GW in practice: Implementation, Approximations, and Numerical Workflows

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HANAMI

MAX DRIVING THE EXASCALE TRANSITION

Yambo ©

Outline:

Why GW approximations

The quasi particle equation and GW approximations

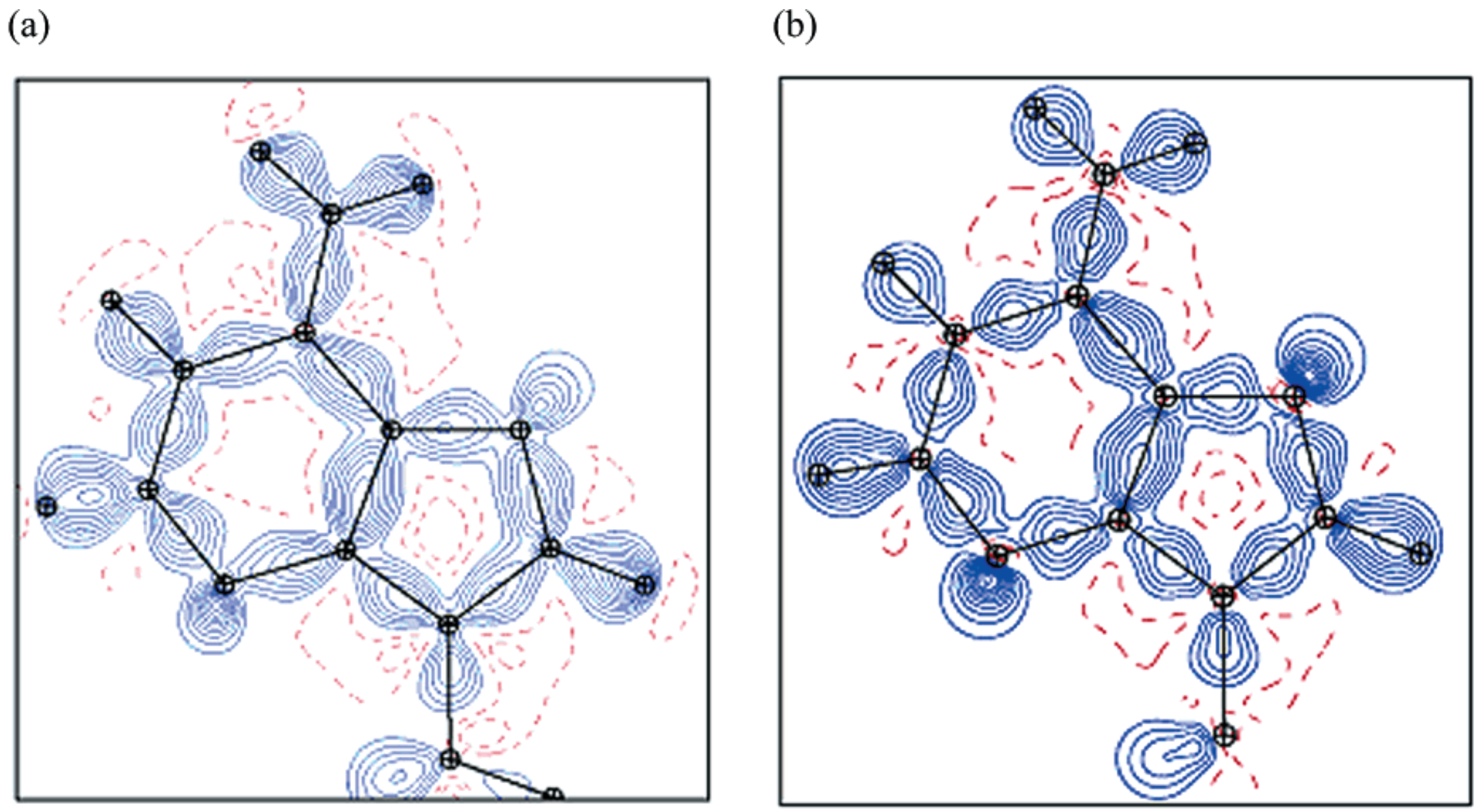
GW in practical calculations: common approximations and best practices

The Yambo code

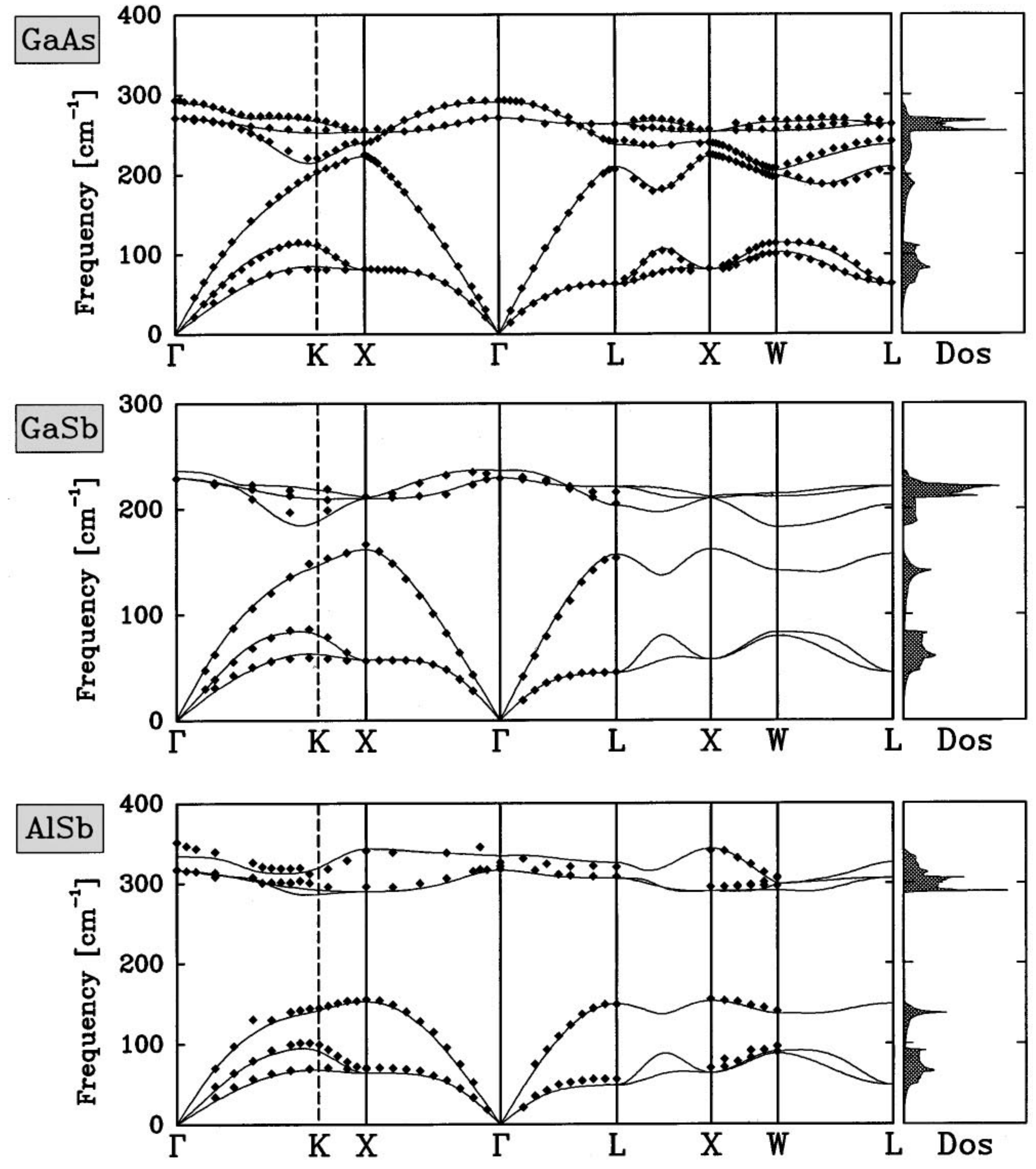
Conclusions and take home messages

Success of Density Functional Theory

from X ray experiment | DFT calculation (PBE)

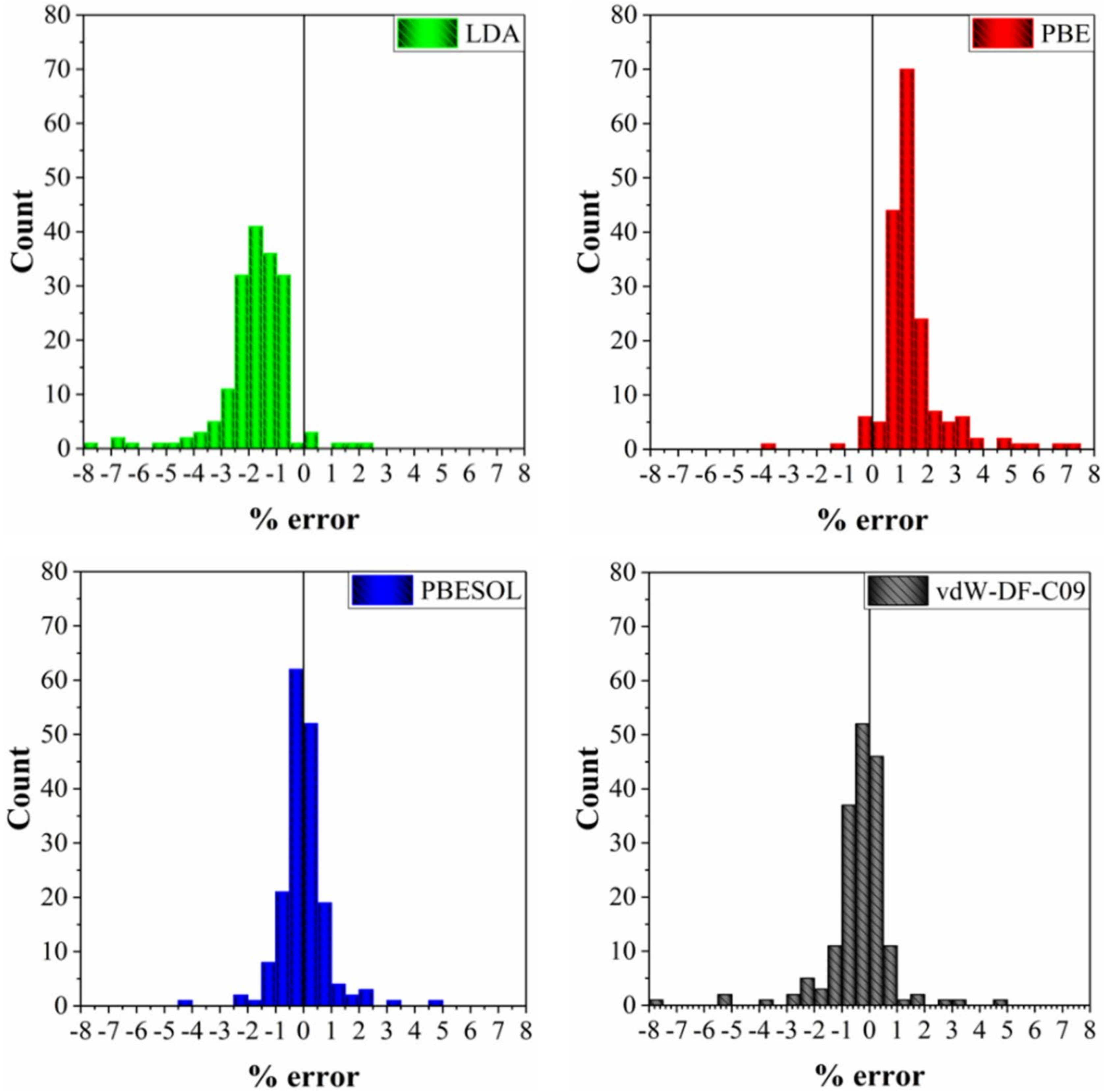


B. Guillot et al. J. Phys. Chem. B 107, 9109 (2003)



Giannozzi, P., S. de Gironcoli, P. Pavone, and S. Baroni, Phys. Rev. B 43, 7231 (1991)

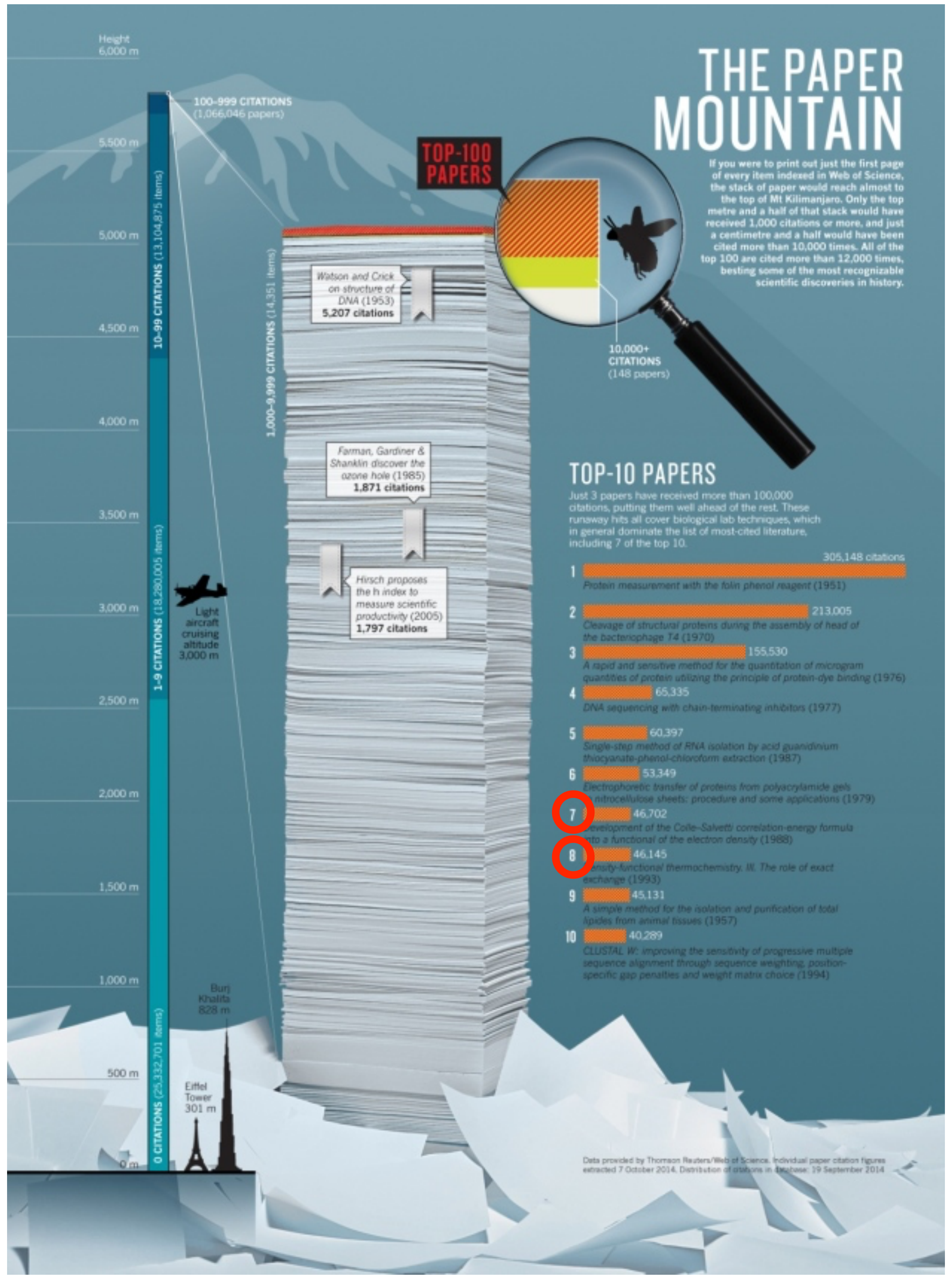
141 binary and ternary oxides
Optimised Lattice Constants



Yuk, Simuck F., et al. Scientific Reports 14. 20219 (2024)

see also: P. Haas et al. Phys. Rev, B. **79**, 085104 (2009)

Impact of Density Functional Theory



Nature News 514, 550 (2014)

TOP TEN CITED PAPERS

Just 3 papers have more than 200,000 citations each, according to the Web of Science database. All three cover biological laboratory techniques. This update to a 2014 list of most-cited articles shows that the top three papers remain unchanged. But there have been shifts in the positions of others (triangles), and some additions that were not on the previous list (orange stars). For alternative rankings from two other databases, and a median ranking across all three, see Supplementary information (go.nature.com/425g9dn).

Rank	Citations	Paper
1	355,968 citations	*Protein measurement with the folin phenol reagent* (1951)
2	259,187	*Cleavage of structural proteins during the assembly of the head of bacteriophage T4* (1970)
3	242,864	*A rapid and sensitive method for the quantitation of microgram quantities of protein utilizing the principle of protein-dye binding* (1976)
▲4 (16)	174,137	*Generalized gradient approximation made simple* (1996)
▲5 (21)	148,626	*Analysis of relative gene expression data using real-time quantitative PCR and the $2^{-\Delta\Delta C_T}$ method* (2001)
★6	133,965	*Preferred reporting items for systematic reviews and meta-analyses: the PRISMA statement* (2009)*
★7	116,706	*Deep residual learning for image recognition* (2016, preprint 2015)
▲8 (43)	101,906	*Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set* (1996)
★9	100,327	*Using thematic analysis in psychology* (2006)†
▼10 (7)	93,223	*Development of the Colle–Salvetti correlation-energy formula into a functional of the electron density* (1988)

Data show citations from Web of Science 'Core Collection' journals as of March 2025, to permit comparison with 2014 list (*Nature* **514**, 550–553; 2014). Orders would change if citation metrics from other databases were included (see Supplementary information).
*Paper was published in multiple journals simultaneously. This total aggregates citations to all journal versions.
†Corrected for data error in Web of Science, which lists a different paper by the same authors.

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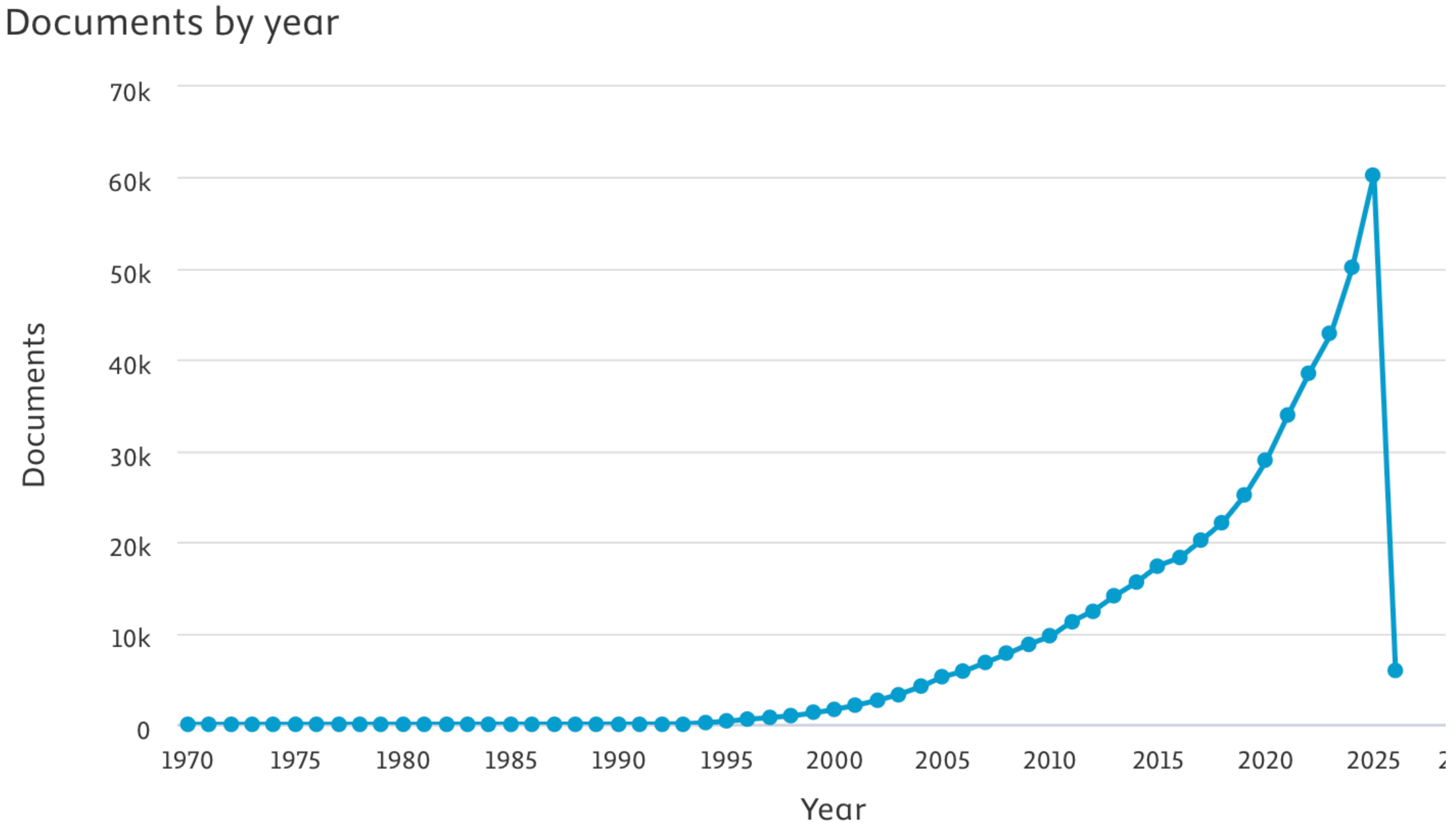
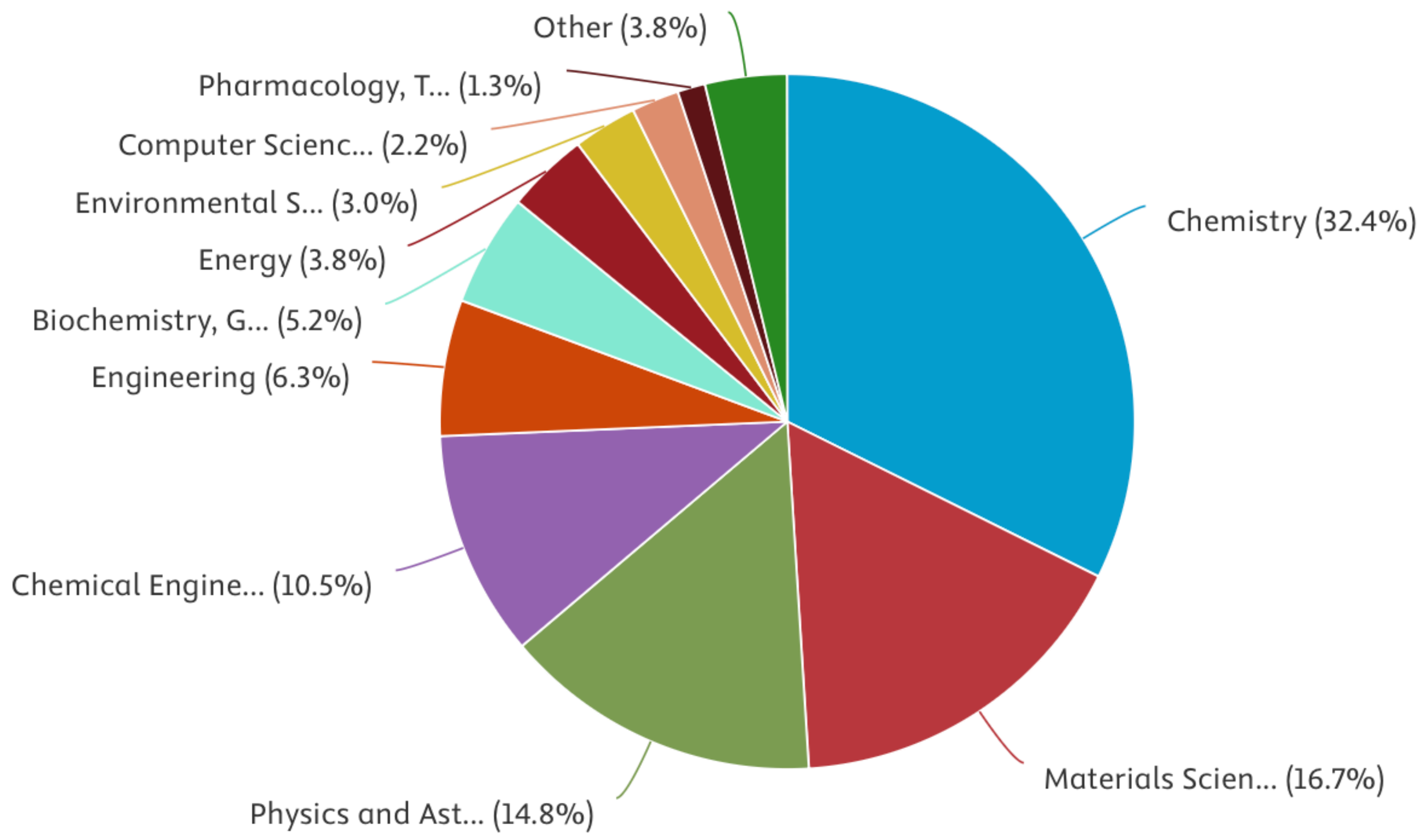
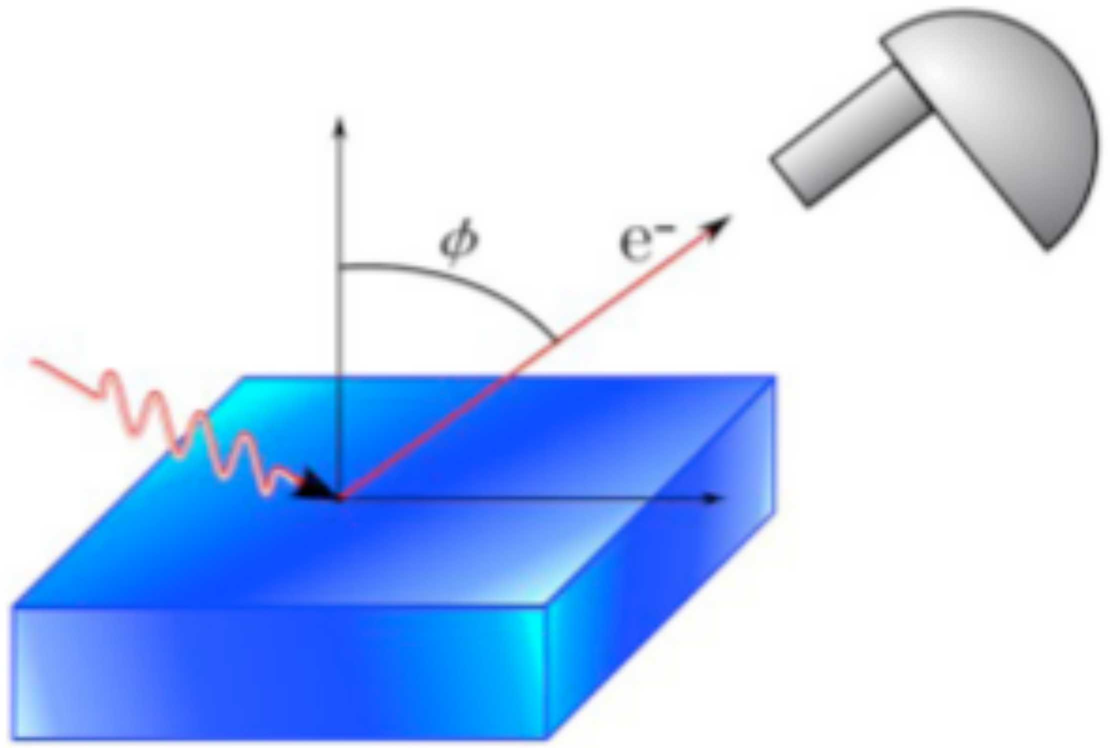
Nature 640, 591 (2025)





