES.OUT
BAND.OUT
BAND-QP.OUT
bandstructure.dat
bandstructure-qp.dat
bandstructure-qp.xml
bandstructure.xml
BONDLENGTH.OUT
dos.xml
EFERMI_GW.OUT
EFERMI.OUT
EIGVAL.OUT
eigval.xml
EPS00_GW.OUT
EQATOMS.OUT
EVALCORE.OUT
evalcore.xml
EVALFV_GW.OUT
EVALFV.OUT
EVALQP.DAT
EVALQP.OUT
EVALSV_GW.OUT
EVALSV.OUT
EVECFV_GW.OUT
EVECFV.OUT
EVECSV_GW.OUT
EVECSV.OUT
geometry.xml
GW_INFO.OUT
INFO.OUT
info.xml
input.xml
KPOINTS.OUT
LATTICE.OUT
LINENGY.OUT
OCCSV.OUT
PLOT.eps
PMATVV.OUT
RMSDVEFF.OUT
SELFC.OUT
SELFX.OUT
si-gw-dos-KS.GW.png
si-gw-ef.png
si-gw-vbm.png
Si_ini.xml
Si_scf.xml
STATE.OUT
SYMCRYS.OUT
SYMGENR.OUT
SYMINV.OUT
SYMLAT.OUT
SYMMULT.OUT
SYMSITE.OUT
SYMT2.OUT
TDOS.OUT
TDOS-QP.OUT
TOTENERGY.OUT
VXCNN.DAT
VXCNN.OUT
```

# exciting Usage

```
.                        EPS00_GW.OUT    INFO.OUT                 Si_scf.xml
..                       EQATOMS.OUT     info.xml                 STATE.OUT
atoms.xml                EVALCORE.OUT    input.xml                SYMCRYS.OUT
BANDLINES.OUT            evalcore.xml    KPOINTS.OUT              SYMGENR.OUT
BAND.OUT                 EVALFV_GW.OUT   LATTICE.OUT              SYMINV.OUT
BAND-QP.OUT              EVALFV.OUT      LINENGY.OUT              SYMLAT.OUT
bandstructure.dat        EVALQP.DAT      OCCSV.OUT                SYMMULT.OUT
bandstructure-qp.dat     EVALQP.OUT      PLOT.eps                 SYMSITE.OUT
bandstructure-qp.xml     EVALSV_GW.OUT   PMATVV.OUT               SYMT2.OUT
bandstructure.xml        EVALSV.OUT      RMSDVEFF.OUT             TDOS.OUT
BONDLENGTH.OUT           EVECFV_GW.OUT   SELFC.OUT                TDOS-QP.OUT
dos.xml                  EVECFV.OUT      SELFX.OUT                TOTENERGY.OUT
EFERMI_GW.OUT            EVECSV_GW.OUT   si-gw-dos-KS.GW.png      VXCNN.DAT
EFERMI.OUT               EVECSV.OUT      si-gw-ef.png             VXCNN.OUT
EIGVAL.OUT               geometry.xml    si-gw-vbm.png
eigval.xml               GW_INFO.OUT     Si_ini.xml
```

# exciting Usage

```
.                           EPS00_GW.OUT     INFO.OUT                  Si_scf.xml
..                          EQATOMS.OUT      info.xml                  STATE.OUT
atoms.xml                   EVALCORE.OUT     input.xml                 SYMCRYS.OUT
BANDLINES.OUT               evalcore.xml     KPOINTS.OUT               SYMGENR.OUT
BAND.OUT                    EVALFV_GW.OUT    LATTICE.OUT               SYMINV.OUT
BAND-QP.OUT                 EVALFV.OUT       LINENGY.OUT               SYMLAT.OUT
bandstructure.dat           EVALQP.DAT       OCCSV.OUT                 SYMMULT.OUT