- Scopus: "DFT" AND "Calculation" Jan. 2026

Excited states of Materials: Direct Photoemission

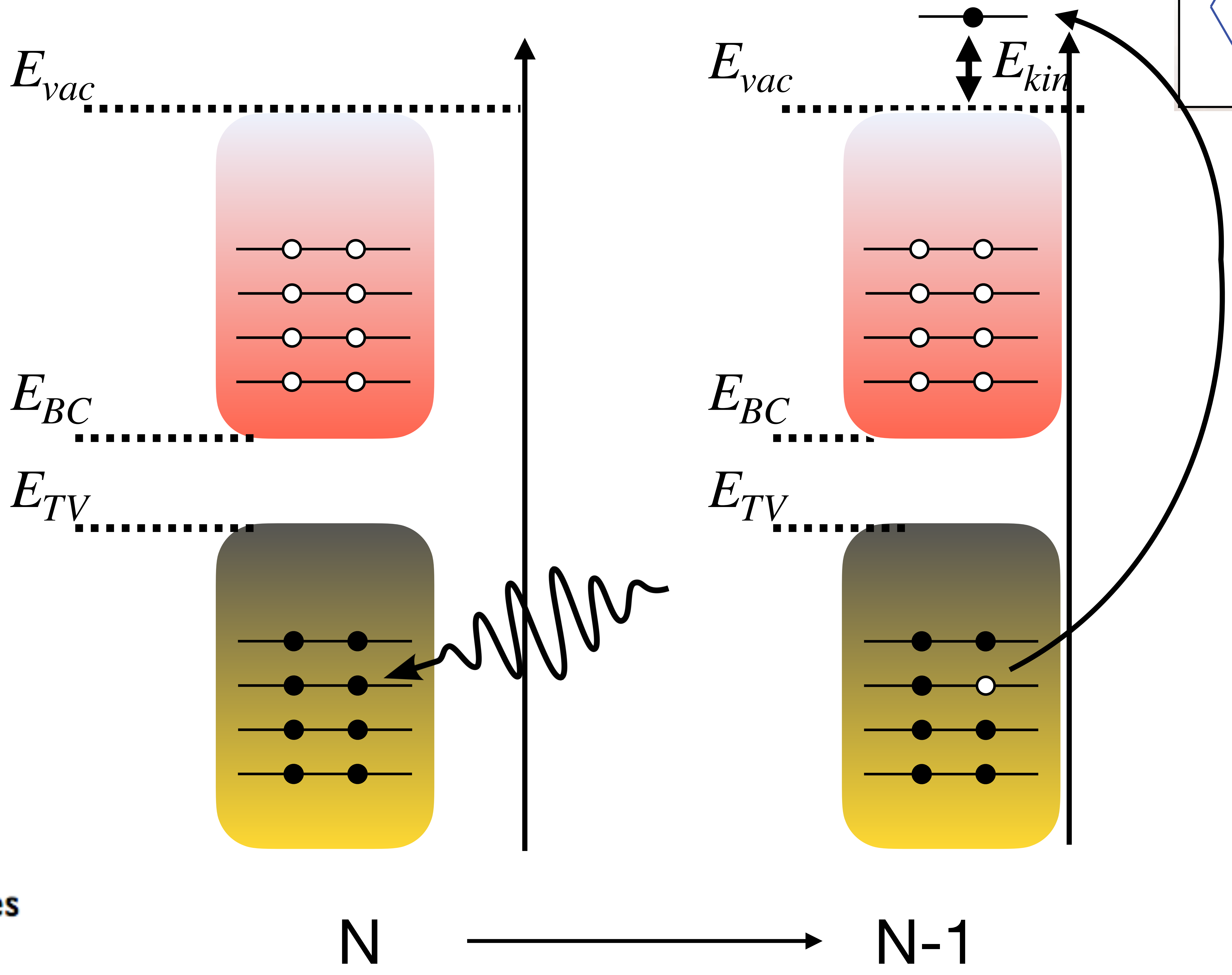


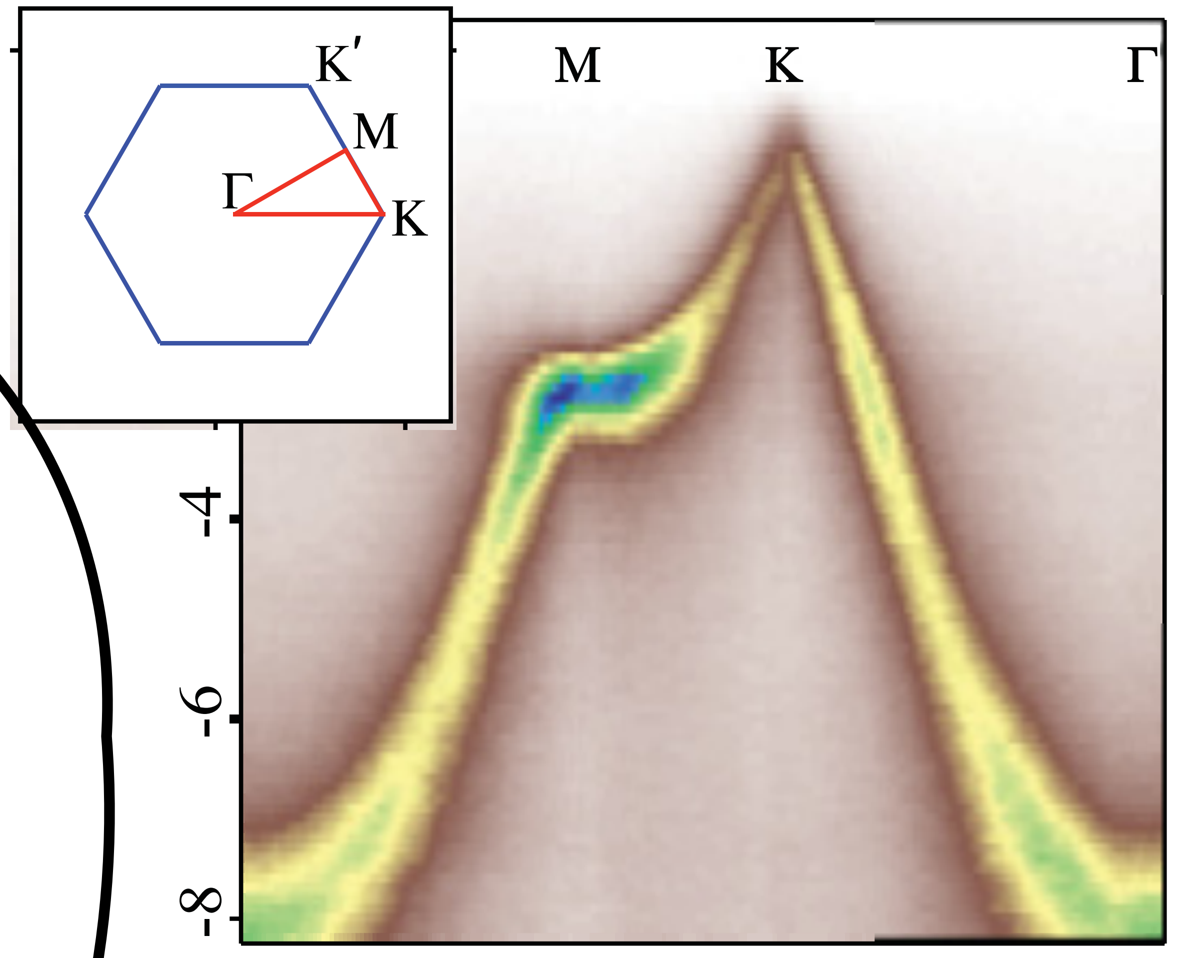
$$E(N) + h\nu = E(N-1) + [\Phi_W + E_{kin}]$$

$$E(N) - E(N-1) = [\Phi_W + E_{kin}] - h\nu$$

...plus momentum conservation ⇒ ARPES

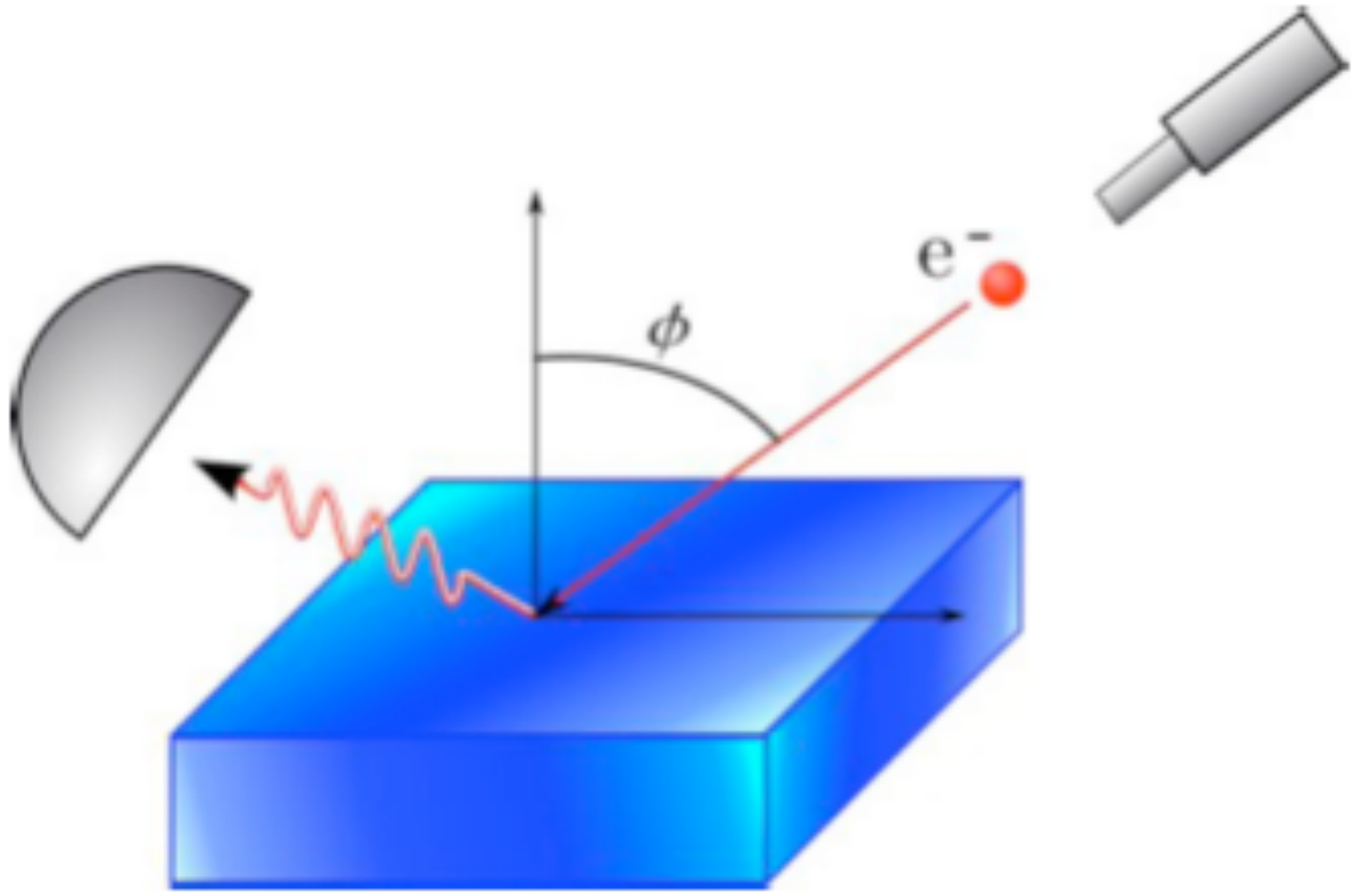
Measure the density of occupied states





Occupied States

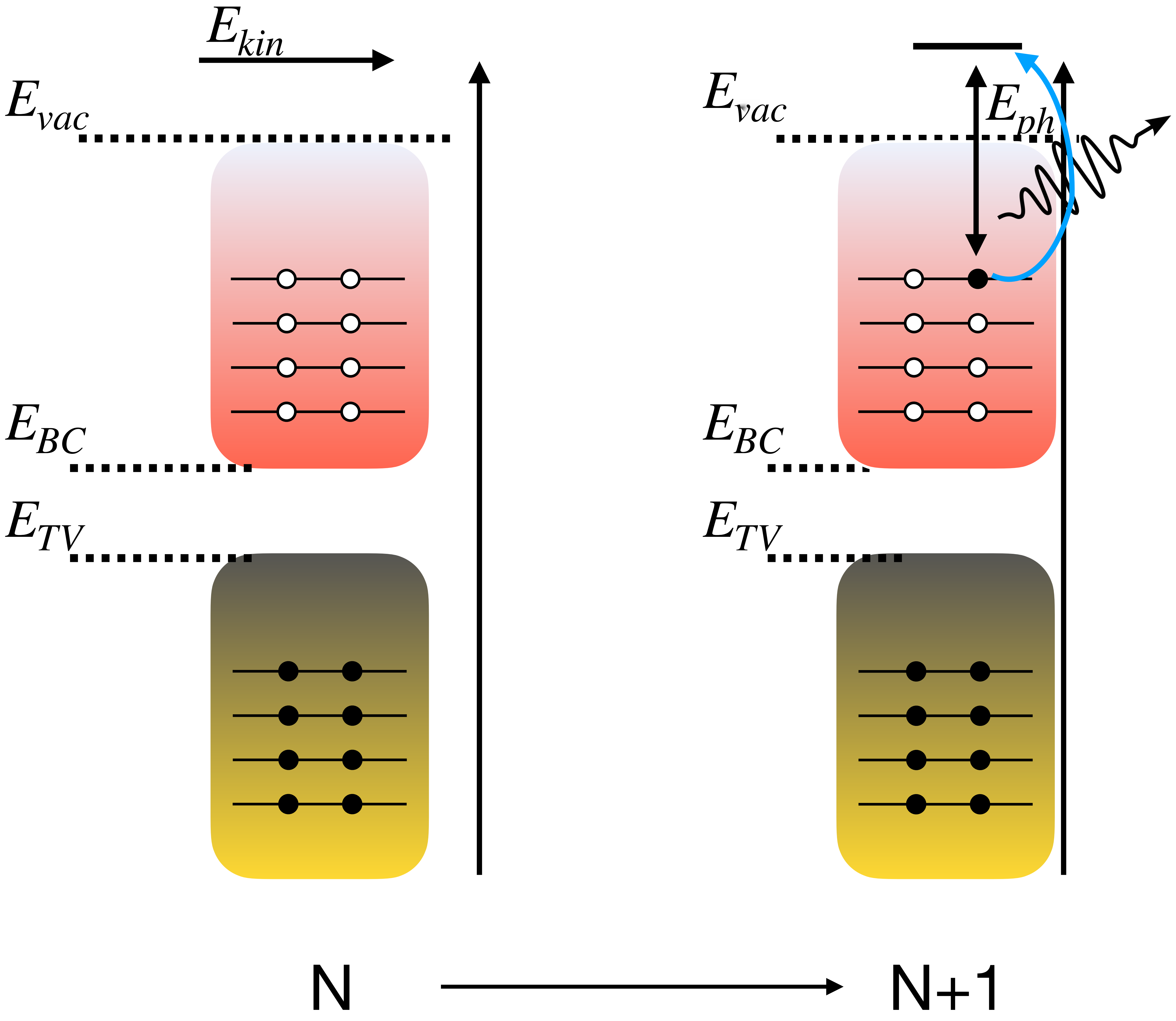
Excited states of Materials: Inverse Photoemission



electron in - photon out

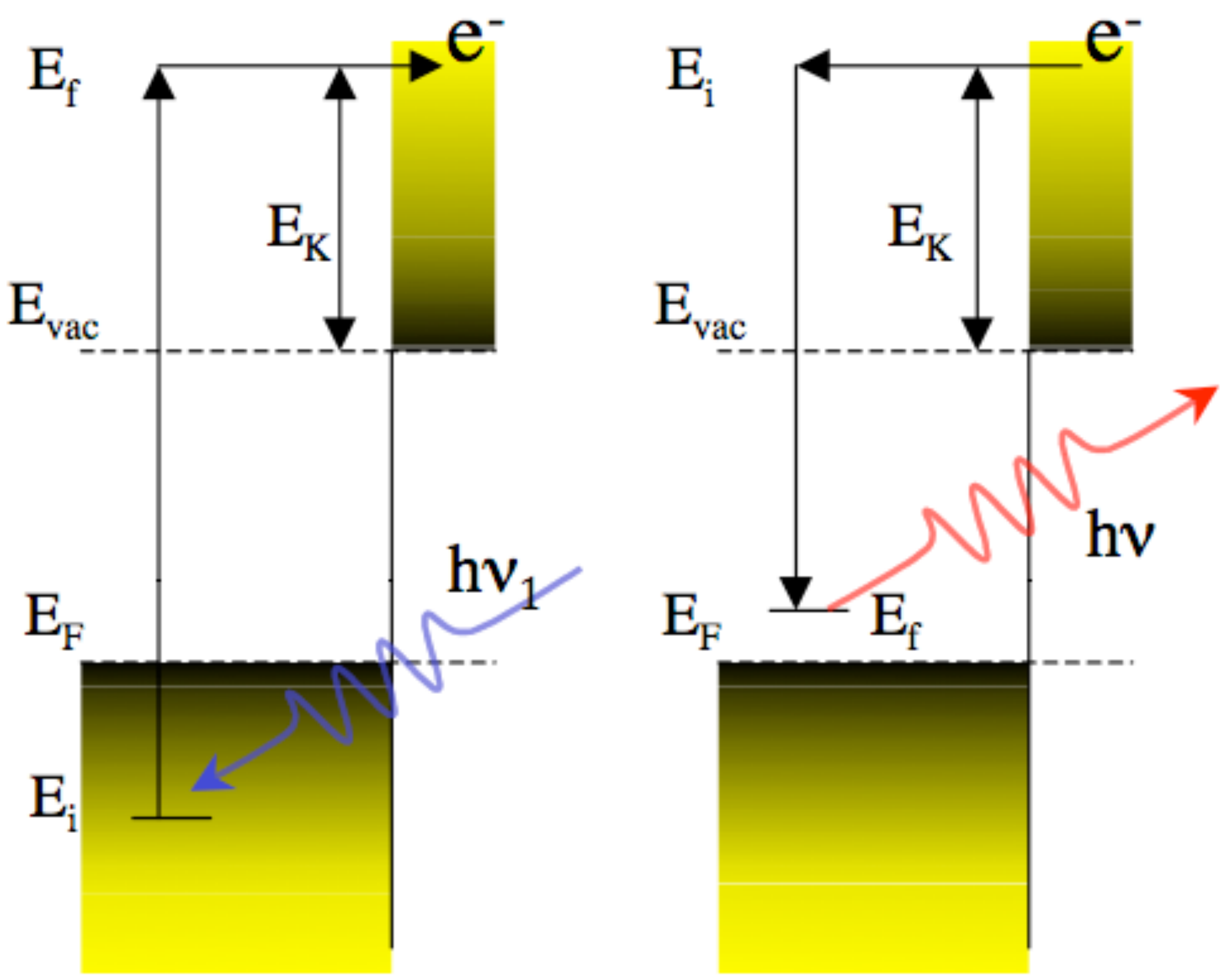
$$E(N+1) - E(N) = E_k + h\nu$$

Measure the density of unoccupied states



Empty States

Excited states of Materials: The Band Gap



Picture from J. Osma Peso PhD Thesis

Direct photoemission

$$\epsilon_i = E_{kin} - \hbar\omega$$

$$\epsilon_i = E_0^N - E_i^{N-1}$$

Total energy difference between the N-particle ground state and the (N-1) particle state that remains after the emission

Inverse photoemission

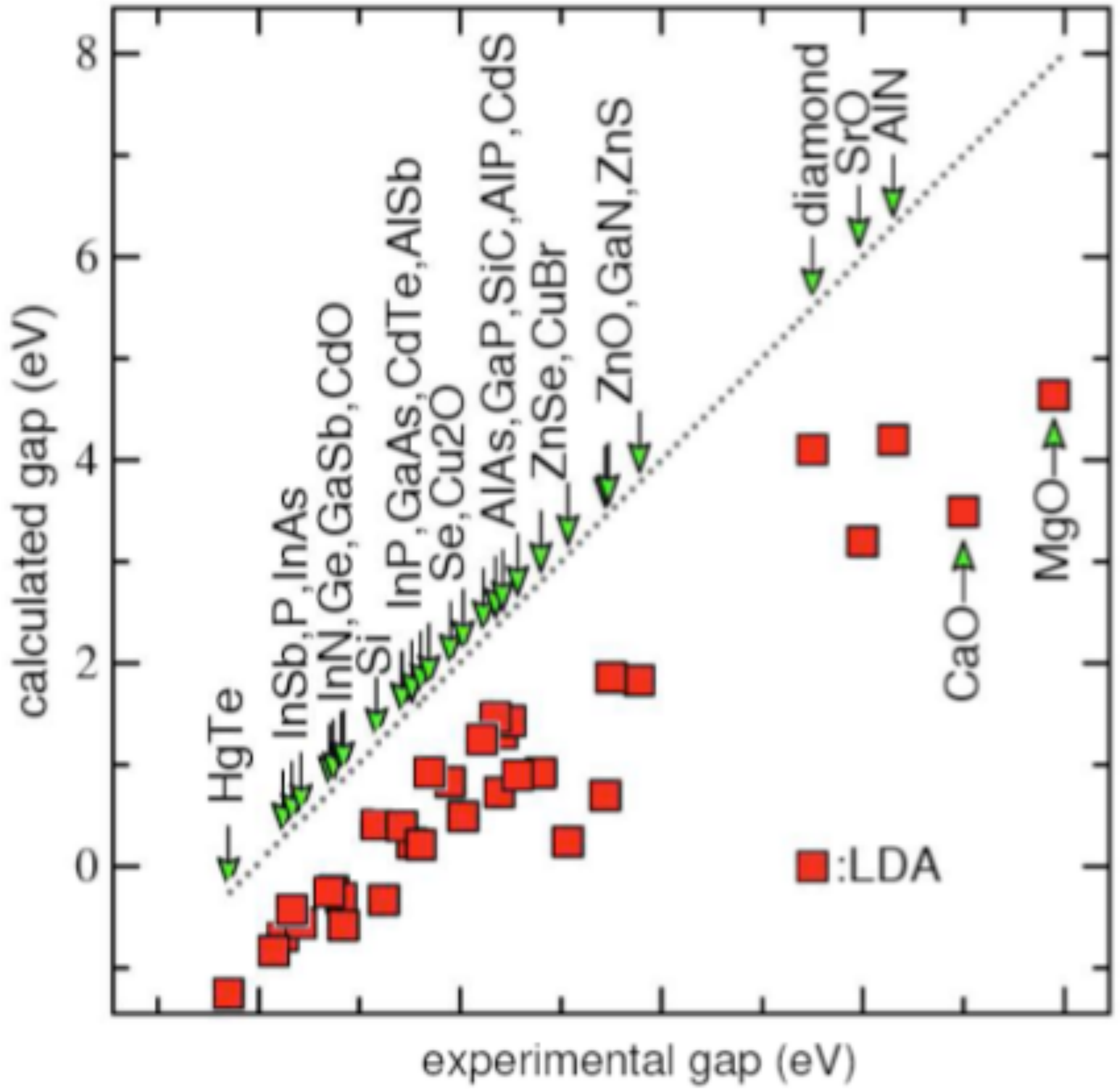
$$\epsilon_i = E_i^{N+1} - E_0^N$$

The ejection (removal) of an electron is a many-body process

$$E_{gap} = (E_{N+1} - E_N) - (E_N - E_{N-1})$$

electron affinity ionization potential

Excited states of Materials: The Band Gap Problem



Adapted from M. van Schilfgaarde et al. PRL **96** (2006)

Si: 0.47 eV (LDA) vs 1.1 eV (expt)

GaAs: 0.30 eV (LDA) vs 1.4 eV (expt)

Huge discrepancy not due to the LDA

Excited states of Materials: The Band Gap Problem

Can we calculate the QP gap directly using total energies from DFT-LDA?

$$E_{gap} = (E_{N+1} - E_N) - (E_N - E_{N-1})$$

electron affinity   ionization potential

$$E_{Gap} = \underline{\epsilon^N_{N+1} - \epsilon^N_N} + \sum_i^{N+1} \Delta\epsilon^L + \sum_i^{N-1} \Delta\epsilon^H - E_{Har}[\Delta\rho^L] - E_{Har}[\Delta\rho^H] + \int V^N_{Har}(\mathbf{r})(\Delta\rho^H(\mathbf{r}) - \Delta\rho^L(\mathbf{r}))d\mathbf{r}$$

Kohn-Sham gap

$$+E_{xc}[\rho^{N+1}] + E_{xc}[\rho^{N-1}] - 2E_{xc}[\rho^N] - \int V^{N+1}_{XC}(\mathbf{r})\rho^{N+1}(\mathbf{r})d\mathbf{r} - \int V^{N-1}_{XC}(\mathbf{r})\rho^{N-1}(\mathbf{r})d\mathbf{r} + 2\int V^N_{XC}(\mathbf{r})\rho^N(\mathbf{r})d\mathbf{r}$$