bandstructure-qp.dat        EVALQP.OUT       PLOT.eps                  SYMSITE.OUT
bandstructure-qp.xml        EVALSV_GW.OUT    PMATVV.OUT                SYMT2.OUT
bandstructure.xml           EVALSV.OUT       RMSDVEFF.OUT              TDOS.OUT
BONDLENGTH.OUT              EVECFV_GW.OUT    SELFC.OUT                 TDOS-QP.OUT
dos.xml                     EVECFV.OUT       SELFX.OUT                 TOTENERGY.OUT
EFERMI_GW.OUT               EVECSV_GW.OUT    si-gw-dos-KS.GW.png       VXCNN.DAT
EFERMI.OUT                  EVECSV.OUT       si-gw-ef.png              VXCNN.OUT
EIGVAL.OUT                  geometry.xml     si-gw-vbm.png
eigval.xml                  GW_INFO.OUT      Si_ini.xml
```

# exciting Usage

k-point # 1: 0.000000 0.000000 0.000000 0.037037

| state | E_KS | E_HF | E_GW | Sx | Re(Sc) | Im(Sc) | Vxc | DE_HF | DE_GW | Znk |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | -0.45134 | -0.69966 | -0.44986 | -0.70105 | 0.25056 | 0.03612 | -0.45273 | -0.24832 | 0.00149 | 0.66555 |
| 2 | -0.01047 | -0.07414 | -0.00378 | -0.56215 | 0.07225 | 0.00015 | -0.49848 | -0.06367 | 0.00670 | 0.78017 |
| 3 | -0.01047 | -0.07414 | -0.00389 | -0.56215 | 0.07211 | 0.00013 | -0.49848 | -0.06367 | 0.00658 | 0.77903 |
| 4 | -0.01047 | -0.07414 | -0.00389 | -0.56215 | 0.07212 | 0.00014 | -0.49848 | -0.06367 | 0.00659 | 0.77917 |
| 5 | 0.08067 | 0.26157 | 0.10936 | -0.25087 | -0.14402 | -0.00125 | -0.43177 | 0.18090 | 0.02869 | 0.77794 |
| 6 | 0.08067 | 0.26157 | 0.10933 | -0.25087 | -0.14409 | -0.00127 | -0.43177 | 0.18090 | 0.02865 | 0.77846 |
| 7 | 0.08067 | 0.26157 | 0.10942 | -0.25087 | -0.14399 | -0.00120 | -0.43177 | 0.18090 | 0.02875 | 0.77888 |
| 8 | 0.10651 | 0.32083 | 0.14503 | -0.34472 | -0.16419 | -0.00147 | -0.55904 | 0.21432 | 0.03852 | 0.76837 |
| 9 | 0.26869 | 0.47704 | 0.28745 | -0.13571 | -0.18444 | -0.00703 | -0.34406 | 0.20835 | 0.01875 | 0.78431 |
| 10 | 0.27253 | 0.49322 | 0.31704 | -0.16678 | -0.16550 | -0.00209 | -0.38748 | 0.22069 | 0.04451 | 0.80646 |

k-point # 2: 0.000000 0.000000 0.333333 0.296296

| state | E_KS | E_HF | E_GW | Sx | Re(Sc) | Im(Sc) | Vxc | DE_HF | DE_GW | Znk |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | -0.40055 | -0.62733 | -0.40035 | -0.69022 | 0.22708 | 0.02707 | -0.46344 | -0.22678 | 0.00020 | 0.68318 |
| 2 | -0.20836 | -0.33803 | -0.20833 | -0.58997 | 0.12970 | 0.00745 | -0.46029 | -0.12968 | 0.00002 | 0.74643 |
| 3 | -0.04760 | -0.12044 | -0.04295 | -0.55914 | 0.07884 | 0.00053 | -0.48631 | -0.07284 | 0.00466 | 0.77473 |