C. E. Patrick and F. Giustino, PRL 109, 116801 (2012)]

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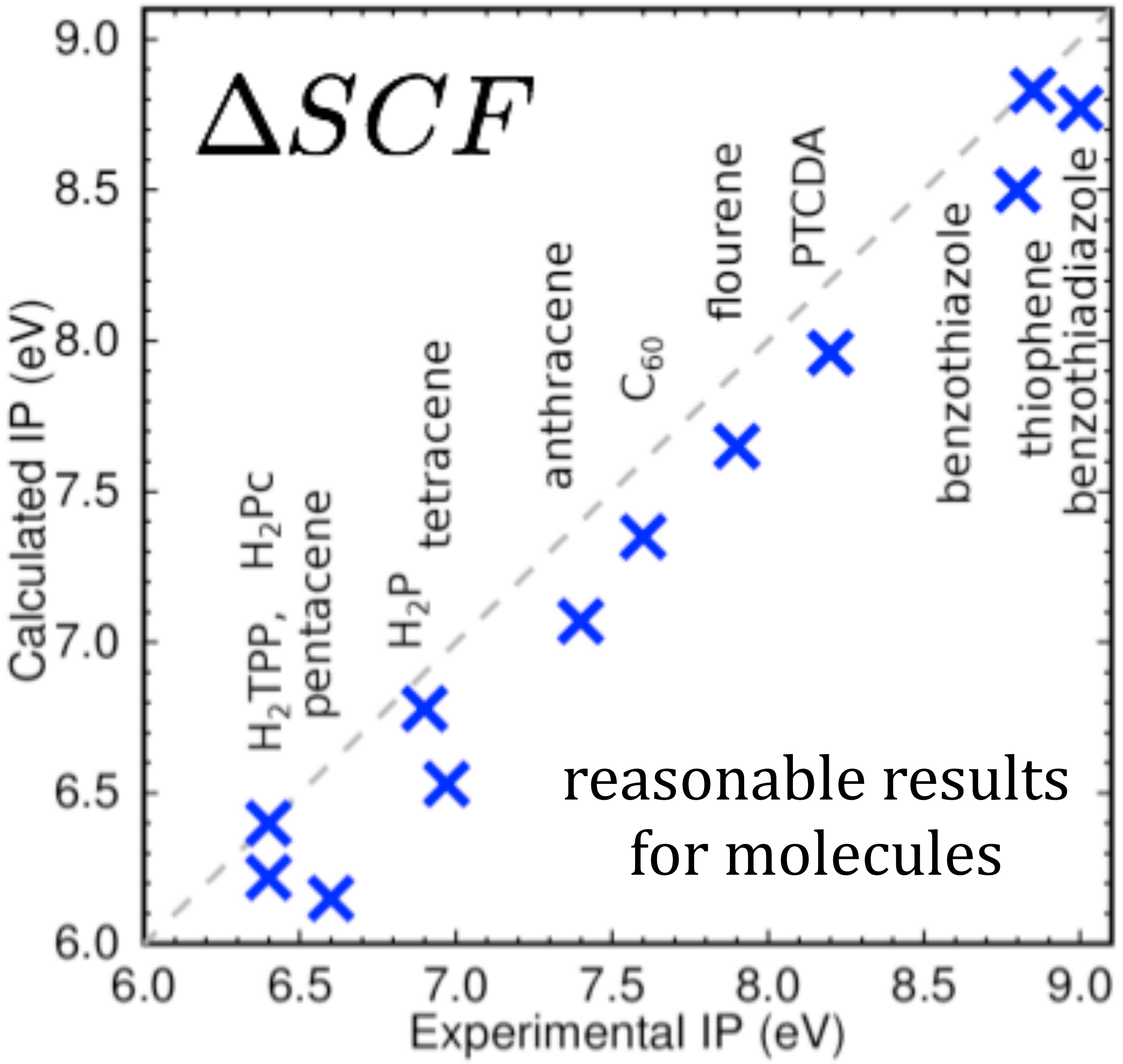

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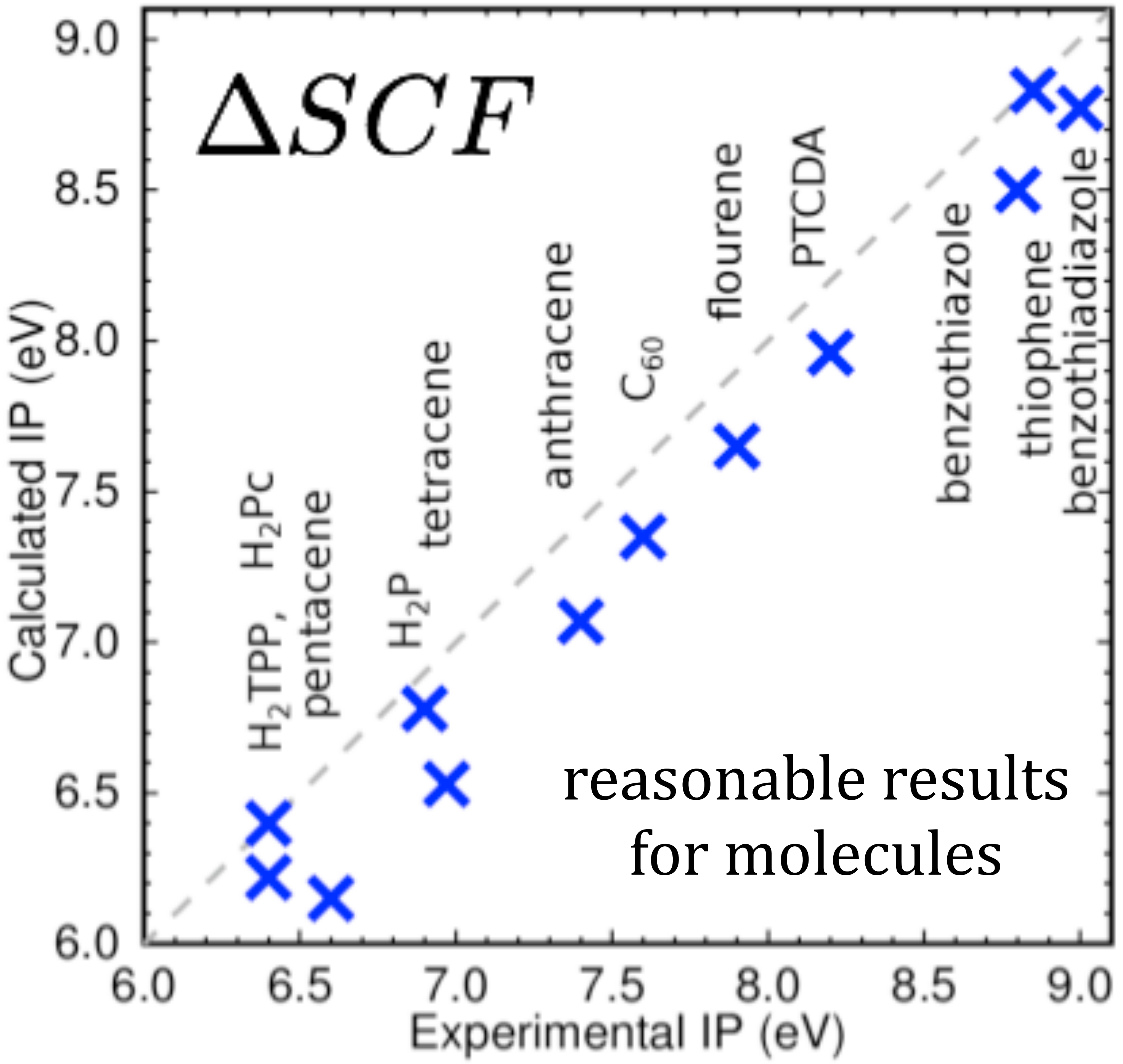
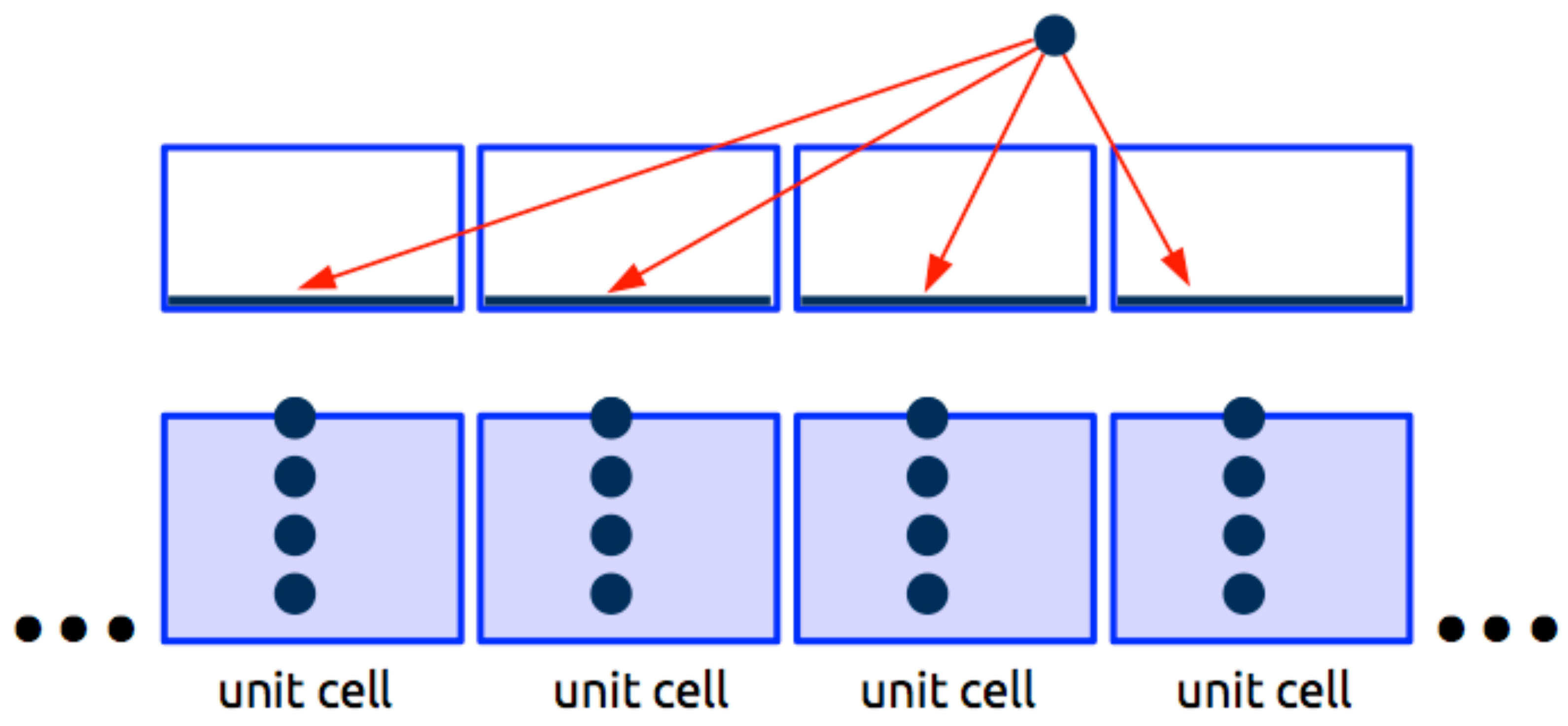


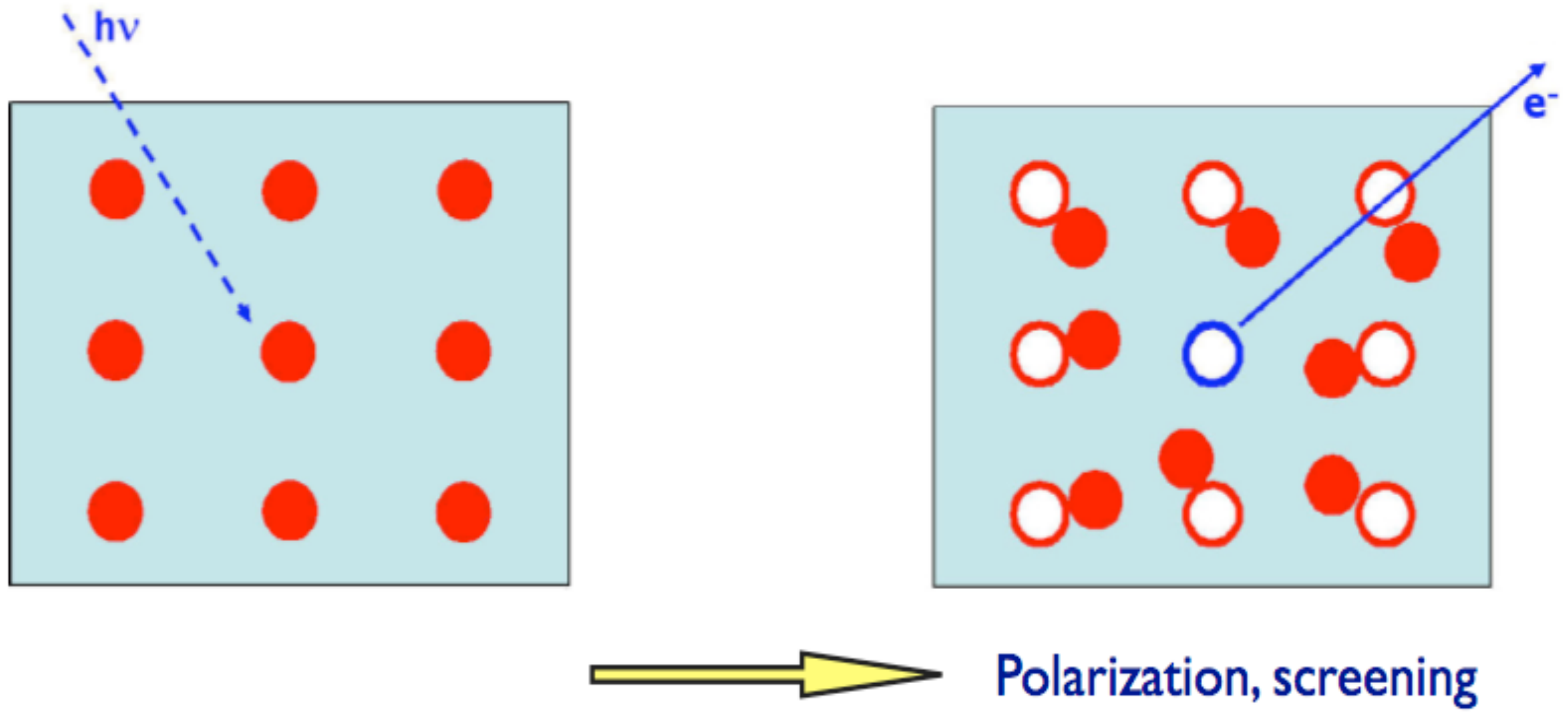
What about periodic solids ?



Infinitesimal extra charge per cell

C. E. Patrick and F. Giustino, PRL 109, 116801 (2012)]

The Green Function



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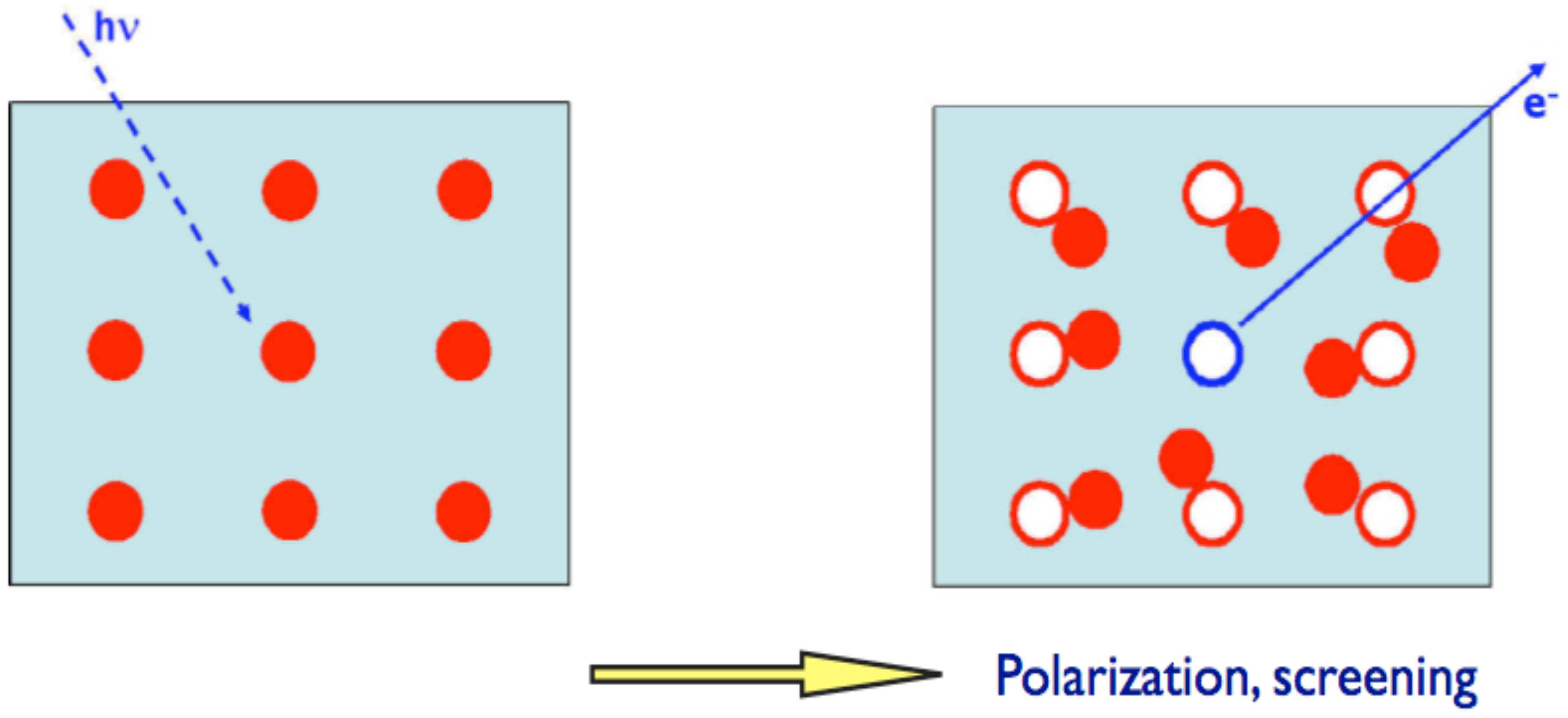
a framework that links the N-particle with the $(N \pm 1)$particle system

The Green Function



Theoretical description for describing the ejection or injection of electrons requires a framework that links the N-particle with the $(N \pm 1)$particle system

$$G(\mathbf{r_1}t_1, \mathbf{r_2}t_2) = -\frac{i}{\hbar} < \Psi_0^N | \hat{T}[\hat{\psi}(\mathbf{r_1}t_1)\hat{\psi}^\dagger(\mathbf{r_2}t_2)] | \Psi_0^N >$$

Green Function has poles at the true many-particle excitation energies

$$G(\mathbf{r_1}, \mathbf{r_2}, \omega) = \sum_j \frac{f_j(\mathbf{r_1}) f_j^*(\mathbf{r_2})}{\omega - \epsilon_j + i\eta sgn(\epsilon_j - \mu)}$$

$$\epsilon_j = \begin{matrix} E(N+1,j) - E(N) \\ E(N) - E(N-1,j) \end{matrix} \qquad f_j(\mathbf{r_1}) = \begin{matrix} \langle \Psi_0^N | \hat{\psi}(\mathbf{r_1}) | \Psi_j^{N+1} \rangle & \epsilon_j > \mu \\ \langle \Psi_j^{N-1} | \hat{\psi}(\mathbf{r_1}) | \Psi_0^N \rangle & \epsilon_j < \mu \end{matrix}$$

In principle provides access to:
excitation lifetime
total energy
expectation value of one-particle operator

How to obtain G?

Perturbation theory starts from what is known to evaluate what is not known ...hoping that the difference is small

We start from a known $G_0(\omega)$ that correspond of the Hamiltonian H_0 (e.g. non interacting electrons) and consider the Hamiltonian $H = H_0 + H_1$, where the interaction is in H_1

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Everything that is unknown is put in

$$\Sigma(\omega) = G_0^{-1}(\omega) - G^{-1}(\omega)$$

This is the definition of the Self Energy

The Quasiparticle Equation

$$[\omega - \hat{H}_0]G(\omega) + i\int \Sigma(\omega)G(\omega) = 1$$

Let's suppose we know the Self Energy

and consider G_0 the Green function of a single particle Hamiltonian

$$H_0 = -\frac{\nabla^2}{2m} + V_{ext} + \frac{e^2}{4\pi\epsilon_0}\int \frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d^3\mathbf{r}'$$

Introducing the Lehmann representation for G:

QP Equation

$$\hat{H}_0(\mathbf{r})f_s(\mathbf{r}) + \int \Sigma(\mathbf{r},\mathbf{r}';\epsilon_s)f_s(\mathbf{r}')d^3\mathbf{r}' = \epsilon_s f_s(\mathbf{r})$$

KS Equation

$$\hat{H}_0(r)\psi_{ks}(r) + V_{xc}(r)\psi_{ks}(r) = \epsilon_{ks}\psi_{ks}(r)$$

Σ contains the many body effects as V_{xc}

Σ is not Hermitian, non-local and frequency dependent

Σ is the potential self by and added (removed) electron to (from) the system

f_s are not orthonormal

ϵ_s are in general complex

V_{xc} is local and not frequency dependent

V_{xc} is part of the potential of a fictitious system

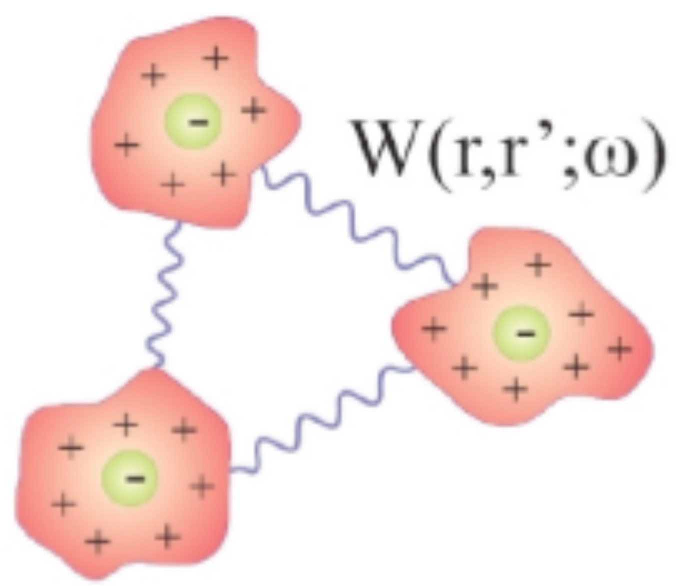
The Quasiparticle Equation

QP equation describes the excitations of the Many-Body system

$$\hat{H}_0(\mathbf{r}) f_s(\mathbf{r}) + \int \Sigma(\mathbf{r}, \mathbf{r}'; \epsilon_s) f_s(\mathbf{r}') d^3\mathbf{r}' = \epsilon_s f_s(\mathbf{r})$$

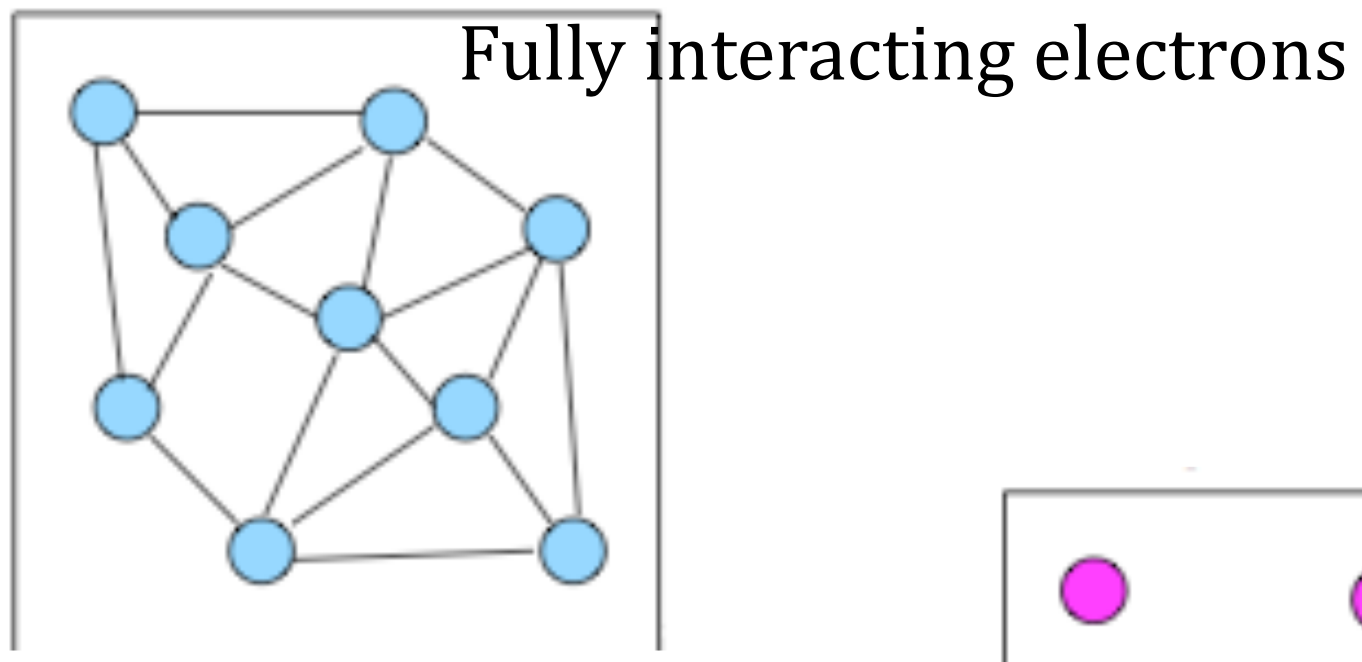
We have to know how is made the operator Σ

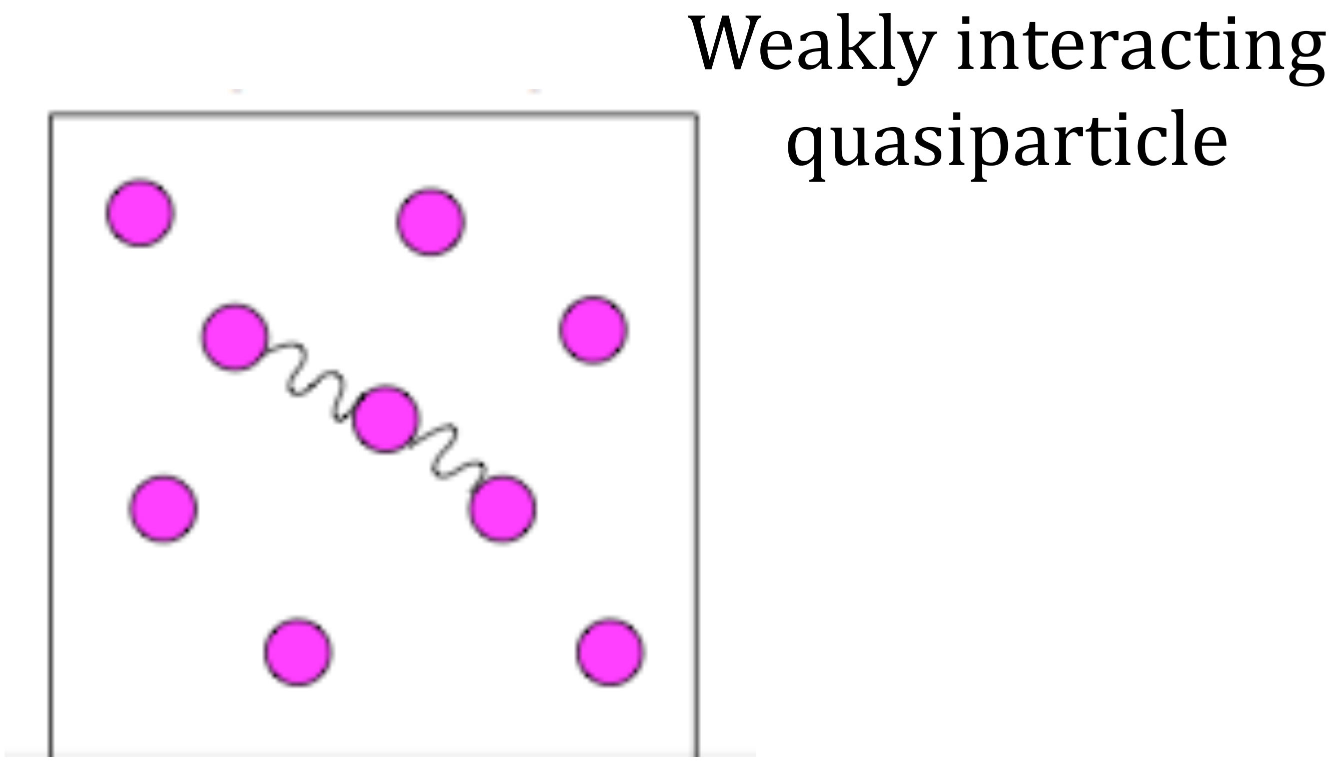
As a perturbation we do not consider the interaction V, but the screened Coulomb W that has reduced strength



W = screened potential:
weaker than bare Coulomb interaction

$$W(r, r', \omega) = \int dr'' \frac{\epsilon^{-1}(r, r'', \omega)}{|r'' - r'|}$$





Hedin's equation:

Set of integro-differential equations, whose self-consistent solution solves the many-electron problem

$$P(12) = -i \int d(34) G(13) G(41^+) \Gamma(34,2)$$

$$W(12) = V(12) + \int d(34) W(13) P(34) V(4,2)$$

$$\Sigma(12) = i \int d(34) G(14) W(1^+3) \Gamma(42,3)$$

$$G(12) = G^0(12) + \int d(34) G^0(13) \Sigma(34) G(42)$$

$$\Gamma(12,3) = \delta(12)\delta(13) + \int d(4567) \frac{\partial \Sigma(12)}{\partial G(45)} G(46) G(75) \Gamma(67,3)$$

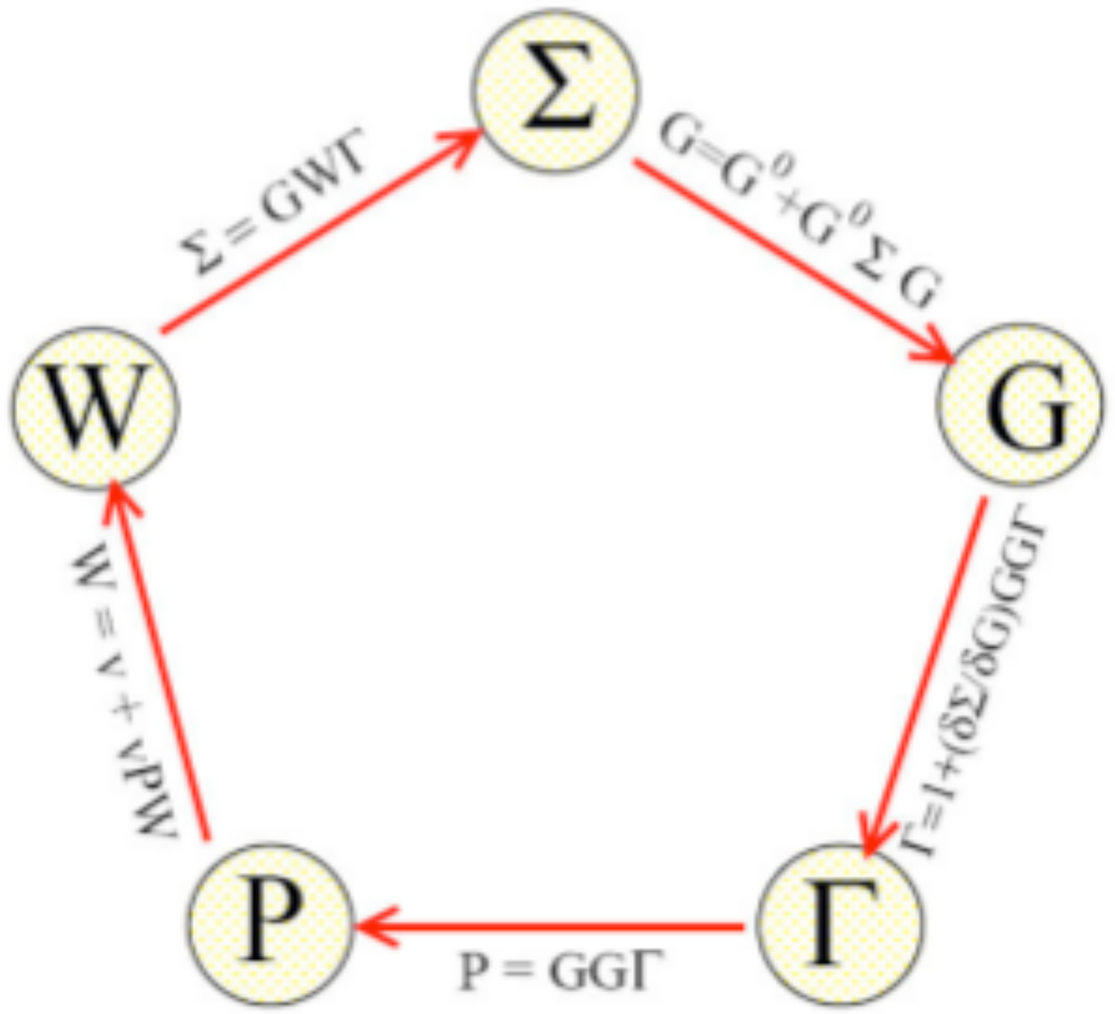
L. Hedin, Phys Rev. 139, A 769 (1965)

Hedin's equation: the GW approximation

How to obtain the Self energy: Iteration of Hedin's Equations and GW

They cannot be solved numerically as they contain functional derivatives, but they can be iterated to derive useful approximations

$$\begin{aligned}
\Sigma &= iGW\Gamma \\
G &= G_0 + G_0\Sigma G \\
\Gamma &= 1 + \frac{\partial\Sigma}{\partial G}GG\Gamma \\
P &= -iGG\Gamma \\
W &= v + vPW
\end{aligned}$$



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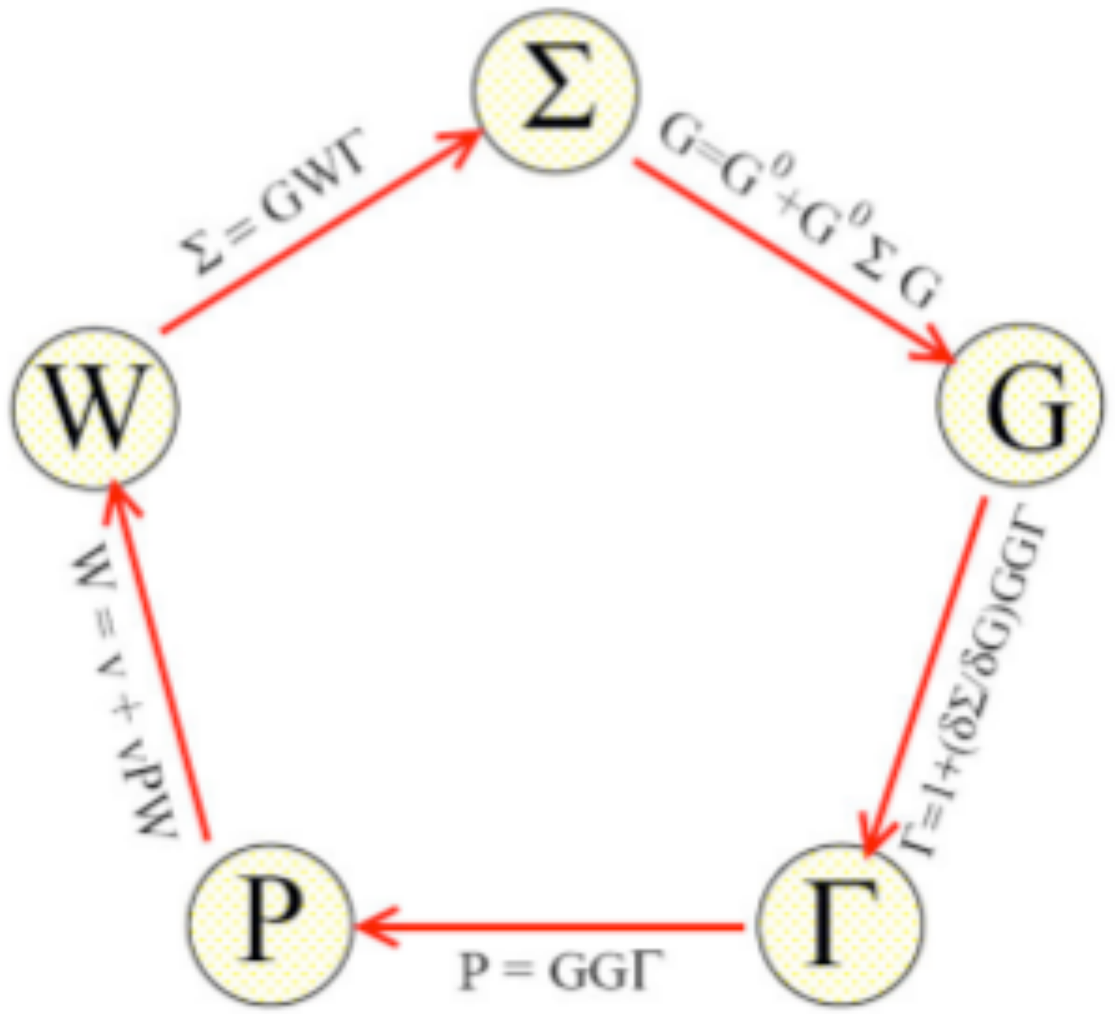

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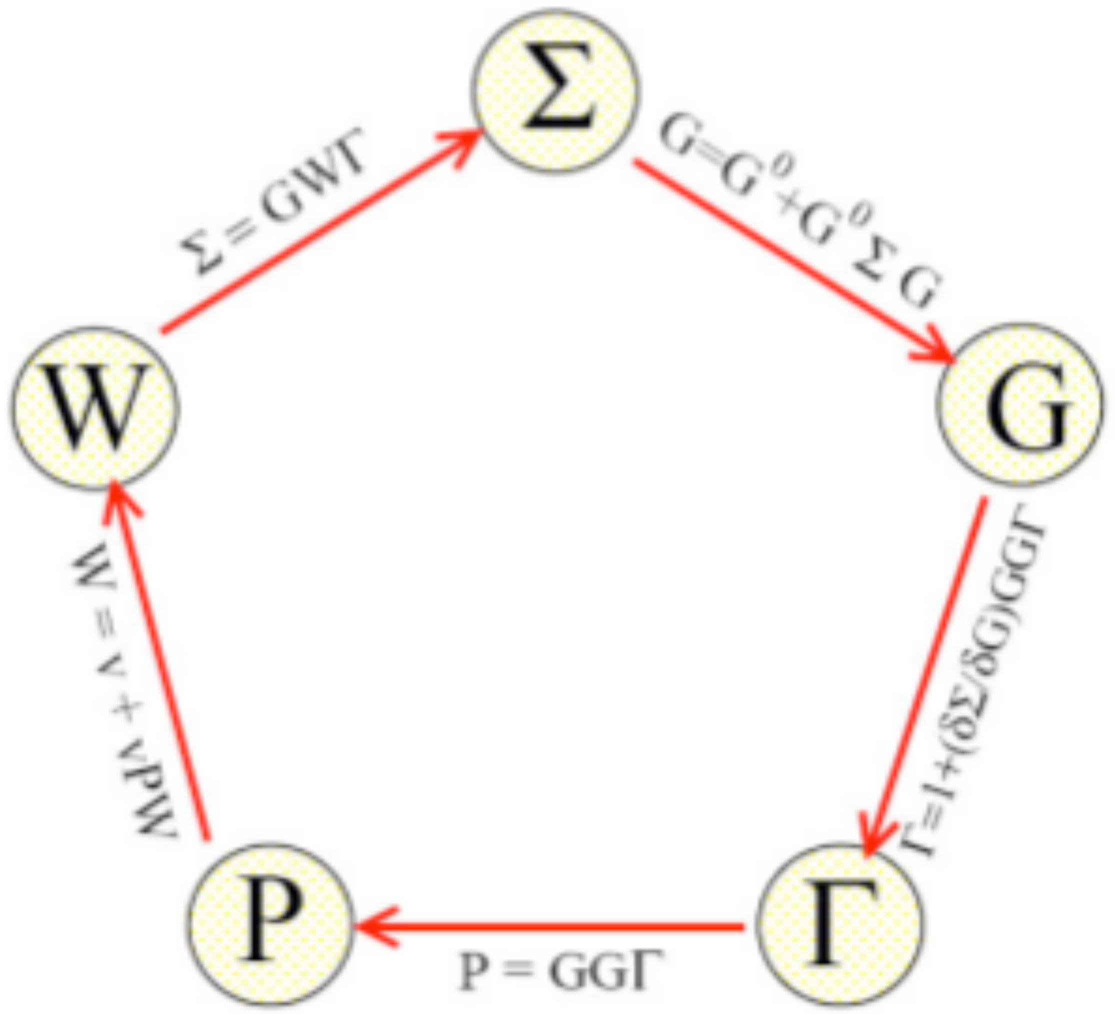

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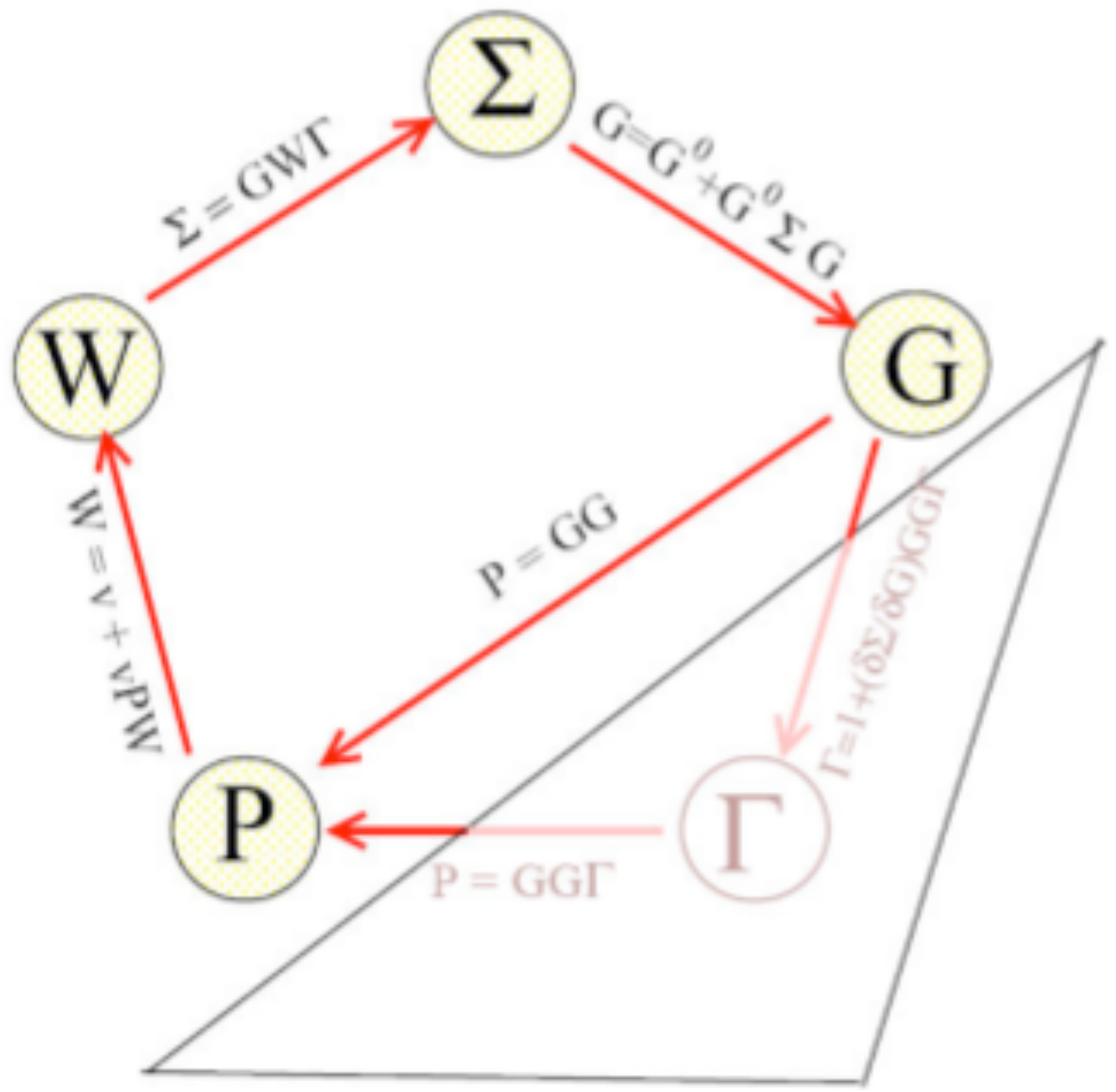

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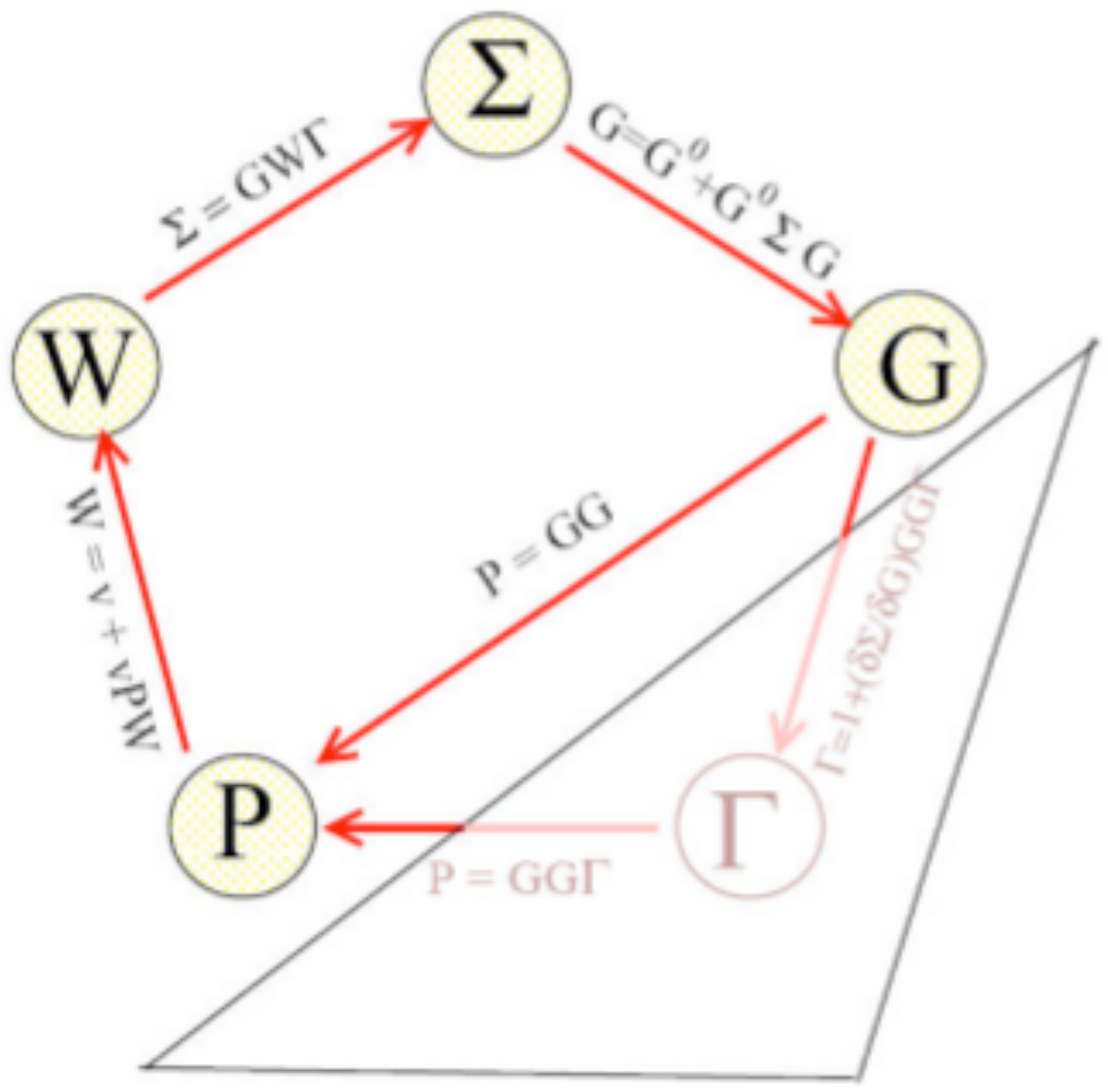

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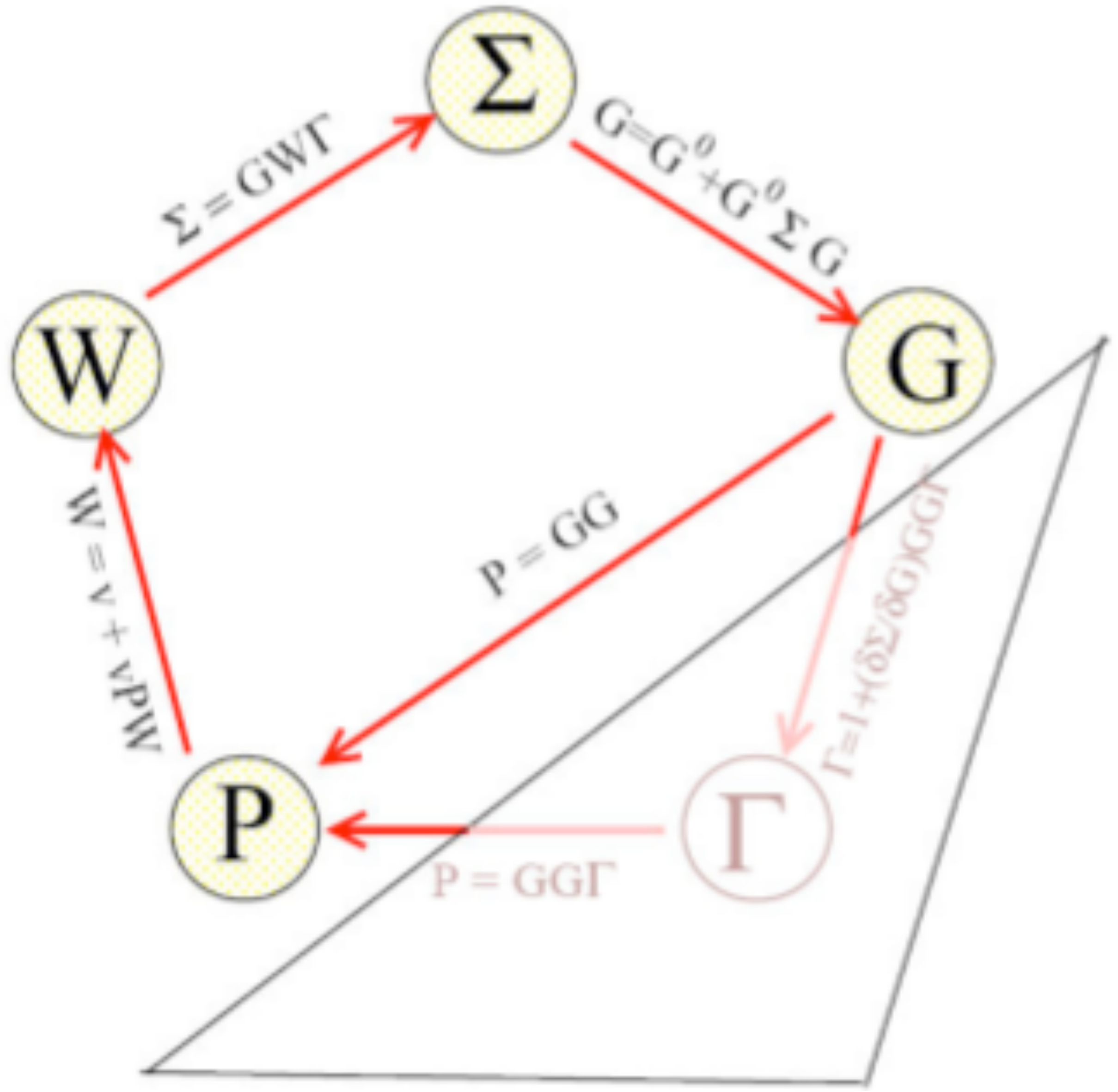

The vertex Γ has been neglected

Remark:

This is an approximation!!

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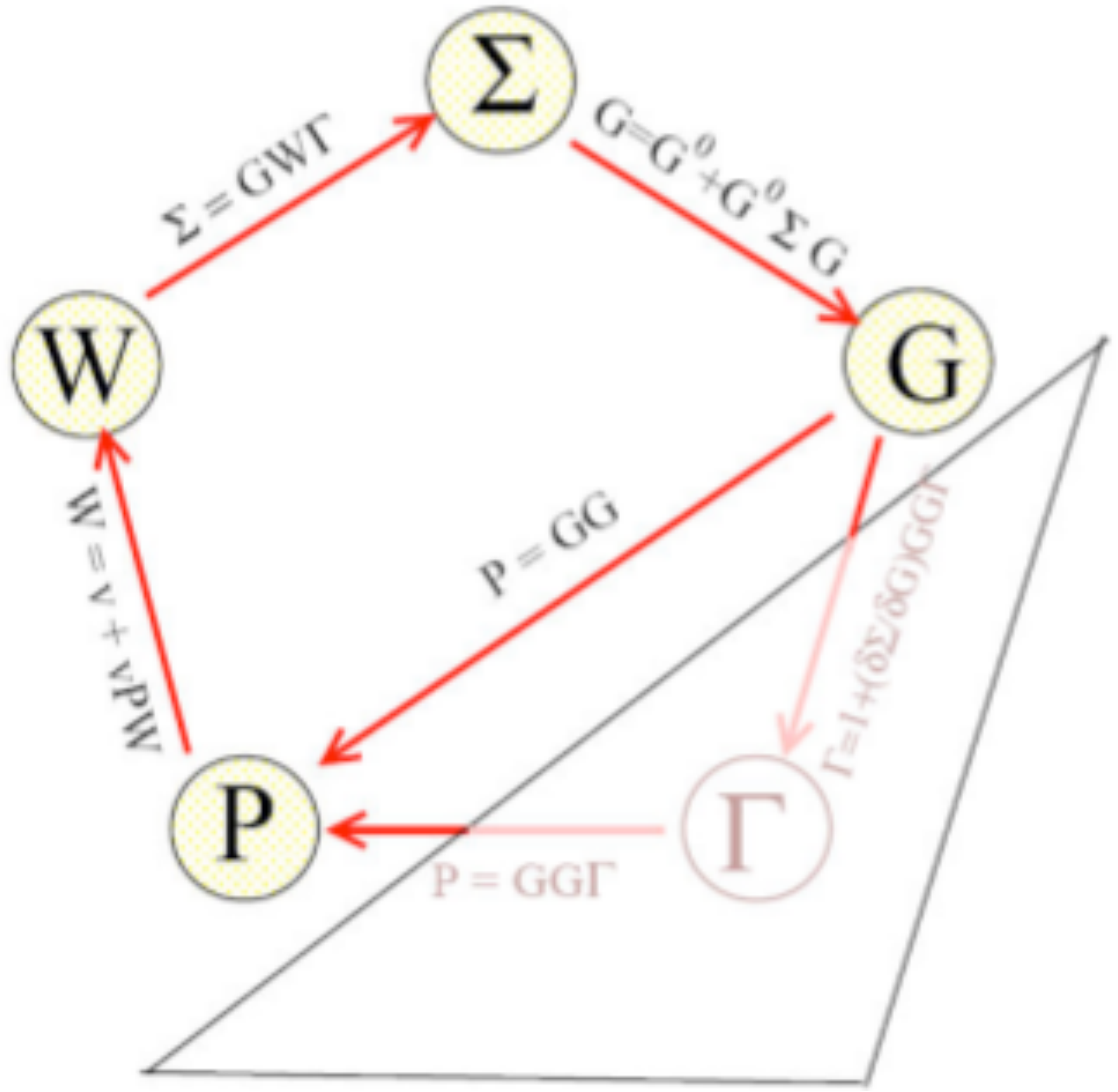

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The set of equation can be solved self-consistently but in most of the applications $G = G_0$ the so called G_0W_0 approximation

This is an approximation!!