| 4 | -0.04760 | -0.12044 | -0.04300 | -0.55914 | 0.07879 | 0.00050 | -0.48631 | -0.07284 | 0.00460 | 0.77383 |
| 5 | 0.04899 | 0.22993 | 0.07841 | -0.28110 | -0.14333 | -0.00053 | -0.46204 | 0.18094 | 0.02942 | 0.78220 |
| 6 | 0.11512 | 0.30416 | 0.14384 | -0.22532 | -0.15215 | -0.00174 | -0.41437 | 0.18905 | 0.02872 | 0.77830 |
| 7 | 0.11512 | 0.30416 | 0.14394 | -0.22532 | -0.15203 | -0.00165 | -0.41437 | 0.18905 | 0.02883 | 0.77885 |
| 8 | 0.26948 | 0.49261 | 0.29430 | -0.15957 | -0.19119 | -0.00829 | -0.38270 | 0.22314 | 0.02483 | 0.77719 |
| 9 | 0.28052 | 0.50287 | 0.31461 | -0.16878 | -0.17908 | -0.00819 | -0.39114 | 0.22236 | 0.03409 | 0.78765 |
| 10 | 0.28052 | 0.50287 | 0.31450 | -0.16878 | -0.17921 | -0.00835 | -0.39114 | 0.22236 | 0.03398 | 0.78768 |

# exciting Usage

```
k-point #     1:    0.000000    0.000000    0.000000    0.037037
 state    E_KS       E_HF       E_GW       Sx         Re(Sc)     Im(Sc)     Vxc        DE_HF      DE_GW      Znk
   1    -0.45134   -0.69966   -0.44986   -0.70105    0.25056    0.03612   -0.45273   -0.24832    0.00149    0.66555
   2    -0.01047   -0.07414   -0.00378   -0.56215    0.07225    0.00015   -0.49848   -0.06367    0.00670    0.78017
   3    -0.01047   -0.07414   -0.00389   -0.56215    0.07211    0.00013   -0.49848   -0.06367    0.00658    0.77903
   4    -0.01047   -0.07414   -0.00389   -0.56215    0.07212    0.00014   -0.49848   -0.06367    0.00659    0.77917
   5     0.08067    0.26157    0.10936   -0.25087   -0.14402   -0.00125   -0.43177    0.18090    0.02869    0.77794
   6     0.08067    0.26157    0.10933   -0.25087   -0.14409   -0.00127   -0.43177    0.18090    0.02865    0.77846
   7     0.08067    0.26157    0.10942   -0.25087   -0.14399   -0.00120   -0.43177    0.18090    0.02875    0.77888
   8     0.10651    0.32083    0.14503   -0.34472   -0.16419   -0.00147   -0.55904    0.21432    0.03852    0.76837
   9     0.26869    0.47704    0.28745   -0.13571   -0.18444   -0.00703   -0.34406    0.20835    0.01875    0.78431
  10     0.27253    0.49322    0.31704   -0.16678   -0.16550   -0.00209   -0.38748    0.22069    0.04451    0.80646

k-point #     2:    0.000000    0.000000    0.333333    0.296296
 state    E_KS       E_HF       E_GW       Sx         Re(Sc)     Im(Sc)     Vxc        DE_HF      DE_GW      Znk
   1    -0.40055   -0.62733   -0.40035   -0.69022    0.22708    0.02707   -0.46344   -0.22678    0.00020    0.68318
   2    -0.20836   -0.33803   -0.20833   -0.58997    0.12970    0.00745   -0.46029   -0.12968    0.00002    0.74643
   3    -0.04760   -0.12044   -0.04295   -0.55914    0.07884    0.00053   -0.48631   -0.07284    0.00466    0.77473
   4    -0.04760   -0.12044   -0.04300   -0.55914    0.07879    0.00050   -0.48631   -0.07284    0.00460    0.77383
   5     0.04899    0.22993    0.07841   -0.28110   -0.14333   -0.00053   -0.46204    0.18094    0.02942    0.78220
   6     0.11512    0.30416    0.14384   -0.22532   -0.15215   -0.00174   -0.41437    0.18905    0.02872    0.77830
   7     0.11512    0.30416    0.14394   -0.22532   -0.15203   -0.00165   -0.41437    0.18905    0.02883    0.77885
   8     0.26948    0.49261    0.29430   -0.15957   -0.19119   -0.00829   -0.38270    0.22314    0.02483    0.77719
   9     0.28052    0.50287    0.31461   -0.16878   -0.17908   -0.00819   -0.39114    0.22236    0.03409    0.78765
  10     0.28052    0.50287    0.31450   -0.16878   -0.17921   -0.00835   -0.39114    0.22236    0.03398    0.78768
```

# exciting Usage

k-point # 1: 0.000000 0.000000 0.000000 0.037037

| state | E_KS | E_HF | E_GW | Sx | Re(Sc) | Im(Sc) | Vxc | DE_HF | DE_GW | Znk |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | -0.45134 | -0.69966 | -0.44986 | -0.70105 | 0.25056 | 0.03612 | -0.45273 | -0.24832 | 0.00149 | 0.66555 |
| 2 | -0.01047 | -0.07414 | -0.00378 | -0.56215 | 0.07225 | 0.00015 | -0.49848 | -0.06367 | 0.00670 | 0.78017 |
| 3 | -0.01047 | -0.07414 | -0.00389 | -0.56215 | 0.07211 | 0.00013 | -0.49848 | -0.06367 | 0.00658 | 0.77903 |
| 4 | -0.01047 | -0.07414 | -0.00389 | -0.56215 | 0.07212 | 0.00014 | -0.49848 | -0.06367 | 0.00659 | 0.77917 |
| 5 | 0.08067 | 0.26157 | 0.10936 | -0.25087 | -0.14402 | -0.00125 | -0.43177 | 0.18090 | 0.02869 | 0.77794 |
| 6 | 0.08067 | 0.26157 | 0.10933 | -0.25087 | -0.14409 | -0.00127 | -0.43177 | 0.18090 | 0.02865 | 0.77846 |
| 7 | 0.08067 | 0.26157 | 0.10942 | -0.25087 | -0.14399 | -0.00120 | -0.43177 | 0.18090 | 0.02875 | 0.77888 |
| 8 | 0.10651 | 0.32083 | 0.14503 | -0.34472 | -0.16419 | -0.00147 | -0.55904 | 0.21432 | 0.03852 | 0.76837 |
| 9 | 0.26869 | 0.47704 | 0.28745 | -0.13571 | -0.18444 | -0.00703 | -0.34406 | 0.20835 | 0.01875 | 0.78431 |
| 10 | 0.27253 | 0.49322 | 0.31704 | -0.16678 | -0.16550 | -0.00209 | -0.38748 | 0.22069 | 0.04451 | 0.80646 |

k-point # 2: 0.000000 0.000000 0.333333 0.296296