GW approximation in practice: GoWo

Goal: $$\hat{H}_0(\mathbf{r})f_s(\mathbf{r}) + \int \Sigma(\mathbf{r},\mathbf{r}';\epsilon_s)f_s(\mathbf{r}')d^3\mathbf{r}' = \epsilon_s f_s(\mathbf{r})$$

$$\Sigma = iGW$$

GW approximation in practice: GoWo

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$$\Sigma = iGW$$

$G = G_0$ Green function of the non-interacting system

GW approximation in practice: GoWo

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$G = G_0$ Green function of the non-interacting system

$$\Sigma^{GW}(\mathbf{r_1},\mathbf{r_2};\tau) = i\hbar G_0(\mathbf{r_1},\mathbf{r_2};\tau)W(\mathbf{r_1},\mathbf{r_2};\tau+\eta)$$

In Fourier space

$$\Sigma^{GW}(\mathbf{r_1},\mathbf{r_2};\omega) = \frac{i\hbar}{2\pi}\int_{-\infty}^{\infty} G_0(\mathbf{r_1},\mathbf{r_2};\omega+\omega')W(\mathbf{r_1},\mathbf{r_2};\omega')e^{i\omega'\eta}d\omega'$$

GW approximation in practice: GoWo

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$$\Sigma = iGW$$

$G = G_0$ Green function of the non-interacting system

$$\Sigma^{GW}(\mathbf{r_1},\mathbf{r_2};\tau) = i\hbar G_0(\mathbf{r_1},\mathbf{r_2};\tau)W(\mathbf{r_1},\mathbf{r_2};\tau+\eta)$$

In Fourier space

$$\Sigma^{GW}(\mathbf{r_1},\mathbf{r_2};\omega) = \frac{i\hbar}{2\pi}\int_{-\infty}^{\infty} G_0(\mathbf{r_1},\mathbf{r_2};\omega+\omega')W(\mathbf{r_1},\mathbf{r_2};\omega')e^{i\omega'\eta}d\omega'$$

Polarization and Screening

$$W = v + vPW$$

$$P(\mathbf{r_1},\mathbf{r_2};\tau) = -i\hbar G_0(\mathbf{r_1},\mathbf{r_2};\tau)G_0(\mathbf{r_2},\mathbf{r_1};-\tau)$$

Polarisation made by non interacting electrons and holes

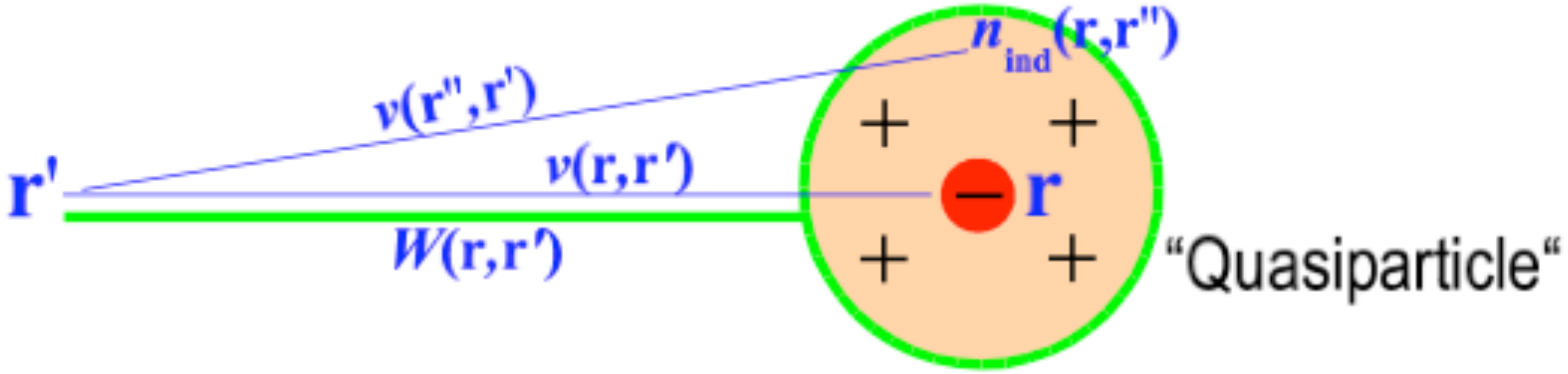
GW approximation in practice: GoWo

$\Sigma = iGW$ $G = G_0$ Green function of the non-interacting system

Screened Potential:

$$W(\mathbf{r_1},\mathbf{r_2};\omega) = \int \epsilon^{-1}(\mathbf{r_1},\mathbf{r}';\omega)v(\mathbf{r}',\mathbf{r_2})d\mathbf{r}' = v(\mathbf{r_1},\mathbf{r_2}) + \int n_{ind}(\mathbf{r_1},\mathbf{r}';\omega)v(\mathbf{r}',\mathbf{r_2})d\mathbf{r}'$$

Classical (Hartree) interaction between additional charge and polarization charge



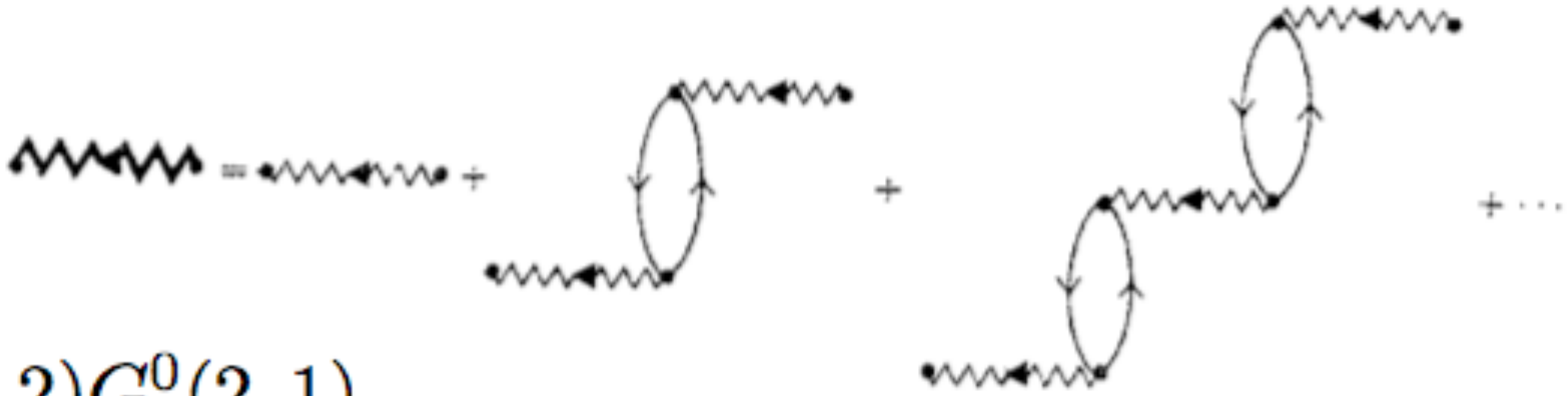
$$n_{ind}(\mathbf{r_1},\mathbf{r_2};\omega) = \int P^0(\mathbf{r_1},\mathbf{r}';\omega)V^{tot}(\mathbf{r}',\mathbf{r_2})d\mathbf{r}'$$

$$\epsilon(\mathbf{r_1},\mathbf{r_2};\omega) = \delta(\mathbf{r_1}-\mathbf{r_2}) - \int v(\mathbf{r_1}-\mathbf{r}')P^0(\mathbf{r}',\mathbf{r_2};\omega)d\mathbf{r}'$$

This is an approximation!!

RPA

$$W = v + vPW$$



Using $P(1,2) = P^0(1,2) = G^0(1,2)G^0(2,1)$

GW approximation in practice:

Evaluation of the Self-Energy

$$\Sigma^{GW} = G_0^{KS} W = G_0^{KS} V + G^{KS}(W - V) = \Sigma_x^{GW} + \Sigma_c^{GW}$$

GW approximation in practice:

Evaluation of the Self-Energy

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$$\Sigma_x^{GW}(\mathbf{r_1}, \mathbf{r_2}; \omega) = \frac{i\hbar}{2\pi} \int_{-\infty}^{\infty} G_0^{KS}(\mathbf{r_1}, \mathbf{r_2}; \omega + \omega') v(\mathbf{r_1}, \mathbf{r_2}) e^{i\omega'\eta} d\omega'$$

can be integrated analytically

$$\langle \phi_i^{KS} | \Sigma_x^{GW} | \phi_i^{KS} \rangle = -\frac{e^2}{4\pi\epsilon_0} \sum_j^{occ.} \int \frac{\phi_i^{KS*}(\mathbf{r})\phi_j^{KS}(\mathbf{r})\phi_j^{KS*}(\mathbf{r}')\phi_i^{KS}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r} d\mathbf{r}'$$

Hartree-Fock exchange term

GW approximation in practice:

Evaluation of the Self-Energy

$$\Sigma^{GW} = G_0^{KS} W = G_0^{KS} V + G^{KS}(W - V) = \Sigma_x^{GW} + \Sigma_c^{GW}$$

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Hartree-Fock exchange term

$$\Sigma_c^{GW}(\mathbf{r_1}, \mathbf{r_2}; \omega) = \frac{i\hbar}{2\pi} \int_{-\infty}^{\infty} G_0^{KS}(\mathbf{r_1}, \mathbf{r_2}; \omega + \omega') [W(\mathbf{r_1}, \mathbf{r_2}; \omega') - v(\mathbf{r_1}, \mathbf{r_2})] e^{i\omega'\eta} d\omega'$$

have to be computed numerically; most time consuming part

Different implementations

Code	Basis set	References
Berkeley*GW*	Plane waves	Deslippe et al., 2012
Yambo	Plane waves	Marini et al., 2009
WEST	Plane waves	Govoni and Galli, 2015
SaX	Plane waves	Martin-Samos and Bussi, 2009
Sternheimer*GW*	Plane waves	Giustino et al., 2010a; Schlipf et al., 2019
ABINIT	Plane waves (PAW)	Gonze et al., 2009
VASP	Plane waves (PAW)	Shishkin and Kresse, 2006a; Liu et al., 2016

Code	Basis set	References
GPAW	Plane waves (PAW)	Hüser et al., 2013b
Fiesta	Gaussian	Blase et al., 2011
Turbomole	Gaussian	van Setten et al., 2013
CP2K	Gaussian	Wilhelm et al., 2016, 2018
MOLGW	Gaussian	Bruneval et al., 2016
FHI-aims	NAO	Ren et al., 2012a; Golze et al., 2018
exciting	FLAPW	Gulans et al., 2014
SPEX	FLAPW	Friedrich et al., 2010
FHI-gap	FLAPW	Jiang et al., 2013
Tombo	Augmented	Ono et al., 2015
Questaal	LMTO	Methfessel et al., 2000; Questaal, 2018

Real Space and Real Time: H.N. Rojas, R. W. Godby and R. J. Needs PRL 74, 1827 (1995)

Use of Wannier Function: P. Umari, G. Stenuit and S. Baroni PRB 79, 201104(R) (2009)

GW approximation in practice:

Plane wave representation:

$$\langle n\mathbf{k}|\Sigma_x(\mathbf{r_1},\mathbf{r_2})|\mathbf{n'k'}\rangle = -\sum_{\mathbf{n_1}}\int_{\mathbf{Bz}}\frac{\mathbf{d^3q}}{(2\pi)^3}\sum_{\mathbf{G}}\mathbf{v}(\mathbf{q}+\mathbf{G})\rho_{\mathbf{n},\mathbf{n_1}}(\mathbf{q},\mathbf{G})\rho^*_{\mathbf{n'n_1}}(\mathbf{q},\mathbf{G})\mathbf{f_{n_1k_1}}$$

$$\rho_{nn1}(\mathbf{q}+\mathbf{G}) = \langle n\mathbf{k}|e^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}}|n1\mathbf{k_1}\rangle$$

$$\langle n\mathbf{k}|\Sigma_c(\mathbf{r_1},\mathbf{r_2};\omega)|\mathbf{n'k'}\rangle = \frac{1}{2}\sum_{\mathbf{n_1}}\int_{\mathbf{Bz}}\frac{\mathbf{d^3q}}{(2\pi)^3}\Big\{\sum_{\mathbf{GG'}}\mathbf{v}(\mathbf{q}+\mathbf{G})\rho_{\mathbf{n},\mathbf{n_1}}(\mathbf{q},\mathbf{G})\rho^*_{\mathbf{n'n_1}}(\mathbf{q},\mathbf{G'})\times$$

$$\times\int\frac{d\omega'}{2\pi}\epsilon^{-1}_{\mathbf{GG'}}(\mathbf{q},\omega')\Big[\frac{f_{n1(\mathbf{k}-\mathbf{q})}}{\omega-\omega'-\epsilon^{LDA}_{n1(\mathbf{k}-\mathbf{q})}-i\delta}+\frac{1-f_{n1(\mathbf{k}-\mathbf{q})}}{\omega-\omega'-\epsilon^{LDA}_{n1(\mathbf{k}-\mathbf{q})}+i\delta}\Big]\Big\}$$

What makes GW calculations even at G0W0 level rather “laborious”:

Careful is needed:

Integration over the Brillouin zone

GW approximation in practice:

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$$\langle n\mathbf{k}|\Sigma_x(\mathbf{r_1},\mathbf{r_2})|\mathbf{n'k'}\rangle = -\sum_{\mathbf{n_1}}\int_{\mathbf{Bz}}\frac{\mathbf{d^3q}}{(2\pi)^3}\sum_{\mathbf{G}}\mathbf{v}(\mathbf{q}+\mathbf{G})\rho_{\mathbf{n,n_1}}(\mathbf{q},\mathbf{G})\rho^*_{\mathbf{n'n_1}}(\mathbf{q},\mathbf{G})\mathbf{f_{n_1k_1}}$$

$$\rho_{nn1}(\mathbf{q}+\mathbf{G}) = \langle n\mathbf{k}|e^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}}|n1\mathbf{k_1}\rangle$$

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What makes GW calculations even at G0W0 level rather “laborious”:

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$$\times\int\frac{d\omega'}{2\pi}\epsilon^{-1}_{\mathbf{GG'}}(\mathbf{q},\omega')\Big[\frac{f_{n1(\mathbf{k}-\mathbf{q})}}{\omega-\omega'-\epsilon^{LDA}_{n1(\mathbf{k}-\mathbf{q})}-i\delta}+\frac{1-f_{n1(\mathbf{k}-\mathbf{q})}}{\omega-\omega'-\epsilon^{LDA}_{n1(\mathbf{k}-\mathbf{q})}+i\delta}\Big]\Big\}$$

What makes GW calculations even at G0W0 level rather “laborious”:

Careful is needed:

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Plane wave cutoff for exchange and dielectric matrix

Sum over unoccupied states

GW approximation in practice:

Plane wave representation:

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$$\rho_{nn1}(\mathbf{q}+\mathbf{G}) = \langle n\mathbf{k}|e^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}}|n1\mathbf{k_1}\rangle$$

$$\langle n\mathbf{k}|\Sigma_c(\mathbf{r_1},\mathbf{r_2};\omega)|\mathbf{n'k'}\rangle = \frac{1}{2}\sum_{\mathbf{n_1}}\int_{\mathbf{Bz}}\frac{\mathbf{d^3q}}{(2\pi)^3}\left\{\sum_{\mathbf{GG'}}\mathbf{v}(\mathbf{q}+\mathbf{G})\rho_{\mathbf{n},\mathbf{n_1}}(\mathbf{q},\mathbf{G})\rho^*_{\mathbf{n'}\mathbf{n_1}}(\mathbf{q},\mathbf{G'})\times\right.$$

$$\left.\times\int\frac{d\omega'}{2\pi}\epsilon^{-1}_{\mathbf{GG'}}(\mathbf{q},\omega')\left[\frac{f_{n1(\mathbf{k}-\mathbf{q})}}{\omega-\omega'-\epsilon^{LDA}_{n1(\mathbf{k}-\mathbf{q})}-i\delta}+\frac{1-f_{n1(\mathbf{k}-\mathbf{q})}}{\omega-\omega'-\epsilon^{LDA}_{n1(\mathbf{k}-\mathbf{q})}+i\delta}\right]\right\}$$

What makes GW calculations even at G0W0 level rather “laborious”:

Careful is needed:

Integration over the Brillouin zone

Plane wave cutoff for exchange and dielectric matrix

Sum over unoccupied states

Integration in energy domain

GW approximation in practice:

GW approximation in practice: Plasmon-Pole approximation

$$\langle n\mathbf{k}|\Sigma_c(\mathbf{r_1},\mathbf{r_2};\omega)|\mathbf{n'k'}\rangle = \frac{\mathbf{1}}{\mathbf{2}}\sum_{\mathbf{n_1}}\int_{\mathbf{Bz}}\frac{\mathbf{d^3q}}{(\mathbf{2}\pi)^{\mathbf{3}}}\Big\{\sum_{\mathbf{GG'}}\mathbf{v}(\mathbf{q}+\mathbf{G})\rho_{\mathbf{n},\mathbf{n_1}}(\mathbf{q},\mathbf{G})\rho^*_{\mathbf{n'}\mathbf{n_1}}(\mathbf{q},\mathbf{G'})\times$$

$$\times\int\frac{d\omega'}{2\pi}\epsilon^{-1}_{\mathbf{GG'}}(\mathbf{q},\omega')\Big[\frac{f_{n1(\mathbf{k}-\mathbf{q})}}{\omega-\omega'-\epsilon^{LDA}_{n1(\mathbf{k}-\mathbf{q})}-i\delta}+\frac{1-f_{n1(\mathbf{k}-\mathbf{q})}}{\omega-\omega'-\epsilon^{LDA}_{n1(\mathbf{k}-\mathbf{q})}+i\delta}\Big]\Big\}$$

GW approximation in practice:

GW approximation in practice: Plasmon-Pole approximation

$$\langle n\mathbf{k}|\Sigma_c(\mathbf{r_1},\mathbf{r_2};\omega)|\mathbf{n'k'}\rangle = \frac{1}{2}\sum_{\mathbf{n_1}}\int_{\mathbf{Bz}}\frac{\mathbf{d^3q}}{(2\pi)^3}\Big\{\sum_{\mathbf{GG'}}\mathbf{v}(\mathbf{q}+\mathbf{G})\rho_{\mathbf{n},\mathbf{n_1}}(\mathbf{q},\mathbf{G})\rho^*_{\mathbf{n'n_1}}(\mathbf{q},\mathbf{G'})\times$$

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$-\Im\{\epsilon^{-1}\}$ Electron Energy Loss spectrum

All components exhibit a peak, otherwise the amplitude is small

Model Dielectric function: Plasmon-Pole approximation

GW approximation in practice: Plasmon-Pole approximation

$$\langle n\mathbf{k}|\Sigma_c(\mathbf{r_1},\mathbf{r_2};\omega)|\mathbf{n'k'}\rangle = \frac{1}{2}\sum_{\mathbf{n_1}}\int_{\mathbf{Bz}}\frac{\mathbf{d^3q}}{(2\pi)^3}\Big\{\sum_{\mathbf{GG'}}\mathbf{v(q+G)}\rho_{\mathbf{n,n_1}}(\mathbf{q},\mathbf{G})\rho^*_{\mathbf{n'n_1}}(\mathbf{q},\mathbf{G'})\times$$

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$-\Im\{\epsilon^{-1}\}$ Electron Energy Loss spectrum

All components exhibit a peak, otherwise the amplitude is small

Model Dielectric function: Plasmon-Pole approximation

$$\Im\epsilon^{-1}_{GG'}(q,\omega) = A_{GG'}(q)\{\delta[\omega-\tilde{\omega}_{GG'}(q)]-\delta[\omega+\tilde{\omega}_{GG'}(q)]\}$$

$$\Re\epsilon^{-1}_{GG'}(q,\omega) = \delta_{GG'}+\frac{\Omega_{GG'}(q)}{\omega-\tilde{\omega}_{GG'}(q)}$$

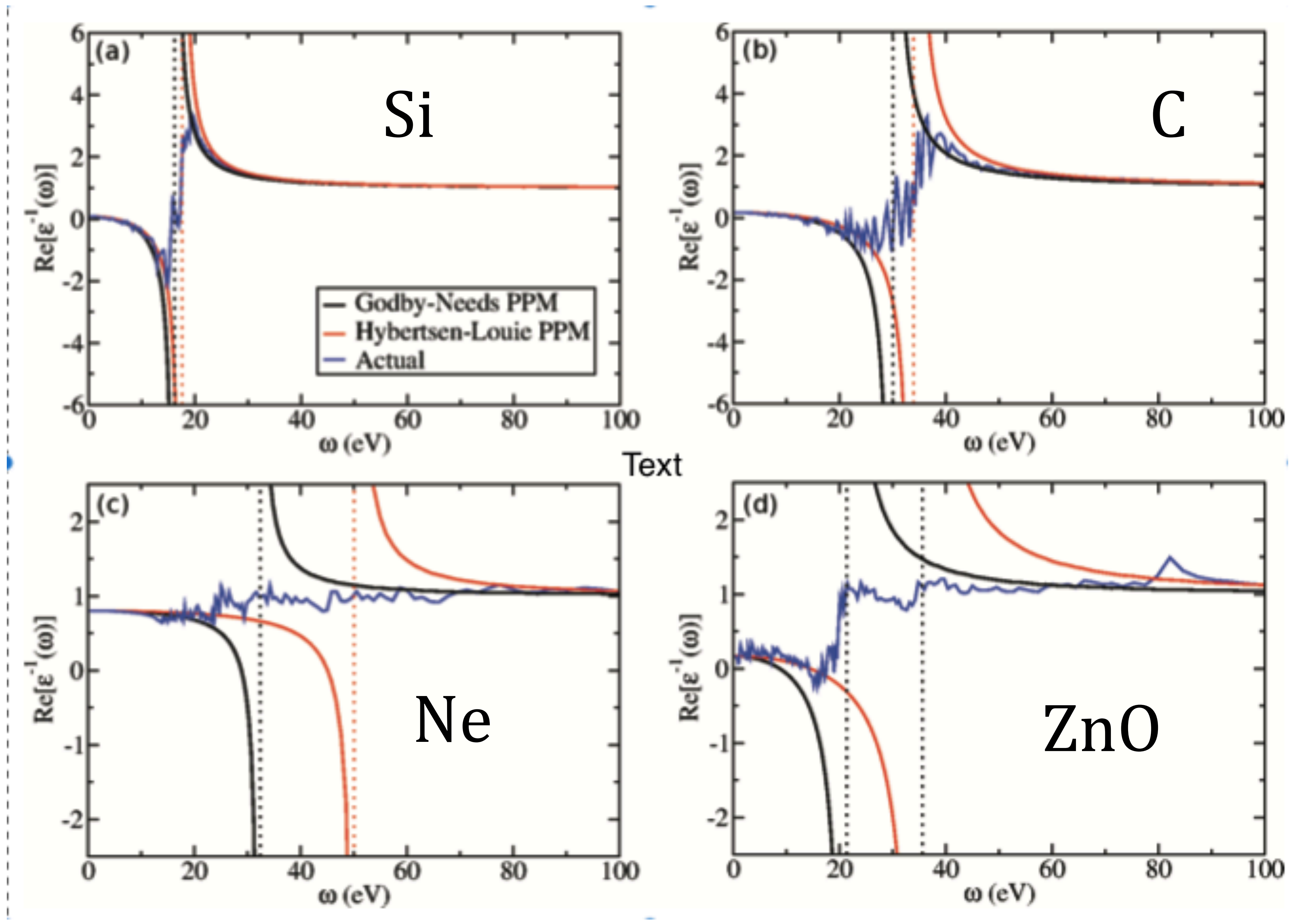
This is an approximation!!

The energy integral is now analytic

Different recipes to evaluate poles and residues

M. Hybertsen and S. Louie PRB **34**, 5390 1986
R. W. Godby and R. J. Needs, PRL. **62**, 1169 (1989).
G. E. Engel and B. Farid, PRB **47**, 15931 (1993).

GW approximation in practice: the Plasmon Pole Approximation



Real part along real axis

P. Larson, M. Dvorak, and Z. Wu Phys Rev. B **88**, 125205 (2013)

ZnO case M. Stankovki et al. Phys Rev. B **84**, 241201 (2011)

	GN	HL	vdLH	EF	Numerical	Expt.
Si	1.20	1.25	1.23	1.26	1.21	1.24
C	6.10	6.25	6.25	6.29	6.15	6.11
Ge	0.68	0.72	0.70	0.71	0.69	0.85
Ne	19.65	20.99	20.51	19.99	19.41	21.50
AlN	5.55	5.73	5.71	5.74	5.59	6.29
GaN	3.51	3.61	3.62	3.66	3.54	3.44
GaAs	1.13	1.15	1.14	1.16	1.13	1.59
MgO	7.13	7.61	7.46	7.39	7.13	7.85
ZnO	2.27	2.80	2.30	2.37	2.17	3.53

PPA become questionable when $\epsilon^{-1}_{GG'}$ differs from single-pole

Ex: interfaces, d electrons in copper: A. Marini, G. Onida, R. Del Sole PRL 88, 01643 (2002)

full integration is needed: alternative methods

GW approximation in practice: QP solution

Goal: $$\hat{H}_0(\mathbf{r})f_s(\mathbf{r}) + \int \Sigma(\mathbf{r},\mathbf{r}';\epsilon_s)f_s(\mathbf{r}')d^3\mathbf{r}' = \epsilon_s f_s(\mathbf{r})$$

$$\Sigma = iGW$$

Once we know $\Sigma^{GW} = G^0 W^0$

$$f_i^{QP}(\mathbf{r}) \approx \phi_i^{KS}(\mathbf{r})$$

⚠ **This is an approximation!! very frequently used but not always valid**

$$E_{nk}^{QP} = \epsilon_{nk} + \langle\psi_{nk}|\Sigma(E_{nk}^{QP}) - V_{xc}|\psi_{nk}\rangle$$

first order expansion around KS eigenvalue ϵ_{nk}

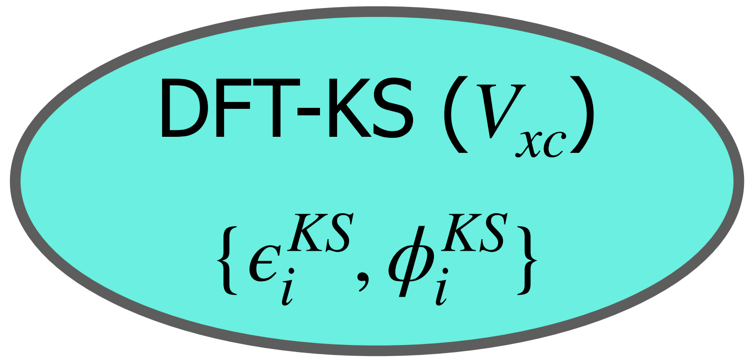
$$E_{nk}^{QP} = \epsilon_{nk} + Z_{nk}\langle\psi_{nk}|\Sigma(\epsilon_{nk}) - V_{xc}|\psi_{nk}\rangle$$

$$Z_{nk} = \left[1 - \frac{d\Sigma_{nk}(\omega)}{d\omega}|_{\omega=\epsilon_{nk}}\right]^{-1}$$

⚠ **This is an approximation!!**

The GW flow in one slide:

DFT: $\{\epsilon_{nk}\}, \{\psi_{nk}\}$

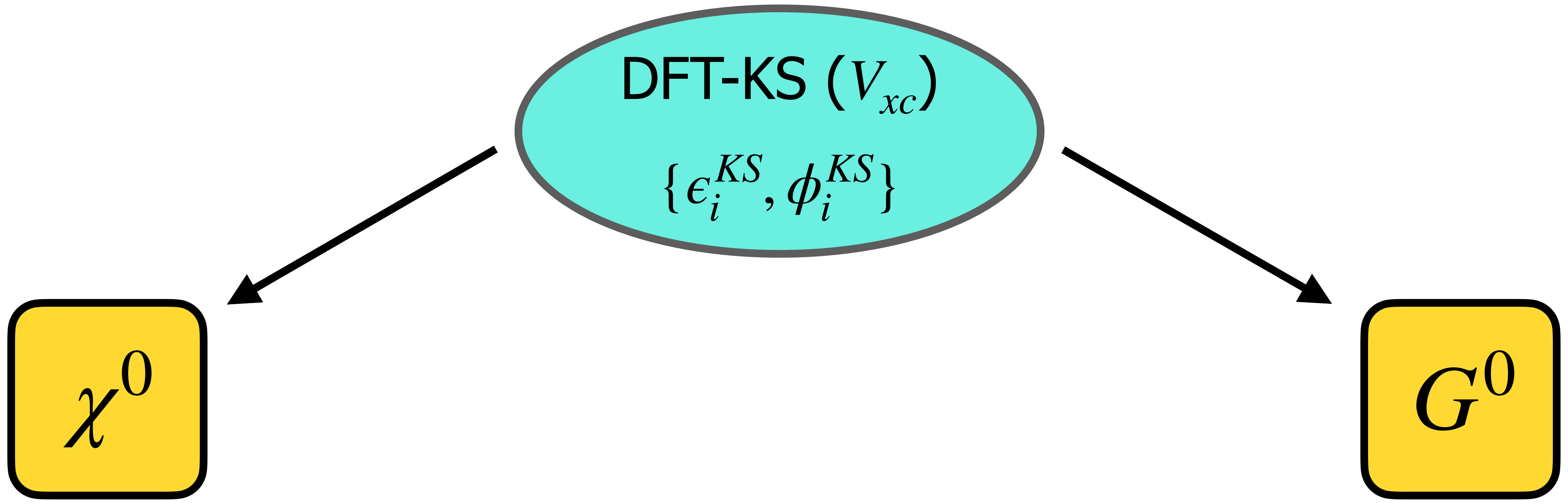


The GW flow in one slide:

DFT: $\{\epsilon_{nk}\}, \{\psi_{nk}\}$

$$G_{0,nk} = \frac{f_{nk}}{\omega - \epsilon_{nk} - i\eta} + \frac{1 - f_{nk}}{\omega - \epsilon_{nk} + i\eta}$$

$$\chi^0_{GG'}(q,\omega) = 2\sum_{vc}\int_{BZ}\frac{dk}{(2\pi)^3}\rho_{cvk}(q,G)\rho^*_{cvk}(q,G')\left[\frac{1}{\omega + \epsilon_{vk-q} - \epsilon_{ck} + i\eta} - \frac{1}{\omega + \epsilon_{ck} - \epsilon_{vk+q} - i\eta}\right]$$



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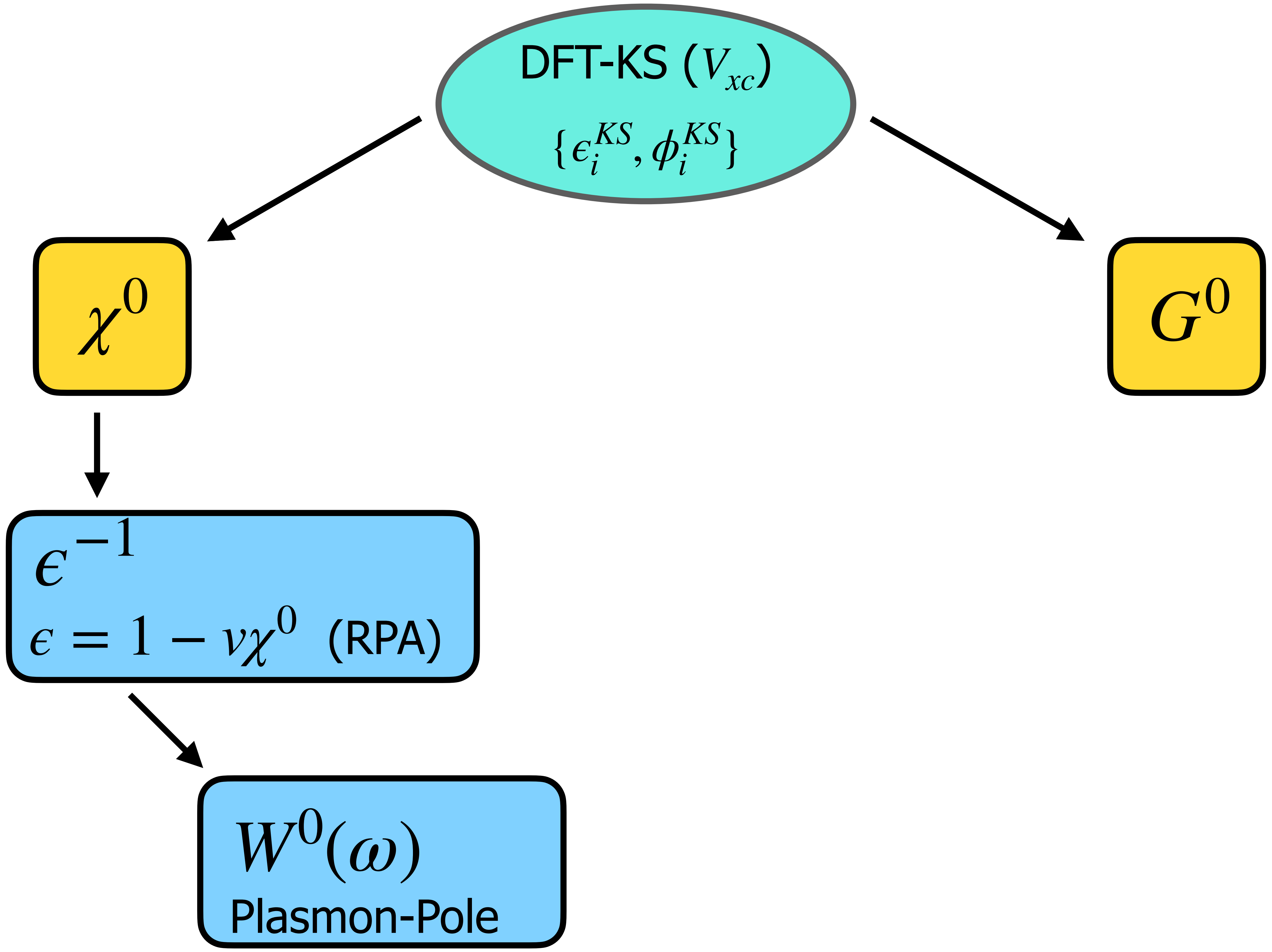
$$\chi_{GG'}(q,\omega) = \sum_{G''}\left[\delta_{GG'} + V(q+G)\chi^0_{GG'}(q,\omega)\right]^{-1}\chi^0_{GG'}(q,\omega)$$

$$\epsilon^{-1}_{GG'}(q,\omega) = \delta_{GG'} + V(q+G)\chi_{GG'}(q,\omega)$$

$$W_{GG'}(q,\omega) = \epsilon^{-1}_{GG'}(q,\omega)V(q+G)$$



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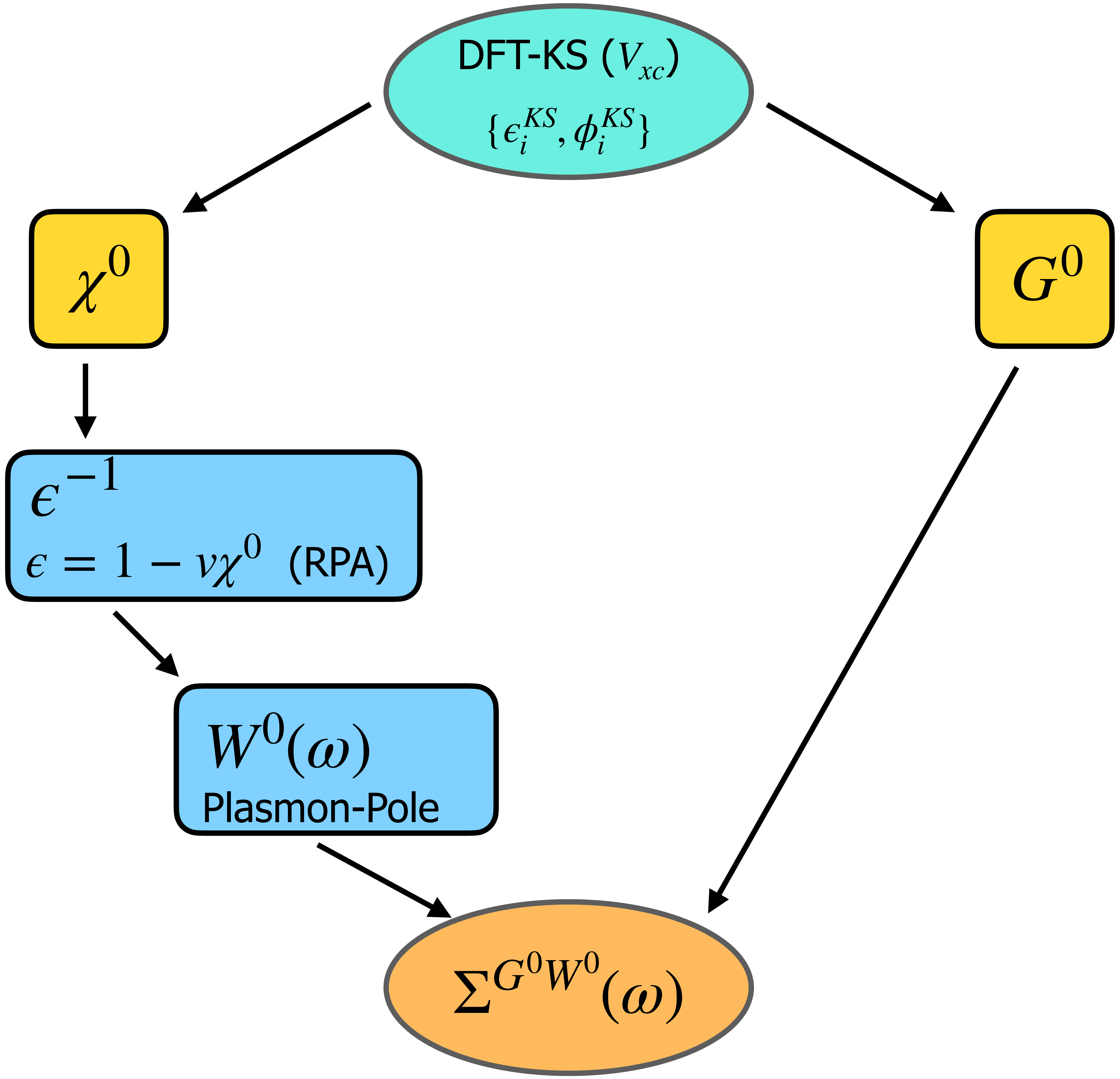
$$W_{GG'}(q,\omega) = \epsilon^{-1}_{GG'}(q,\omega)V(q+G)$$

$$\Sigma^x_{nk} = -\sum_m^{occ}\int_{BZ}\frac{dq}{(2\pi)^3}\sum_G V(q+G)\,|\rho_{nmk}(q,G)|^2$$

$$\Sigma^c_{nk}(\omega) = \sum_m\int_{BZ}\frac{dq}{(2\pi)^3}\sum_{GG'}\frac{\rho_{nmk}(q+G)R_{GG'}(q)\rho^*_{nmk}(q+G')}{\omega - \epsilon_{mk-q} + [\Omega_{GG'}(q) + i\eta]sgn(\mu - \epsilon_{mk-q})}$$



The GW flow in one slide:

DFT: $\{\epsilon_{nk}\}, \{\psi_{nk}\}$

$$G_{0,nk} = \frac{f_{nk}}{\omega - \epsilon_{nk} - i\eta} + \frac{1 - f_{nk}}{\omega - \epsilon_{nk} + i\eta}$$

$$\chi^0_{GG'}(q,\omega) = 2\sum_{vc}\int_{BZ}\frac{dk}{(2\pi)^3}\rho_{cvk}(q,G)\rho^*_{cvk}(q,G')\left[\frac{1}{\omega + \epsilon_{vk-q} - \epsilon_{ck} + i\eta} - \frac{1}{\omega + \epsilon_{ck} - \epsilon_{vk+q} - i\eta}\right]$$

$$\chi_{GG'}(q,\omega) = \sum_{G''}\left[\delta_{GG'} + V(q+G)\chi^0_{GG'}(q,\omega)\right]^{-1}\chi^0_{GG'}(q,\omega)$$

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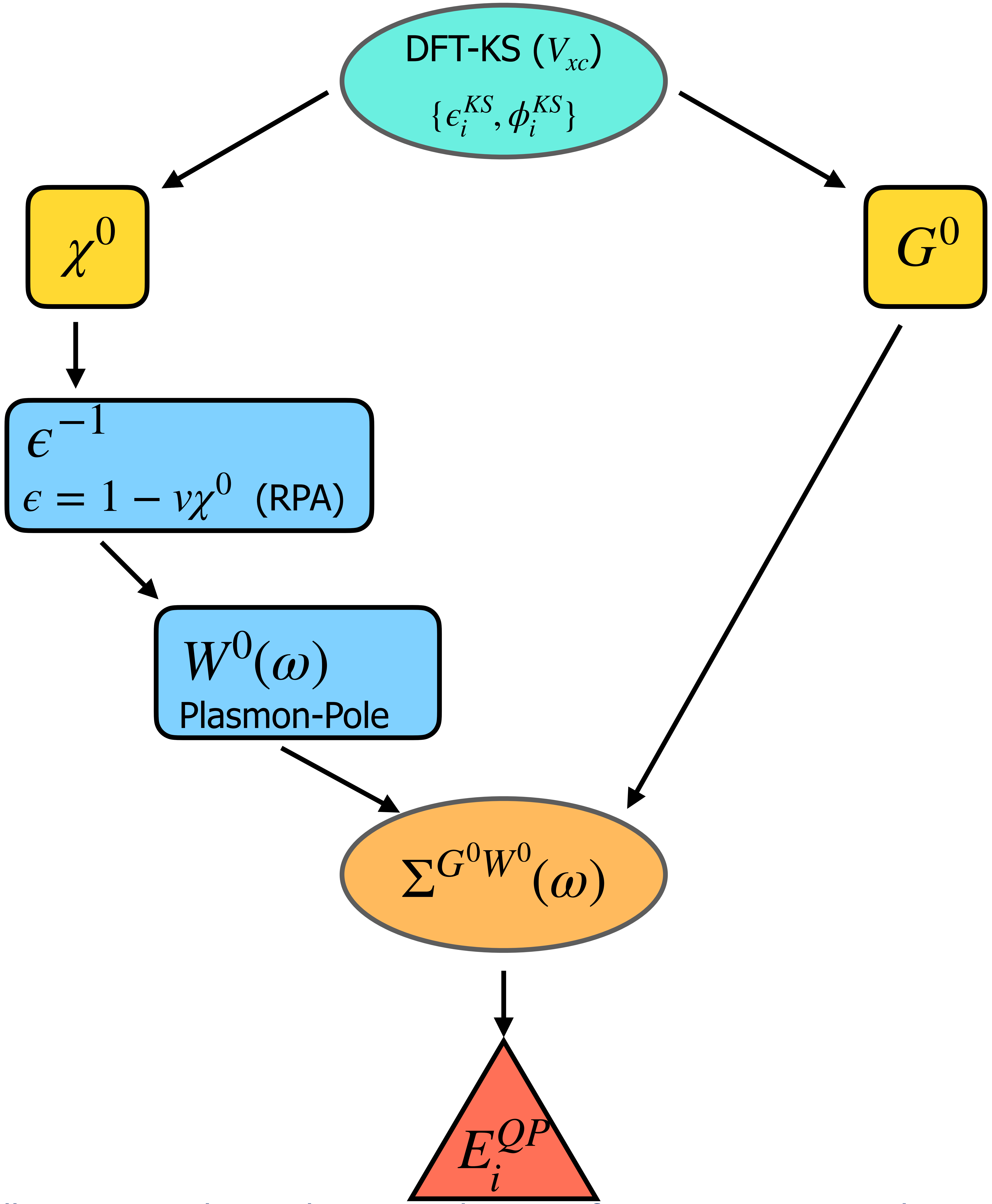
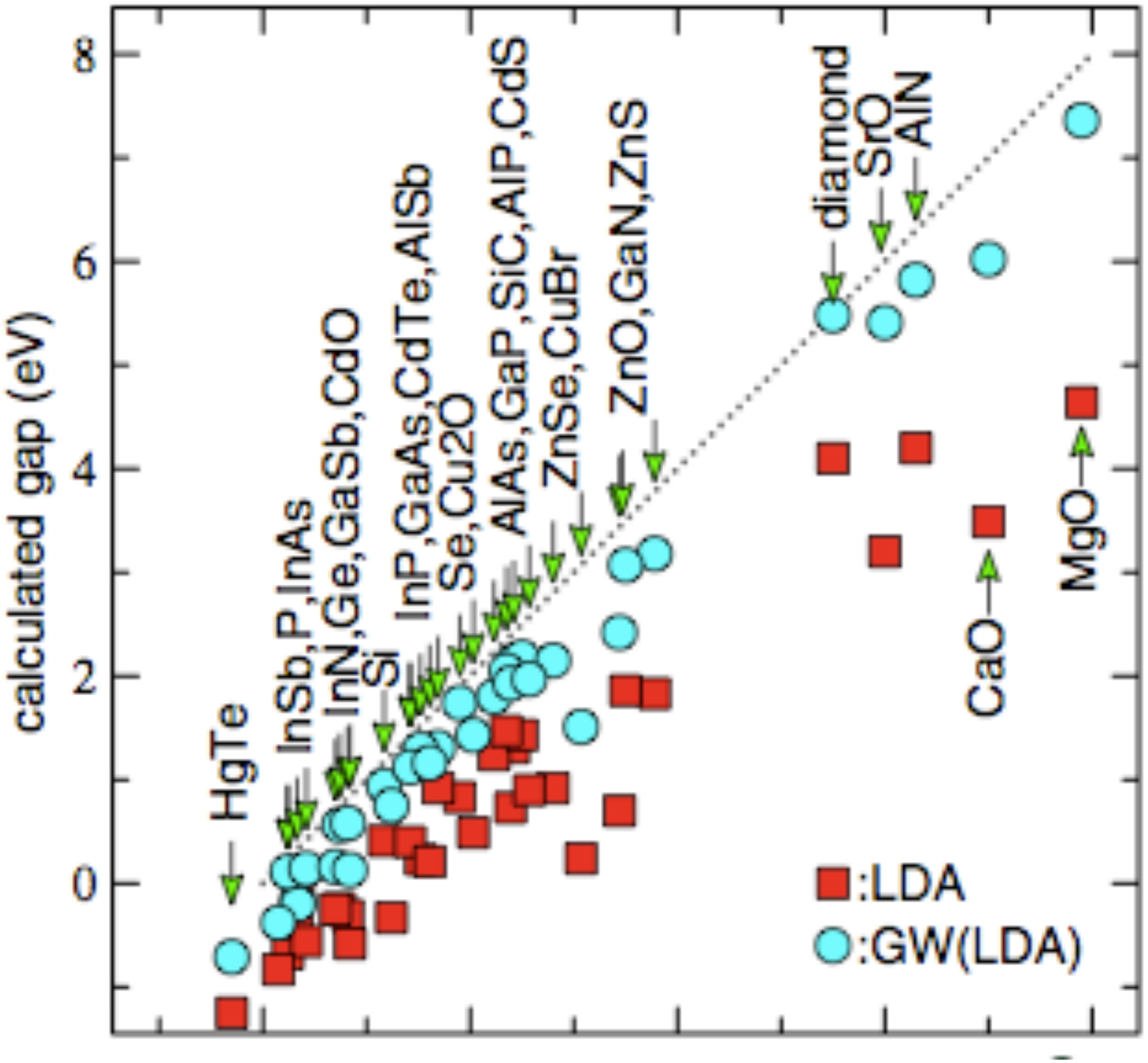
$$\epsilon^{QP}_{nk} = \epsilon_{nk} + Z_{nk}\left[\Sigma_{nk}(\epsilon_{nk}) - V_{xc,nk}\right]$$



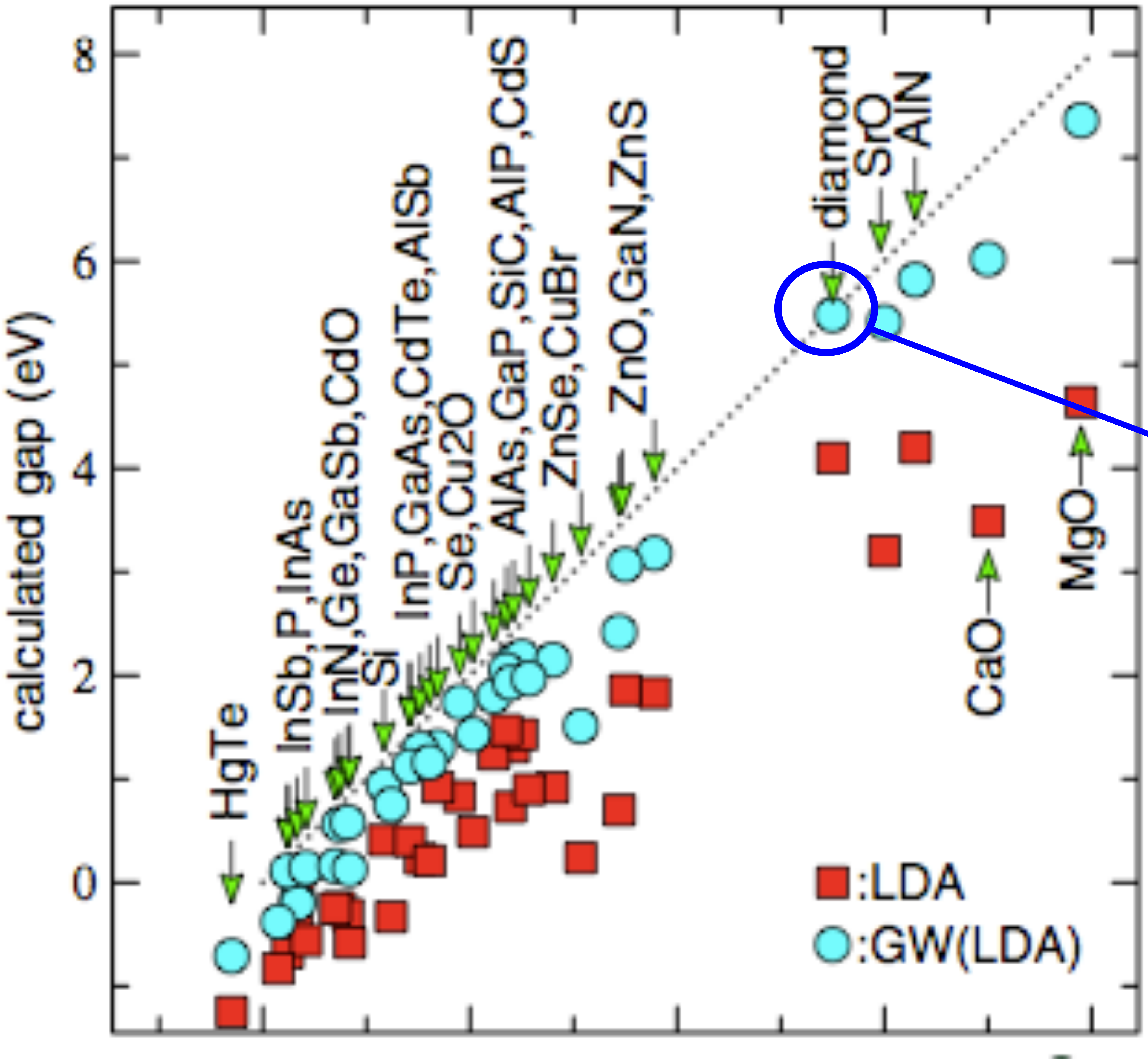
Some GW results: semiconductor band gaps



GW band gaps: huge improvement wrt the LDA

M. van Schilfgaarde, Takao Kotani, and S. Faleev PRL **96,** 226402 (2006)

Some GW results: semiconductor band gaps



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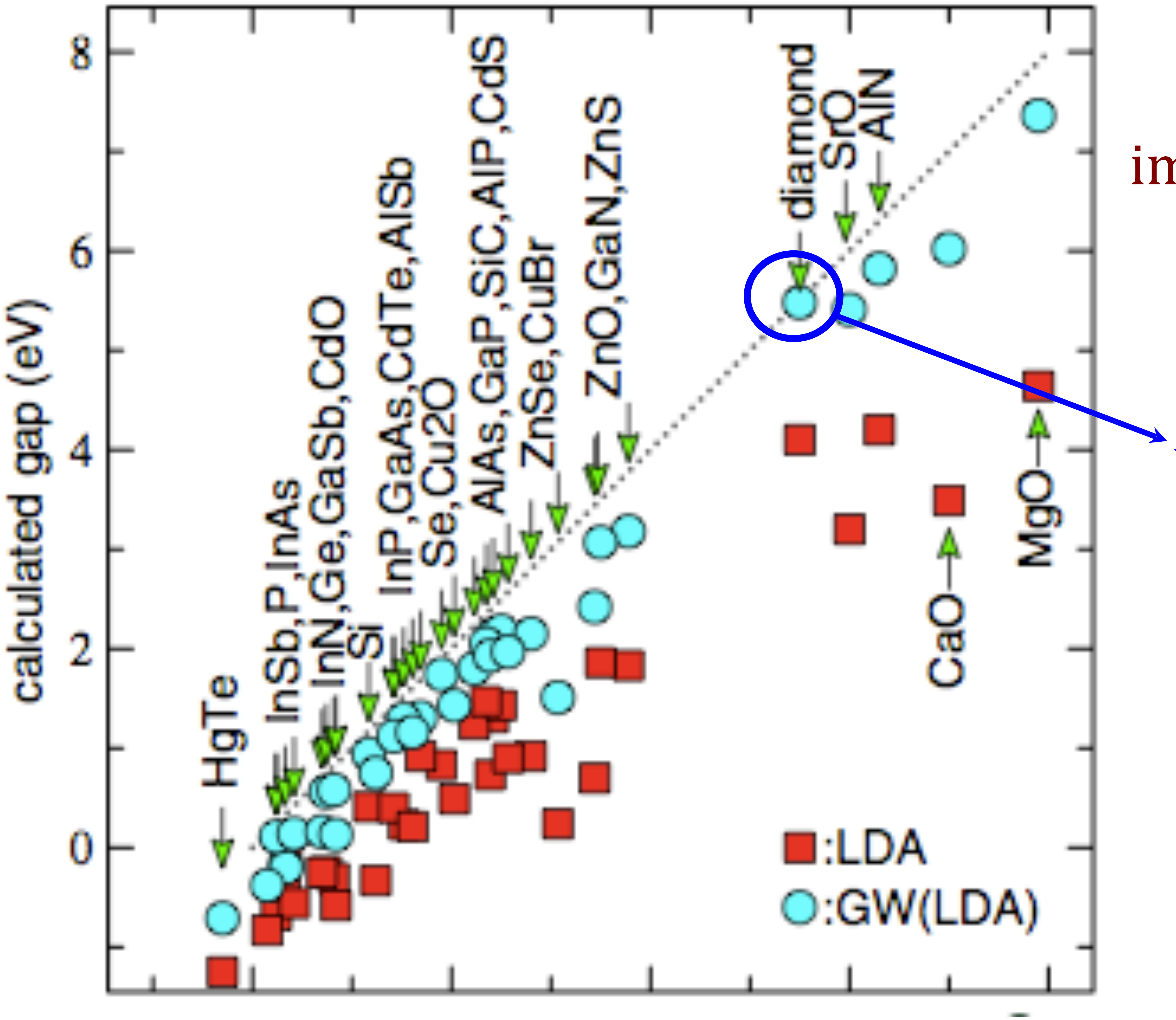

GW band gaps: huge improvement wrt the LDA

Very good agreement with the experiment!!