| state | E_KS | E_HF | E_GW | Sx | Re(Sc) | Im(Sc) | Vxc | DE_HF | DE_GW | Znk |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | -0.40055 | -0.62733 | -0.40035 | -0.69022 | 0.22708 | 0.02707 | -0.46344 | -0.22678 | 0.00020 | 0.68318 |
| 2 | -0.20836 | -0.33803 | -0.20833 | -0.58997 | 0.12970 | 0.00745 | -0.46029 | -0.12968 | 0.00002 | 0.74643 |
| 3 | -0.04760 | -0.12044 | -0.04295 | -0.55914 | 0.07884 | 0.00053 | -0.48631 | -0.07284 | 0.00466 | 0.77473 |
| 4 | -0.04760 | -0.12044 | -0.04300 | -0.55914 | 0.07879 | 0.00050 | -0.48631 | -0.07284 | 0.00460 | 0.77383 |
| 5 | 0.04899 | 0.22993 | 0.07841 | -0.28110 | -0.14333 | -0.00053 | -0.46204 | 0.18094 | 0.02942 | 0.78220 |
| 6 | 0.11512 | 0.30416 | 0.14384 | -0.22532 | -0.15215 | -0.00174 | -0.41437 | 0.18905 | 0.02872 | 0.77830 |
| 7 | 0.11512 | 0.30416 | 0.14394 | -0.22532 | -0.15203 | -0.00165 | -0.41437 | 0.18905 | 0.02883 | 0.77885 |
| 8 | 0.26948 | 0.49261 | 0.29430 | -0.15957 | -0.19119 | -0.00829 | -0.38270 | 0.22314 | 0.02483 | 0.77719 |
| 9 | 0.28052 | 0.50287 | 0.31461 | -0.16878 | -0.17908 | -0.00819 | -0.39114 | 0.22236 | 0.03409 | 0.78765 |
| 10 | 0.28052 | 0.50287 | 0.31450 | -0.16878 | -0.17921 | -0.00835 | -0.39114 | 0.22236 | 0.03398 | 0.78768 |

# exciting Usage

k-point # 1: 0.000000 0.000000 0.000000 0.037037

| state | E_KS | E_HF | E_GW | Sx | Re(Sc) | Im(Sc) | Vxc | DE_HF | DE_GW | Znk |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | -0.45134 | -0.69966 | -0.44986 | -0.70105 | 0.25056 | 0.03612 | -0.45273 | -0.24832 | 0.00149 | 0.66555 |
| 2 | -0.01047 | -0.07414 | -0.00378 | -0.56215 | 0.07225 | 0.00015 | -0.49848 | -0.06367 | 0.00670 | 0.78017 |
| 3 | -0.01047 | -0.07414 | -0.00389 | -0.56215 | 0.07211 | 0.00013 | -0.49848 | -0.06367 | 0.00658 | 0.77903 |
| 4 | -0.01047 | -0.07414 | -0.00389 | -0.56215 | 0.07212 | 0.00014 | -0.49848 | -0.06367 | 0.00659 | 0.77917 |
| 5 | 0.08067 | 0.26157 | 0.10936 | -0.25087 | -0.14402 | -0.00125 | -0.43177 | 0.18090 | 0.02869 | 0.77794 |
| 6 | 0.08067 | 0.26157 | 0.10933 | -0.25087 | -0.14409 | -0.00127 | -0.43177 | 0.18090 | 0.02865 | 0.77846 |
| 7 | 0.08067 | 0.26157 | 0.10942 | -0.25087 | -0.14399 | -0.00120 | -0.43177 | 0.18090 | 0.02875 | 0.77888 |
| 8 | 0.10651 | 0.32083 | 0.14503 | -0.34472 | -0.16419 | -0.00147 | -0.55904 | 0.21432 | 0.03852 | 0.76837 |
| 9 | 0.26869 | 0.47704 | 0.28745 | -0.13571 | -0.18444 | -0.00703 | -0.34406 | 0.20835 | 0.01875 | 0.78431 |
| 10 | 0.27253 | 0.49322 | 0.31704 | -0.16678 | -0.16550 | -0.00209 | -0.38748 | 0.22069 | 0.04451 | 0.80646 |

k-point # 2: 0.000000 0.000000 0.333333 0.296296