But for a wrong reason!!!!

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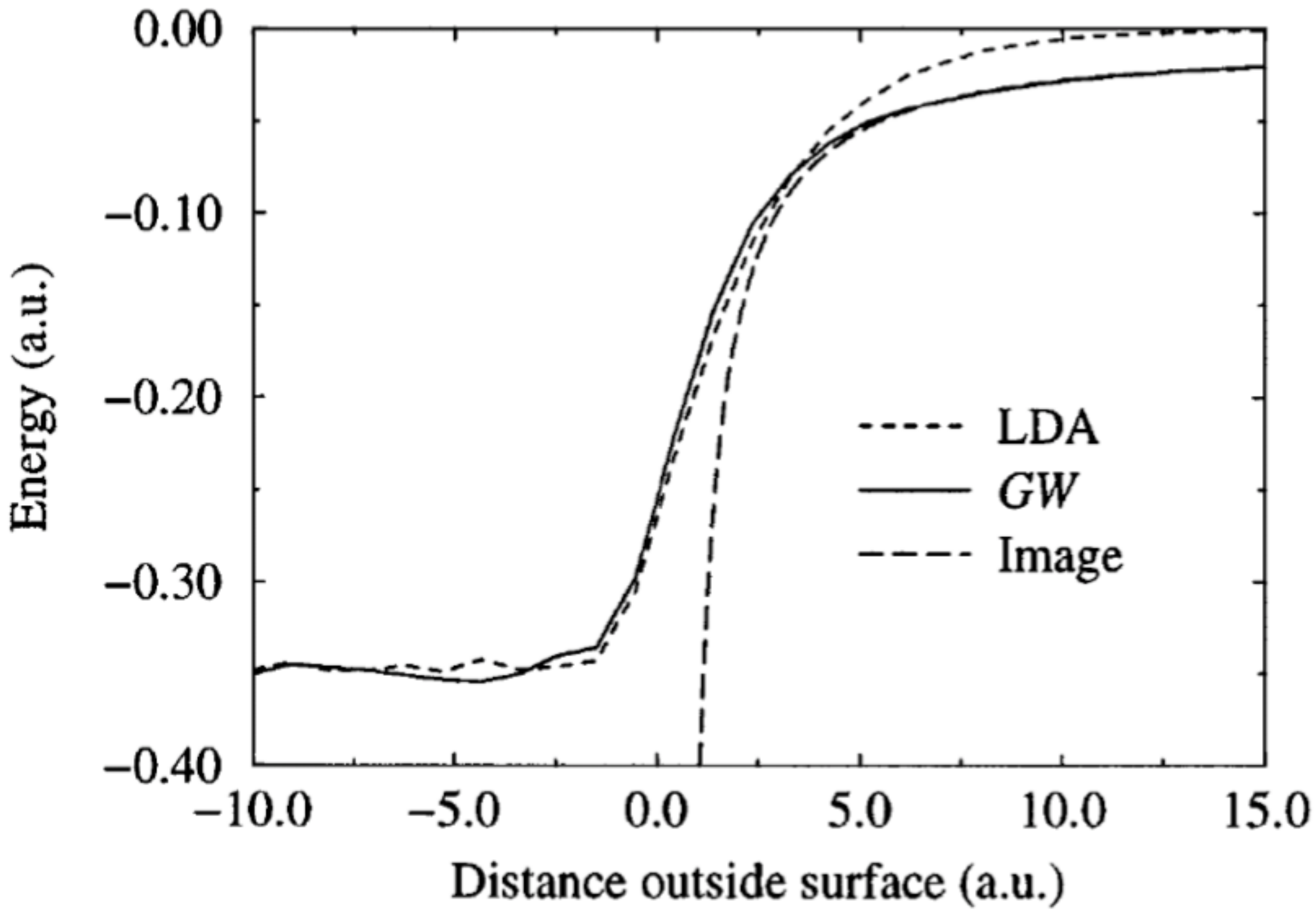
GW potential

$$V_{loc}(\mathbf{r})\psi_{QP}(\mathbf{r}) = \int d\mathbf{r}'\Sigma(\mathbf{r},\mathbf{r}',E_{QP})\psi_{QP}(\mathbf{r}')$$

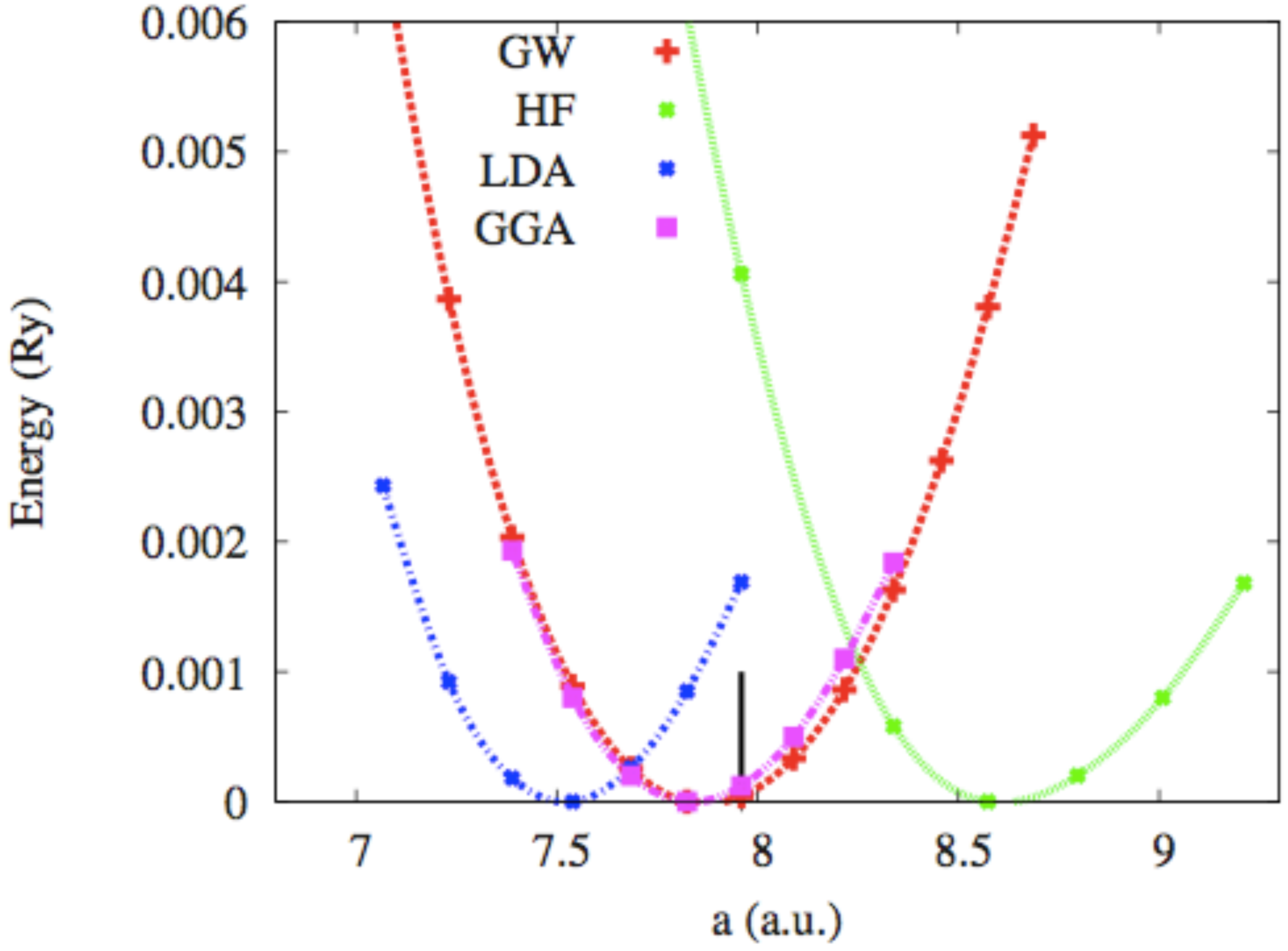
Metallic surfaces: Al (111)



I. D. White et. al., Phys. Rev. Lett. 80 (1988)

Energies by GW

Total Energy of Na vs lattice parameter



Kutepov et al. PRB 80, 041103 (2009)

Bulk Silicon band Gap

Bulk Silicon Band Gap (eV)	
Experiment	1.17
LDA	0.46
HF	6.27
G^0W^0	1.14
scGW	1.55

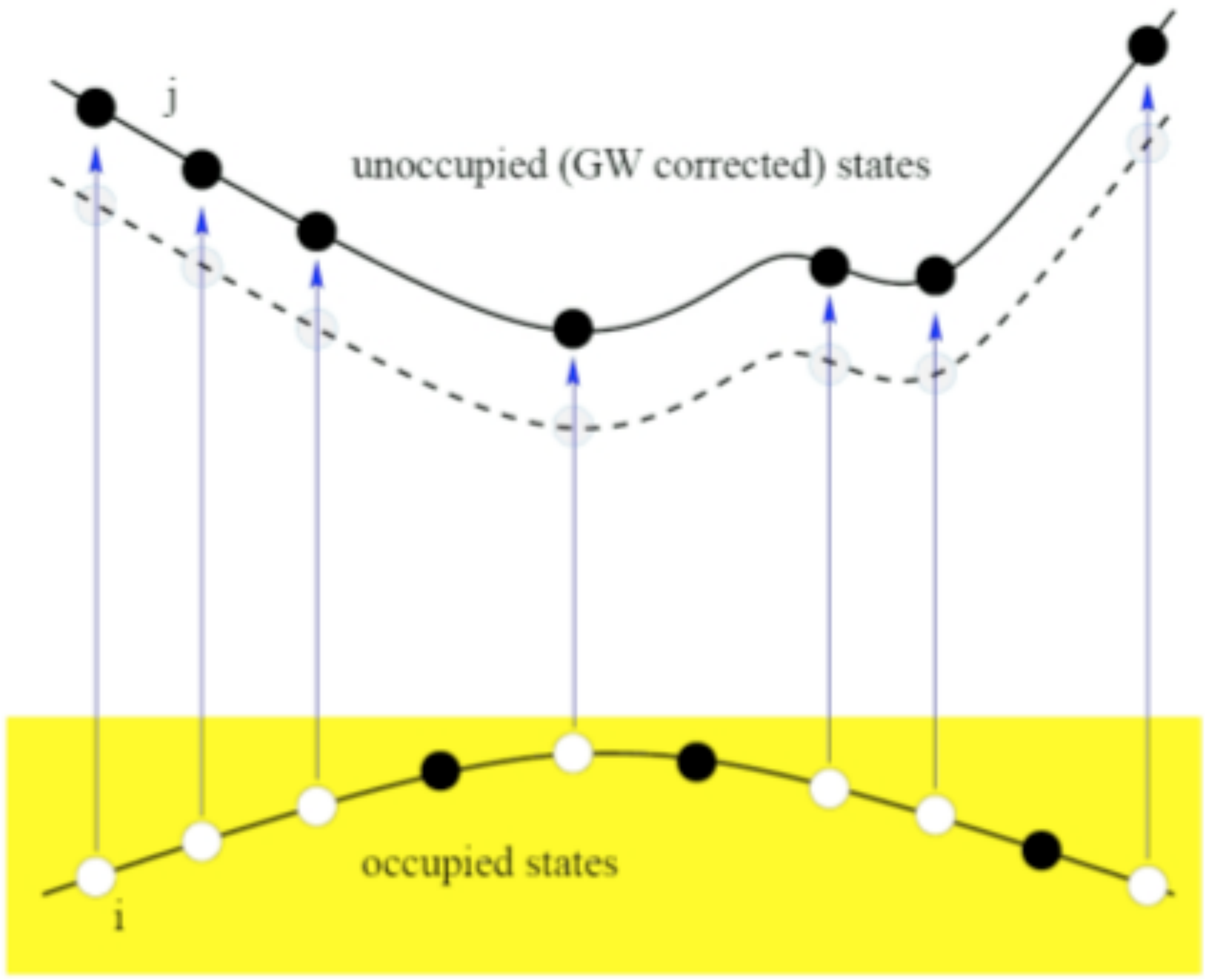
Good energy ...comparable with GGA

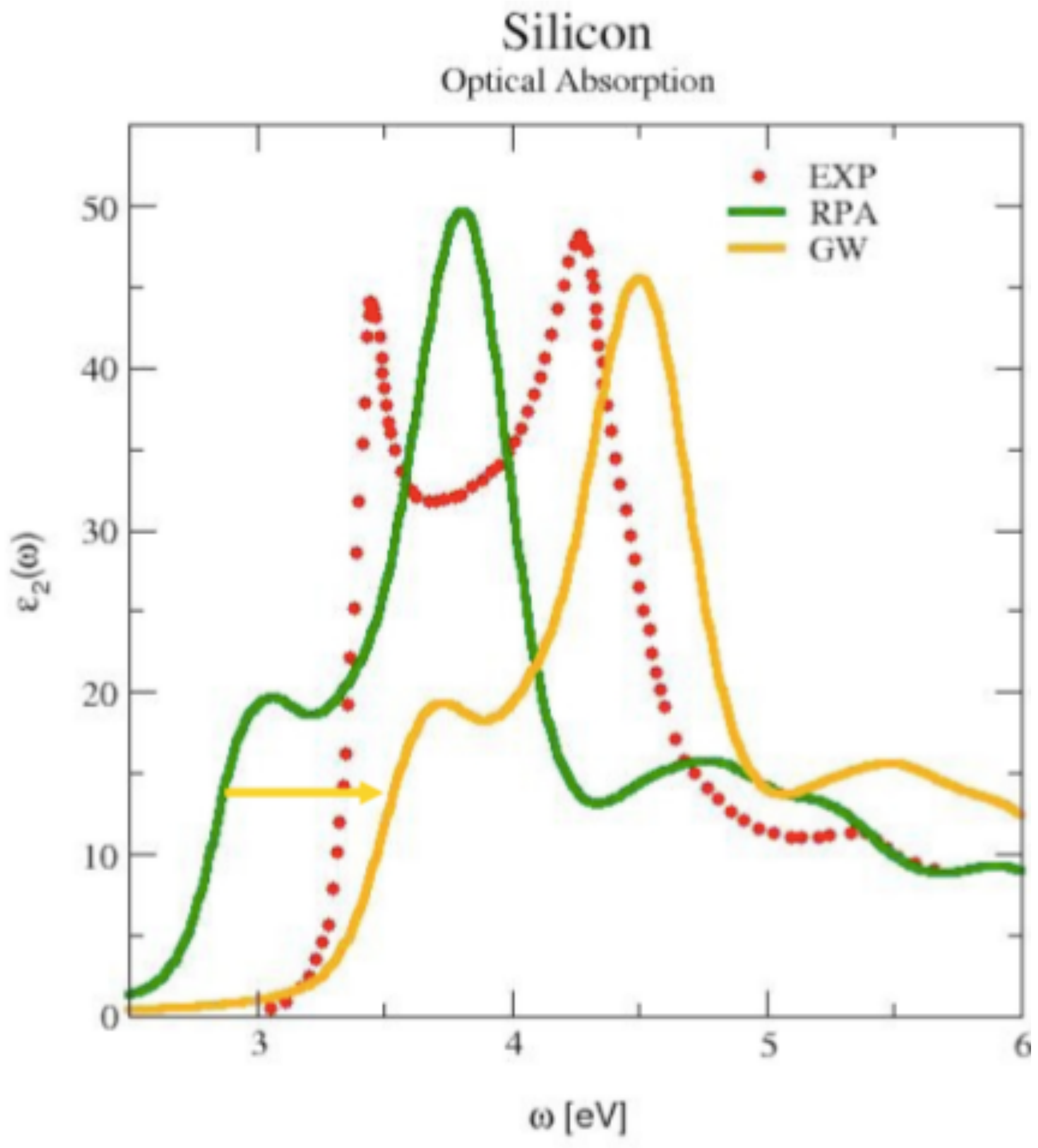
...but one-electron spectra are worse

What about absorption spectra?

Independent transitions:

$$\epsilon_2(\omega) = \frac{8\pi^2}{\Omega\omega^2} \sum_{ij} |\langle \varphi_j | \mathbf{e}\cdot\mathbf{v} | \varphi_i \rangle|^2 \delta(E_j - E_i - \omega)$$





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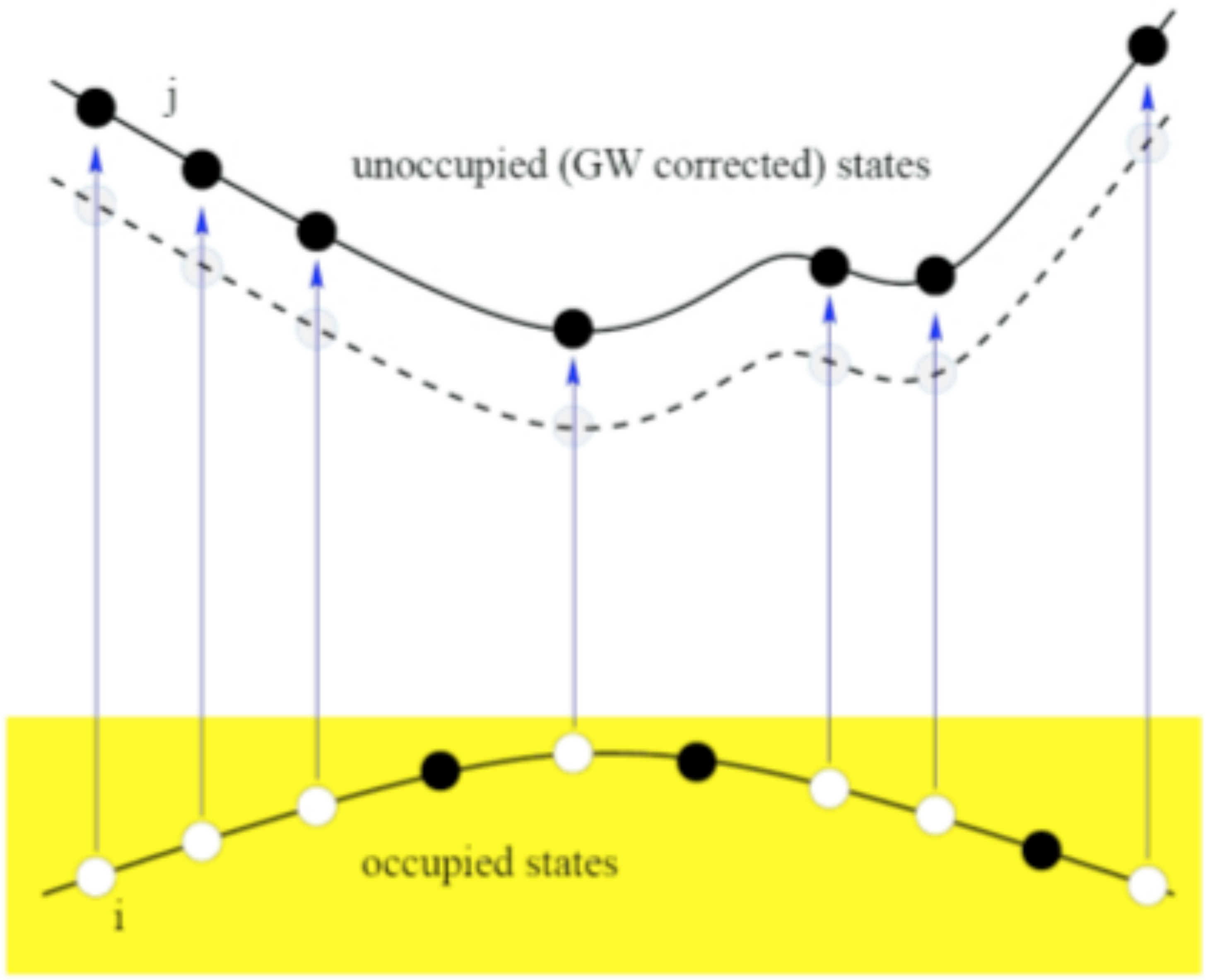

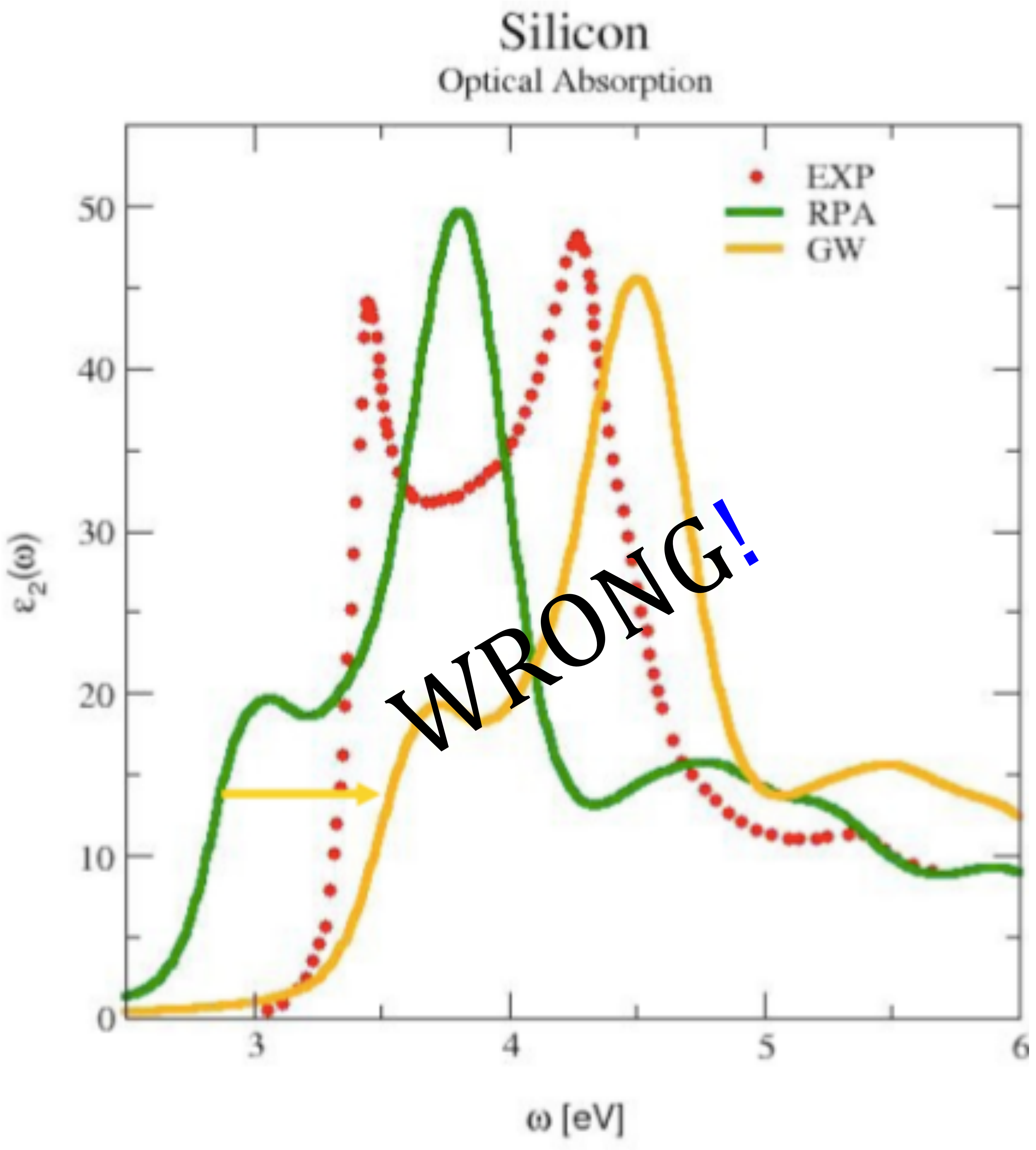

Something important is missing!!!

GW: an exascale-Class Problem

GW represents the intersection of worst-case scaling, memory intensity, and communication, making it an **ideal stress test for exascale computing.**

Why GW Is Computationally Extreme

- **Unfavourable scaling**
  - Typical cost in system size. $\mathcal{O}(N^4 - N^5)$
- **Dense linear algebra + global FFTs**
  - Heavy all-to-all communication
- **Memory pressure**
  - Tens to hundreds of TB for realistic systems
- **Limited algorithmic shortcuts**
  - Accuracy depends on explicitly resolving BZ integration

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Advancing Quantum Many-Body GW Calculations on Exascale Supercomputing Platforms (BerkeleyGW)
ACM Gordon Bell Prize Finalist (2025) B.Zhang et al. arXiv:2509.23018 (2025)

- GW calculation of a 17000 atom system
- many-body GW calculations achieving **O(1) exaFLOP/s** with strong scaling to full machines. (Frontiers, Aurora)
- Strong scaling to ~10^5 GPUs (Frontier)
- Makes predictive excited-state simulations feasible at material sizes previously unreachable by GW.