| state | E_KS | E_HF | E_GW | Sx | Re(Sc) | Im(Sc) | Vxc | DE_HF | DE_GW | Znk |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | -0.40055 | -0.62733 | -0.40035 | -0.69022 | 0.22708 | 0.02707 | -0.46344 | -0.22678 | 0.00020 | 0.68318 |
| 2 | -0.20836 | -0.33803 | -0.20833 | -0.58997 | 0.12970 | 0.00745 | -0.46029 | -0.12968 | 0.00002 | 0.74643 |
| 3 | -0.04760 | -0.12044 | -0.04295 | -0.55914 | 0.07884 | 0.00053 | -0.48631 | -0.07284 | 0.00466 | 0.77473 |
| 4 | -0.04760 | -0.12044 | -0.04300 | -0.55914 | 0.07879 | 0.00050 | -0.48631 | -0.07284 | 0.00460 | 0.77383 |
| 5 | 0.04899 | 0.22993 | 0.07841 | -0.28110 | -0.14333 | -0.00053 | -0.46204 | 0.18094 | 0.02942 | 0.78220 |
| 6 | 0.11512 | 0.30416 | 0.14384 | -0.22532 | -0.15215 | -0.00174 | -0.41437 | 0.18905 | 0.02872 | 0.77830 |
| 7 | 0.11512 | 0.30416 | 0.14394 | -0.22532 | -0.15203 | -0.00165 | -0.41437 | 0.18905 | 0.02883 | 0.77885 |
| 8 | 0.26948 | 0.49261 | 0.29430 | -0.15957 | -0.19119 | -0.00829 | -0.38270 | 0.22314 | 0.02483 | 0.77719 |
| 9 | 0.28052 | 0.50287 | 0.31461 | -0.16878 | -0.17908 | -0.00819 | -0.39114 | 0.22236 | 0.03409 | 0.78765 |
| 10 | 0.28052 | 0.50287 | 0.31450 | -0.16878 | -0.17921 | -0.00835 | -0.39114 | 0.22236 | 0.03398 | 0.78768 |

# exciting Usage

k-point # 1: 0.000000 0.000000 0.000000 0.037037

| state | E_KS | E_HF | E_GW | Sx | Re(Sc) | Im(Sc) | Vxc | DE_HF | DE_GW | Znk |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | -0.45134 | -0.69966 | -0.44986 | -0.70105 | 0.25056 | 0.03612 | -0.45273 | -0.24832 | 0.00149 | 0.66555 |
| 2 | -0.01047 | -0.07414 | -0.00378 | -0.56215 | 0.07225 | 0.00015 | -0.49848 | -0.06367 | 0.00670 | 0.78017 |
| 3 | -0.01047 | -0.07414 | -0.00389 | -0.56215 | 0.07211 | 0.00013 | -0.49848 | -0.06367 | 0.00658 | 0.77903 |
| 4 | -0.01047 | -0.07414 | -0.00389 | -0.56215 | 0.07212 | 0.00014 | -0.49848 | -0.06367 | 0.00659 | 0.77917 |
| 5 | 0.08067 | 0.26157 | 0.10936 | -0.25087 | -0.14402 | -0.00125 | -0.43177 | 0.18090 | 0.02869 | 0.77794 |
| 6 | 0.08067 | 0.26157 | 0.10933 | -0.25087 | -0.14409 | -0.00127 | -0.43177 | 0.18090 | 0.02865 | 0.77846 |
| 7 | 0.08067 | 0.26157 | 0.10942 | -0.25087 | -0.14399 | -0.00120 | -0.43177 | 0.18090 | 0.02875 | 0.77888 |
| 8 | 0.10651 | 0.32083 | 0.14503 | -0.34472 | -0.16419 | -0.00147 | -0.55904 | 0.21432 | 0.03852 | 0.76837 |
| 9 | 0.26869 | 0.47704 | 0.28745 | -0.13571 | -0.18444 | -0.00703 | -0.34406 | 0.20835 | 0.01875 | 0.78431 |
| 10 | 0.27253 | 0.49322 | 0.31704 | -0.16678 | -0.16550 | -0.00209 | -0.38748 | 0.22069 | 0.04451 | 0.80646 |

k-point # 2: 0.000000 0.000000 0.333333 0.296296

| state | E_KS | E_HF | E_GW | Sx | Re(Sc) | Im(Sc) | Vxc | DE_HF | DE_GW | Znk |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | -0.40055 | -0.62733 | -0.40035 | -0.69022 | 0.22708 | 0.02707 | -0.46344 | -0.22678 | 0.00020 | 0.68318 |
| 2 | -0.20836 | -0.33803 | -0.20833 | -0.58997 | 0.12970 | 0.00745 | -0.46029 | -0.12968 | 0.00002 | 0.74643 |
| 3 | -0.04760 | -0.12044 | -0.04295 | -0.55914 | 0.07884 | 0.00053 | -0.48631 | -0.07284 | 0.00466 | 0.77473 |
| 4 | -0.04760 | -0.12044 | -0.04300 | -0.55914 | 0.07879 | 0.00050 | -0.48631 | -0.07284 | 0.00460 | 0.77383 |
| 5 | 0.04899 | 0.22993 | 0.07841 | -0.28110 | -0.14333 | -0.00053 | -0.46204 | 0.18094 | 0.02942 | 0.78220 |
| 6 | 0.11512 | 0.30416 | 0.14384 | -0.22532 | -0.15215 | -0.00174 | -0.41437 | 0.18905 | 0.02872 | 0.77830 |
| 7 | 0.11512 | 0.30416 | 0.14394 | -0.22532 | -0.15203 | -0.00165 | -0.41437 | 0.18905 | 0.02883 | 0.77885 |
| 8 | 0.26948 | 0.49261 | 0.29430 | -0.15957 | -0.19119 | -0.00829 | -0.38270 | 0.22314 | 0.02483 | 0.77719 |
| 9 | 0.28052 | 0.50287 | 0.31461 | -0.16878 | -0.17908 | -0.00819 | -0.39114 | 0.22236 | 0.03409 | 0.78765 |
| 10 | 0.28052 | 0.50287 | 0.31450 | -0.16878 | -0.17921 | -0.00835 | -0.39114 | 0.22236 | 0.03398 | 0.78768 |

# exciting Usage

k-point # 1: 0.000000 0.000000 0.000000 0.037037

| state | E_KS | E_HF | E_GW | Sx | Re(Sc) | Im(Sc) | Vxc | DE_HF | DE_GW | Znk |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | -0.45134 | -0.69966 | -0.44986 | -0.70105 | 0.25056 | 0.03612 | -0.45273 | -0.24832 | 0.00149 | 0.66555 |
| 2 | -0.01047 | -0.07414 | -0.00378 | -0.56215 | 0.07225 | 0.00015 | -0.49848 | -0.06367 | 0.00670 | 0.78017 |
| 3 | -0.01047 | -0.07414 | -0.00389 | -0.56215 | 0.07211 | 0.00013 | -0.49848 | -0.06367 | 0.00658 | 0.77903 |
| 4 | -0.01047 | -0.07414 | -0.00389 | -0.56215 | 0.07212 | 0.00014 | -0.49848 | -0.06367 | 0.00659 | 0.77917 |
| 5 | 0.08067 | 0.26157 | 0.10936 | -0.25087 | -0.14402 | -0.00125 | -0.43177 | 0.18090 | 0.02869 | 0.77794 |
| 6 | 0.08067 | 0.26157 | 0.10933 | -0.25087 | -0.14409 | -0.00127 | -0.43177 | 0.18090 | 0.02865 | 0.77846 |
| 7 | 0.08067 | 0.26157 | 0.10942 | -0.25087 | -0.14399 | -0.00120 | -0.43177 | 0.18090 | 0.02875 | 0.77888 |
| 8 | 0.10651 | 0.32083 | 0.14503 | -0.34472 | -0.16419 | -0.00147 | -0.55904 | 0.21432 | 0.03852 | 0.76837 |
| 9 | 0.26869 | 0.47704 | 0.28745 | -0.13571 | -0.18444 | -0.00703 | -0.34406 | 0.20835 | 0.01875 | 0.78431 |
| 10 | 0.27253 | 0.49322 | 0.31704 | -0.16678 | -0.16550 | -0.00209 | -0.38748 | 0.22069 | 0.04451 | 0.80646 |

k-point # 2: 0.000000 0.000000 0.333333 0.296296

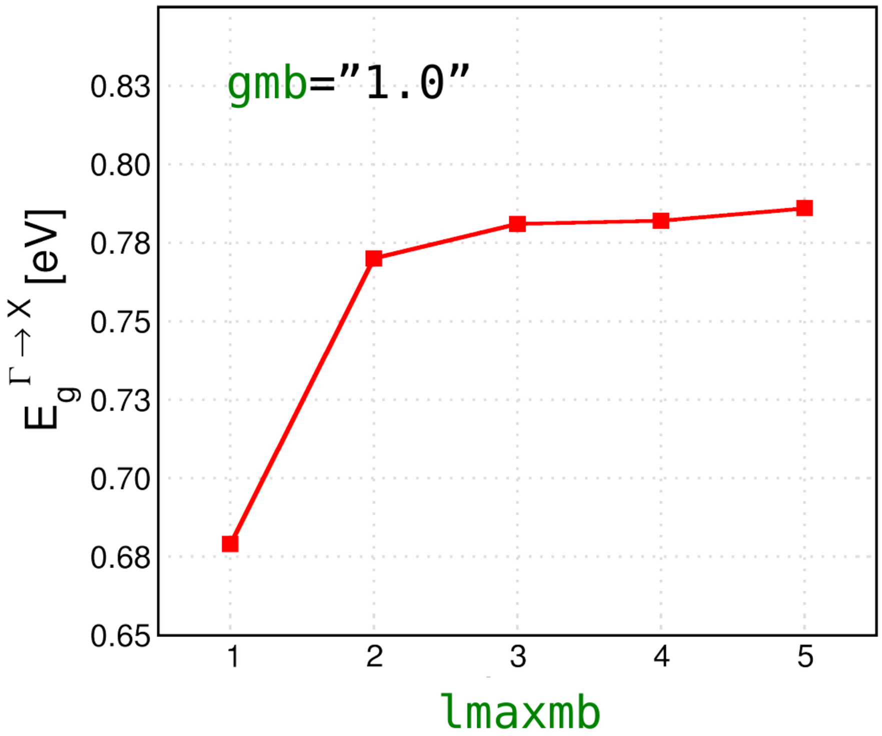
| state | E_KS | E_HF | E_GW | Sx | Re(Sc) | Im(Sc) | Vxc | DE_HF | DE_GW | Znk |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | -0.40055 | -0.62733 | -0.40035 | -0.69022 | 0.22708 | 0.02707 | -0.46344 | -0.22678 | 0.00020 | 0.68318 |
| 2 | -0.20836 | -0.33803 | -0.20833 | -0.58997 | 0.12970 | 0.00745 | -0.46029 | -0.12968 | 0.00002 | 0.74643 |
| 3 | -0.04760 | -0.12044 | -0.04295 | -0.55914 | 0.07884 | 0.00053 | -0.48631 | -0.07284 | 0.00466 | 0.77473 |
| 4 | -0.04760 | -0.12044 | -0.04300 | -0.55914 | 0.07879 | 0.00050 | -0.48631 | -0.07284 | 0.00460 | 0.77383 |
| 5 | 0.04899 | 0.22993 | 0.07841 | -0.28110 | -0.14333 | -0.00053 | -0.46204 | 0.18094 | 0.02942 | 0.78220 |
| 6 | 0.11512 | 0.30416 | 0.14384 | -0.22532 | -0.15215 | -0.00174 | -0.41437 | 0.18905 | 0.02872 | 0.77830 |
| 7 | 0.11512 | 0.30416 | 0.14394 | -0.22532 | -0.15203 | -0.00165 | -0.41437 | 0.18905 | 0.02883 | 0.77885 |
| 8 | 0.26948 | 0.49261 | 0.29430 | -0.15957 | -0.19119 | -0.00829 | -0.38270 | 0.22314 | 0.02483 | 0.77719 |
| 9 | 0.28052 | 0.50287 | 0.31461 | -0.16878 | -0.17908 | -0.00819 | -0.39114 | 0.22236 | 0.03409 | 0.78765 |
| 10 | 0.28052 | 0.50287 | 0.31450 | -0.16878 | -0.17921 | -0.00835 | -0.39114 | 0.22236 | 0.03398 | 0.78768 |

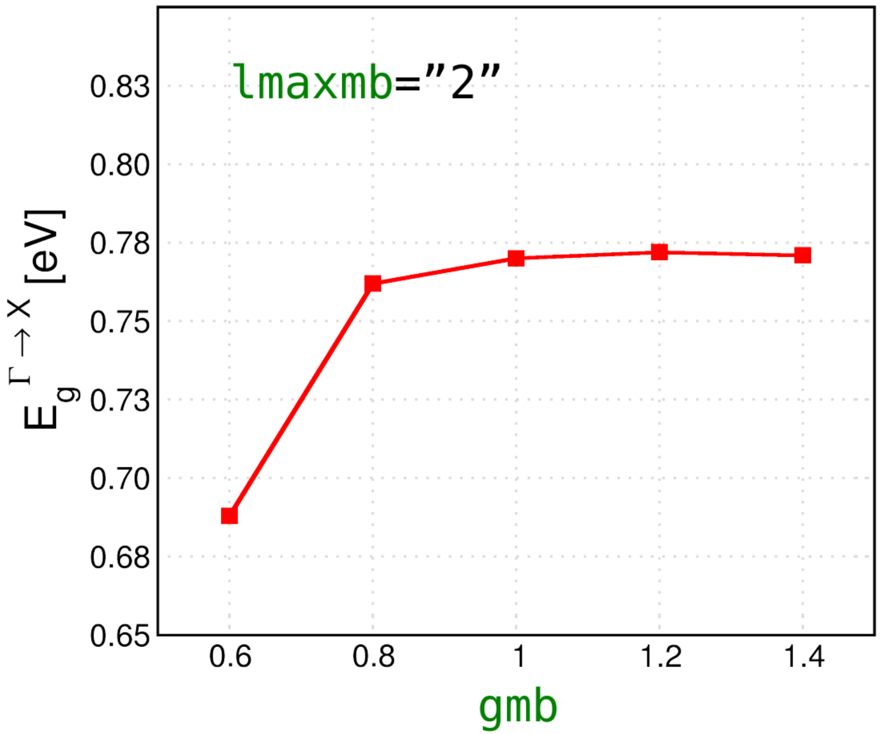
# Convergence test

/input/gw/mixbasis/@lmaxmb

/input/gw/mixbasis/@gmb

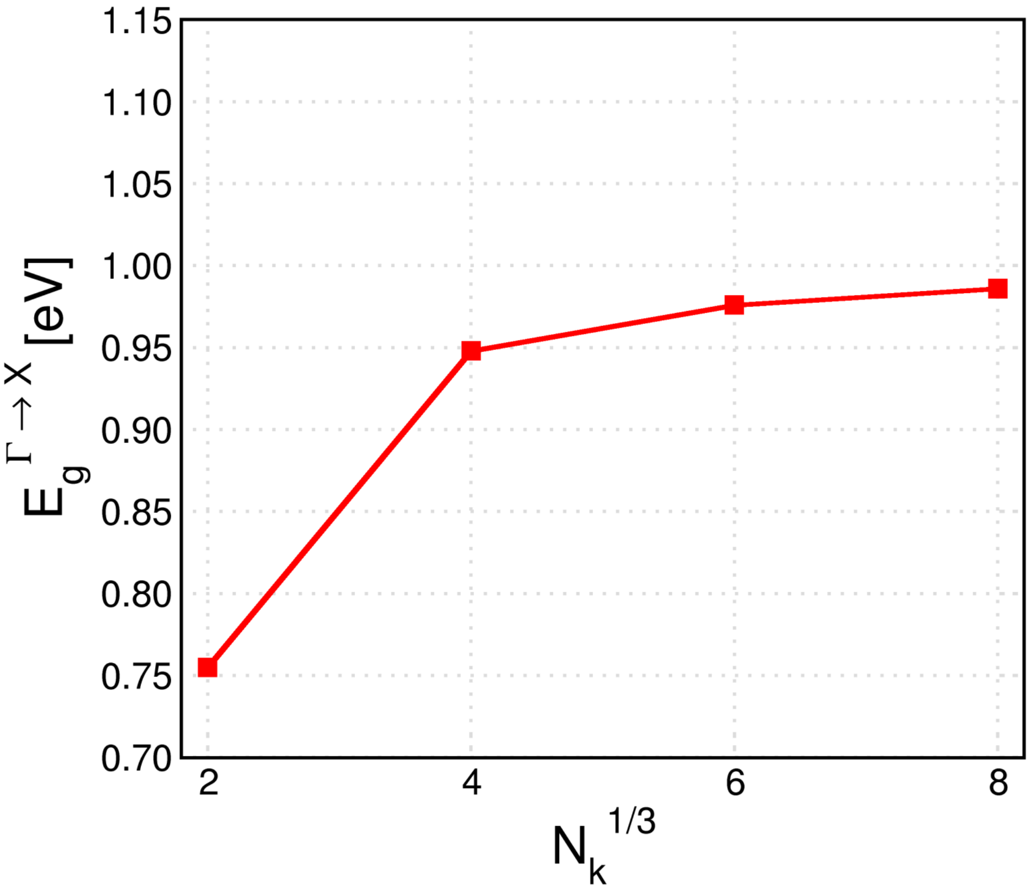
nempty="17", ngridk="2 2 2"



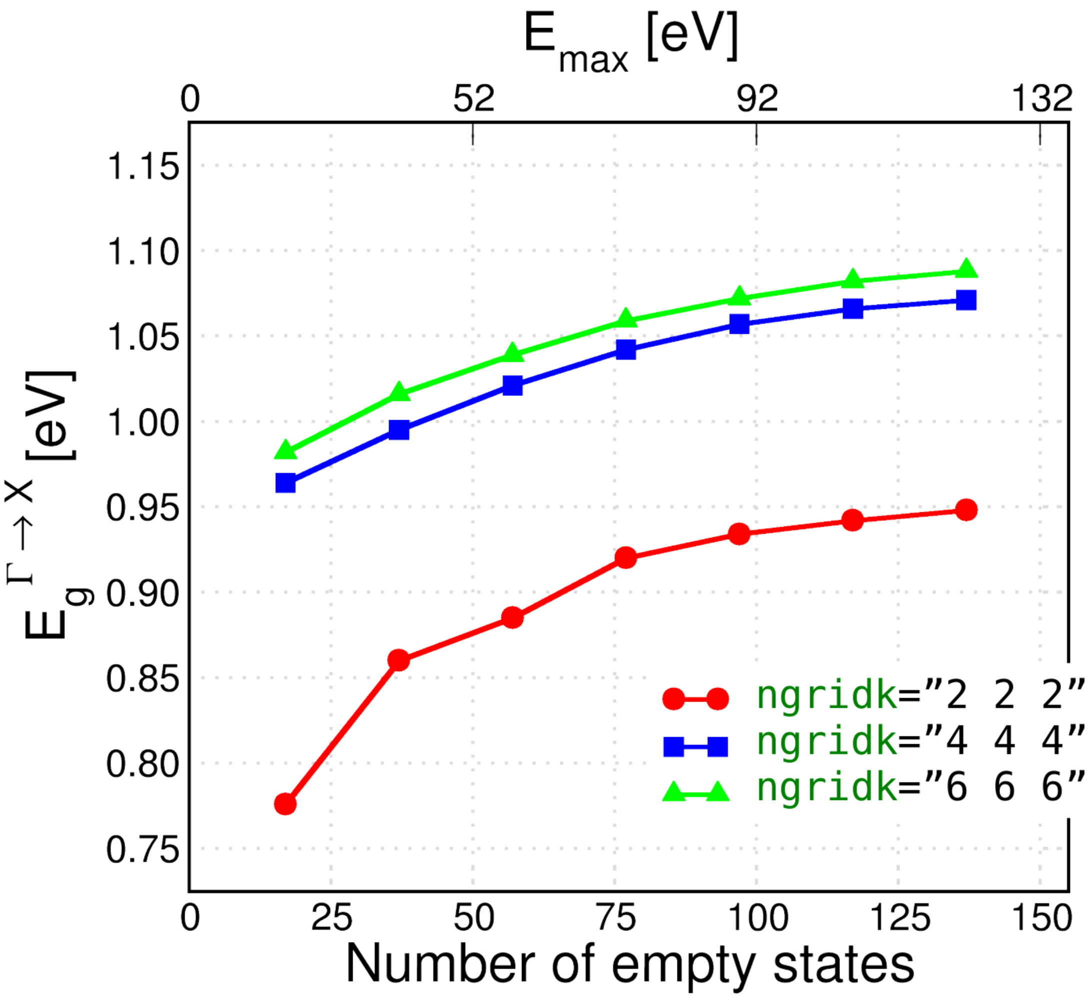



# Convergence test

`lmaxmb="3", gmb="1.0", nempty="17"`



# Convergence test



# Summary

- GW approximation and implementation in **`exciting`**
- Inputs for GW@**`exciting`**
- Key factors to run GW in **`exciting`**
- Perform the convergence tests

# Summary

- GW approximation and implementation in **exciting**
- Inputs for GW@**exciting**
- Key factors to run GW in **exciting**
- Perform the convergence tests
- Do not use as a **BLACK BOX**

# Summary

- GW approximation and implementation in **exciting**
- Inputs for GW@**exciting**
- Key factors to run GW in **exciting**
- Perform the convergence tests
- Do not use as a **BLACK BOX**

**exciting**

**best code**

exciting

neon

# Next

Low scaling GW algorithm

$\mathcal{O}(N^3)$

NOMAD Center of Excellence


# Thank you