Ab-initio Quantum Transport with the GW Approximation, 42,240 Atoms, and Sustained Exascale Performance
ACM Honorable Mention (2025) N. Vetsch et al. https://doi.org/10.1145/3712285.377178 (2025)

Ab initio many-body perturbation theory (MBPT)

$$\left[-\frac{1}{2}\nabla^2 + v^{\mathrm{KS}}(\mathbf{x})\right]\psi_{n\mathbf{k}}(\mathbf{x}) = \epsilon_{n\mathbf{k}}\psi_{n\mathbf{k}}(\mathbf{x})$$

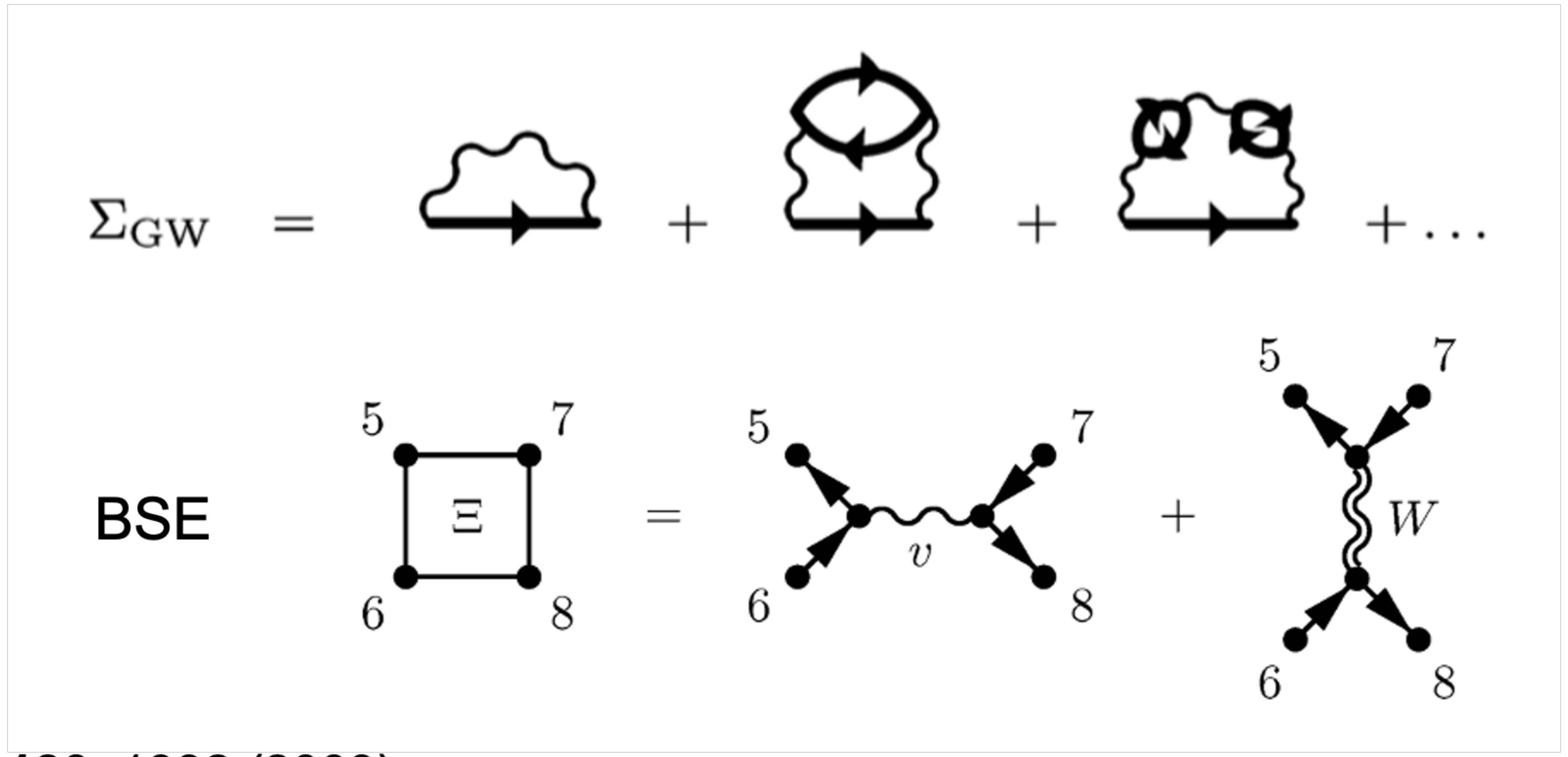
- **DFT** simulation as **input**
- interfaced to QE (MaX), Abinit

$$G(\mathbf{x},\mathbf{x}',\omega) = \sum_{n\mathbf{k}} \frac{\psi_{n\mathbf{k}}(\mathbf{x})\psi^*_{n\mathbf{k}}(\mathbf{x}')}{\omega - \epsilon_{n\mathbf{k}} \pm i0^+}$$

- the **DFT Green's function** used to compute **MBPT** quantities

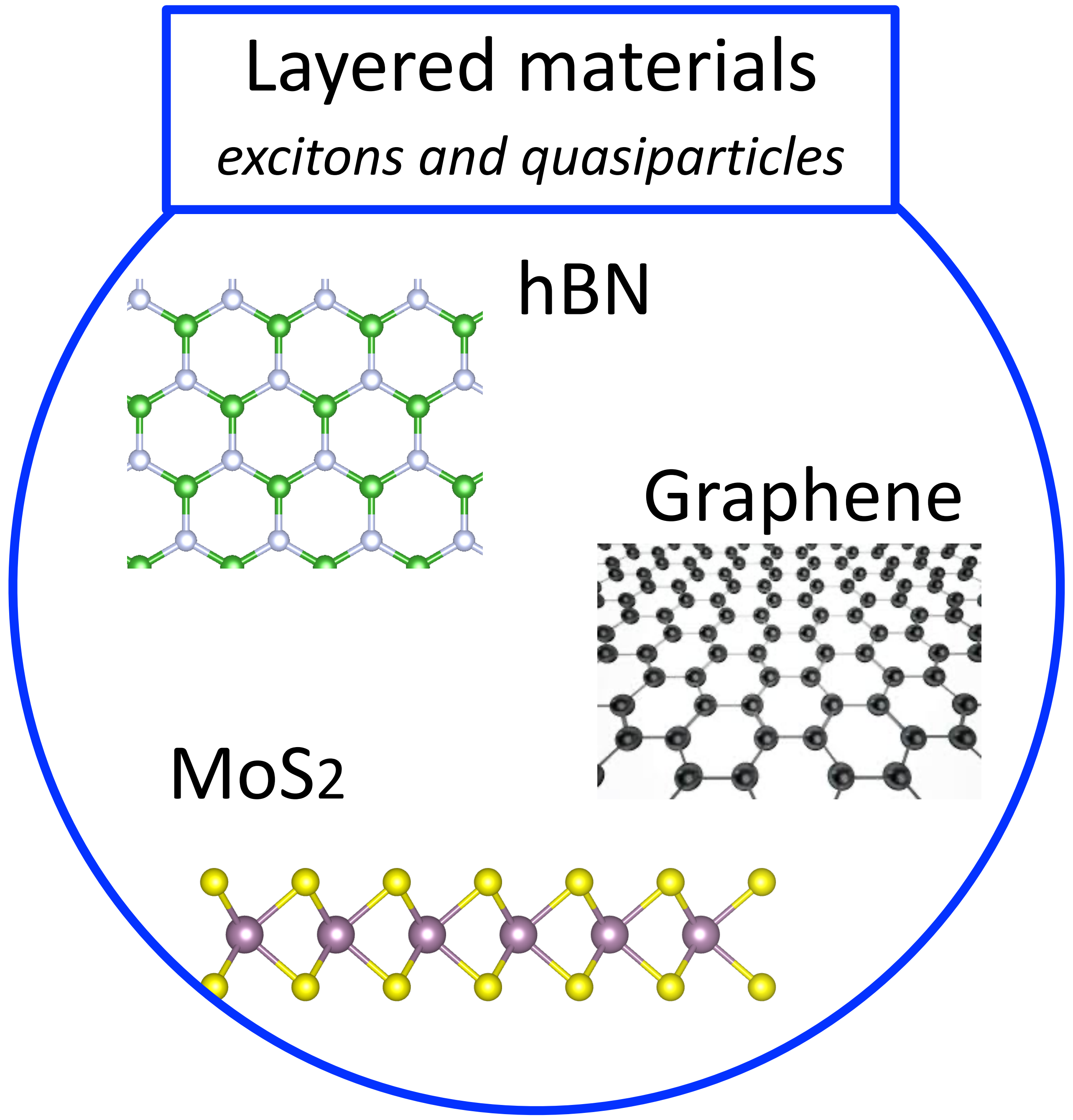
- microscopic screening

$$\chi_{\mathbf{q}}(\mathbf{G},\mathbf{G}',\omega)$$



A. Marini, C. Hogan, M. Gruning, D. Varsano, Comp.Phys.Comm. **180**, 1392 (2009)
D. Sangalli, et al, J. Phys.: Condens. Matter. **31**, 325902 (2019)

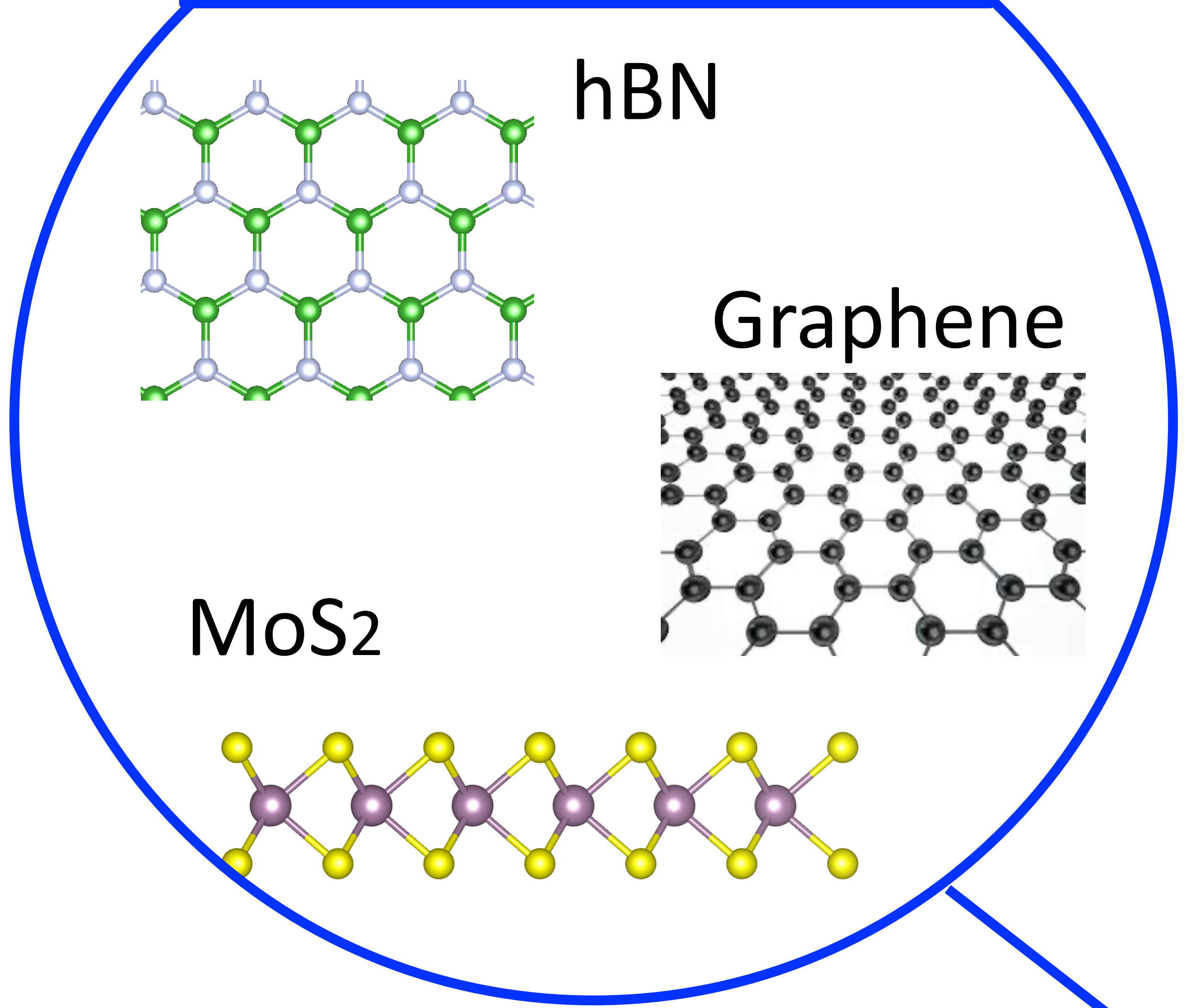
Many Body technique for spectroscopy:



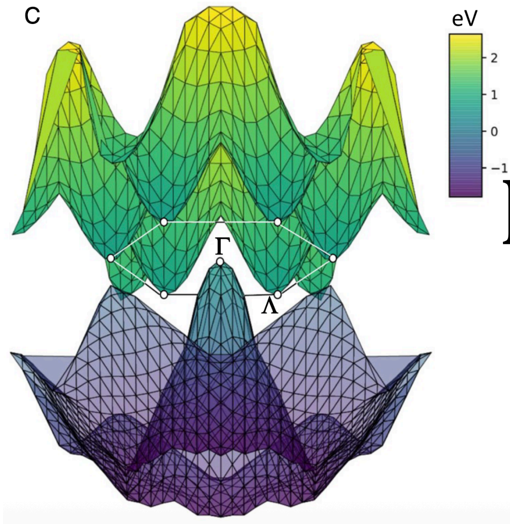
Many Body technique for spectroscopy:

Layered materials

excitons and quasiparticles



Photoemission/quasiparticles



MoS2 GW band structure

Ataei, Varsano, Molinari, Rontani PNAS (2021)

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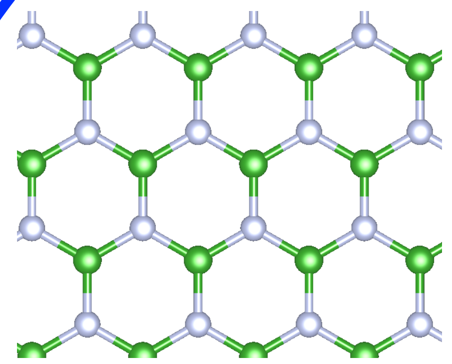
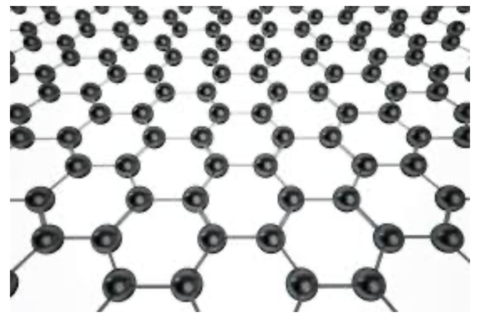
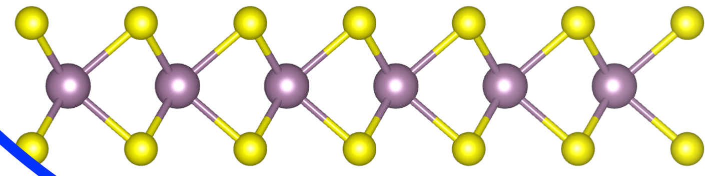


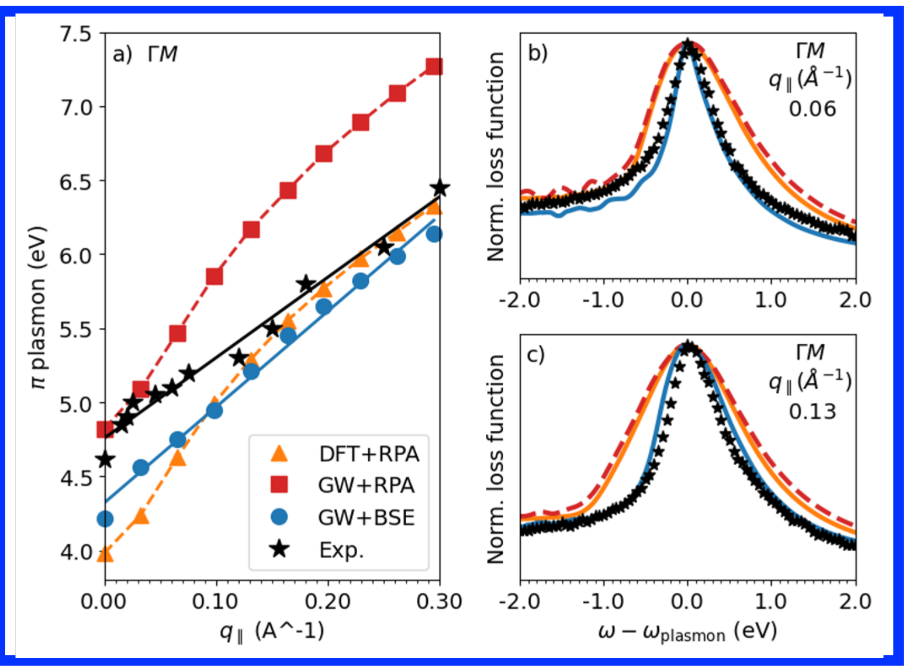
Graphene



MoS2



EELS/IXS



EELS free-standing graphene

Guandalini, Varsano, Ferretti…Nano Lett. (2023)

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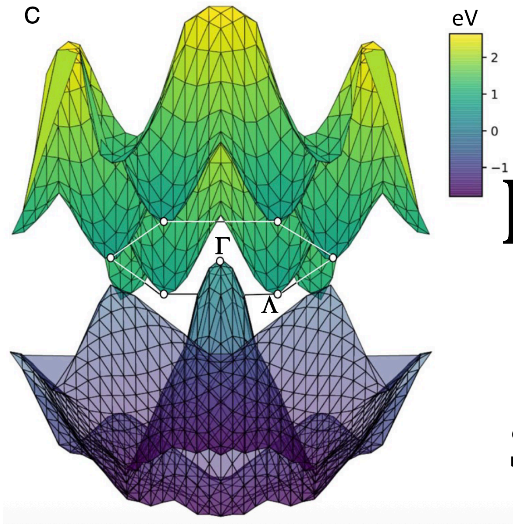

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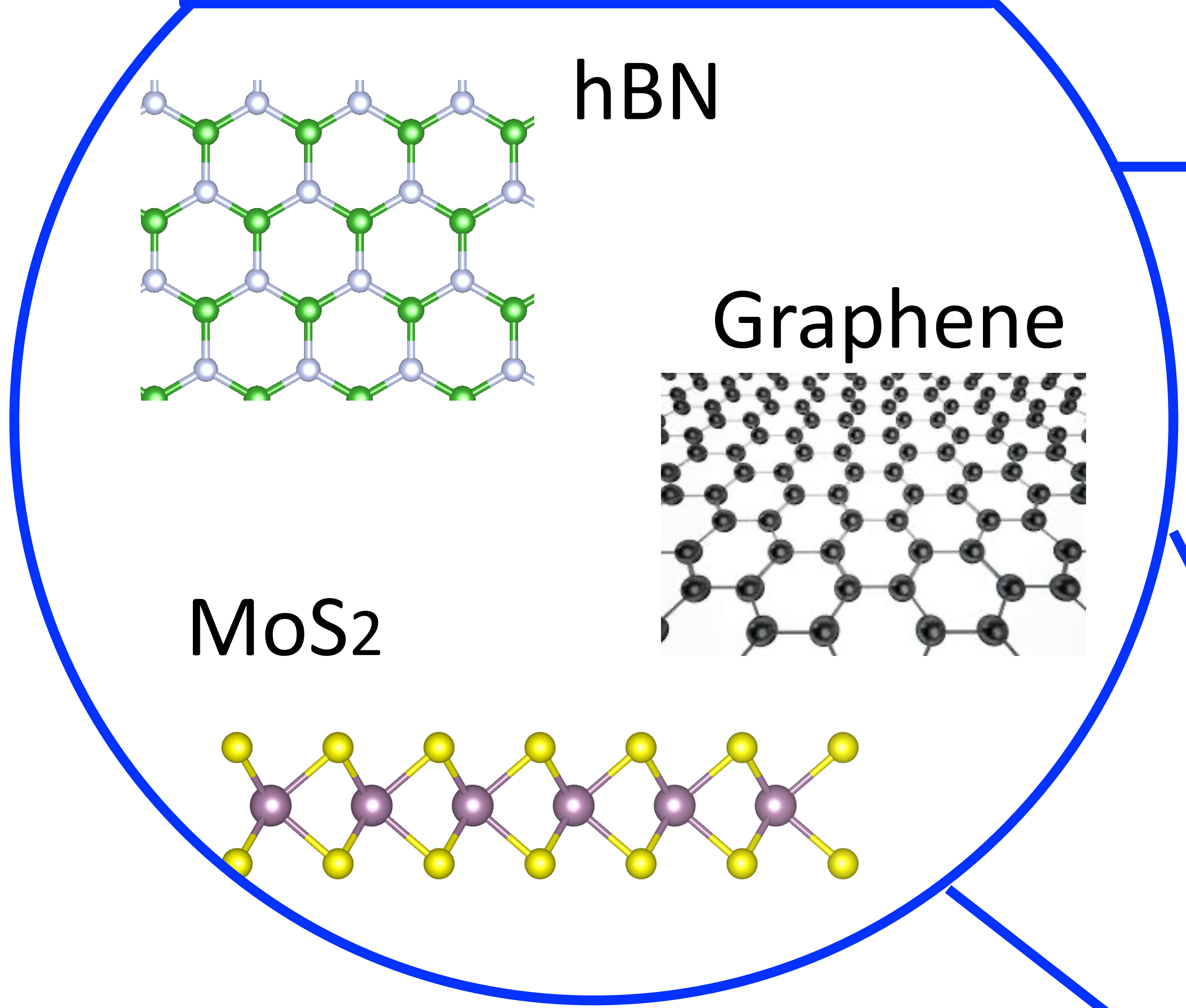
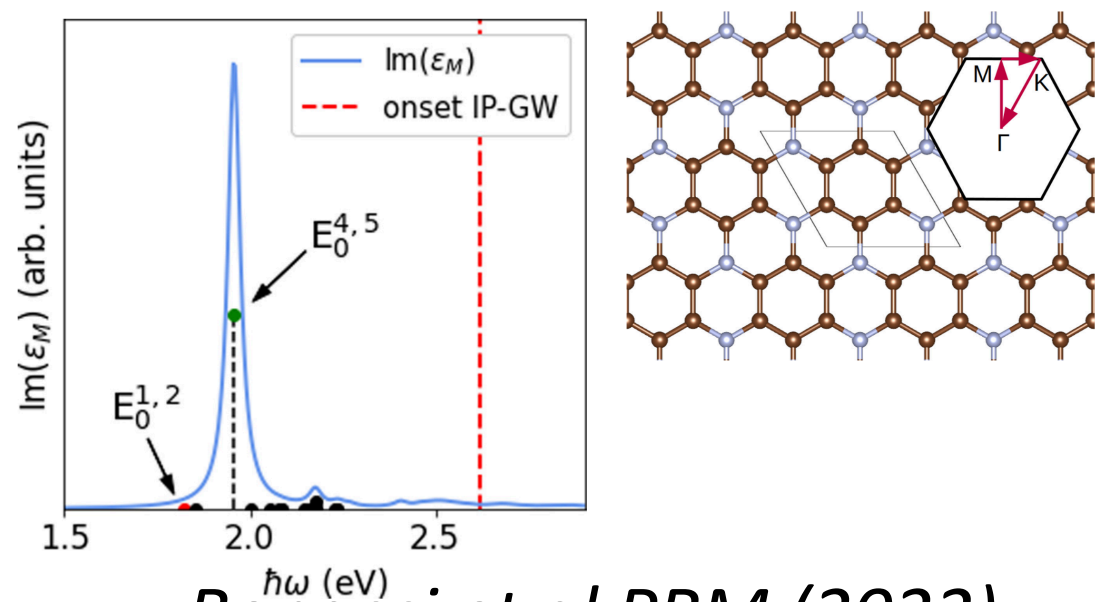


Optical absorption: Excitons



Bonacci et al PRM (2022)

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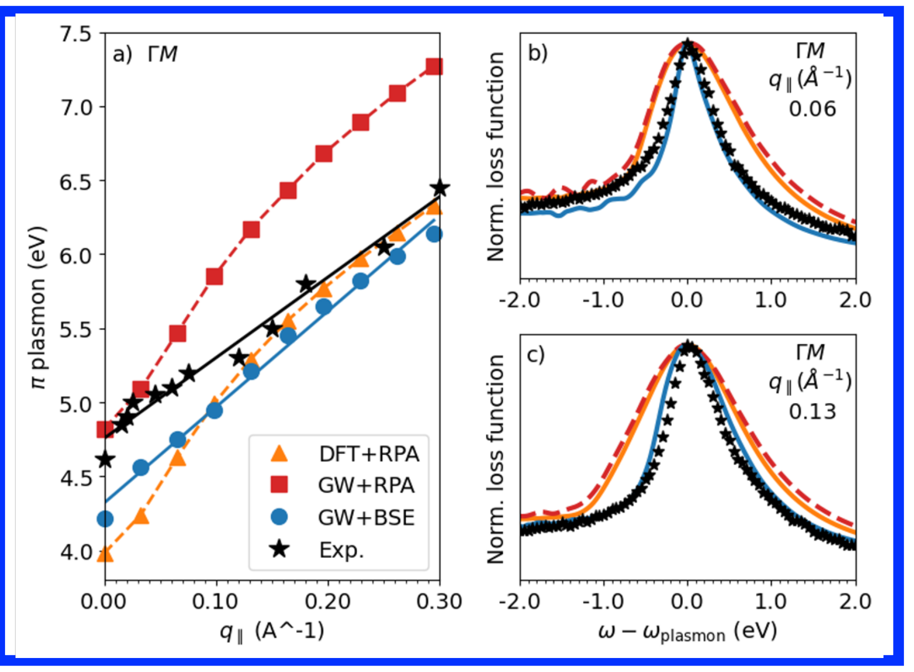

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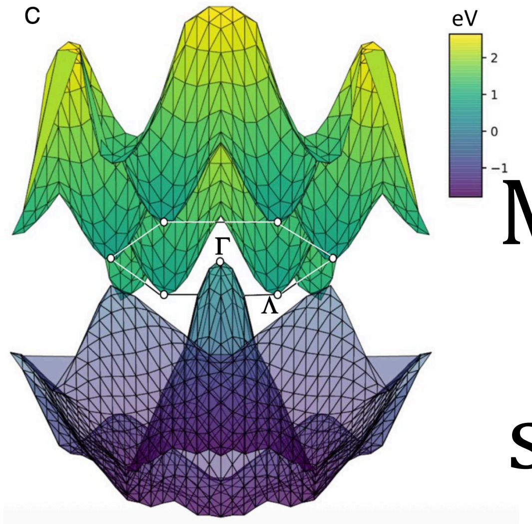

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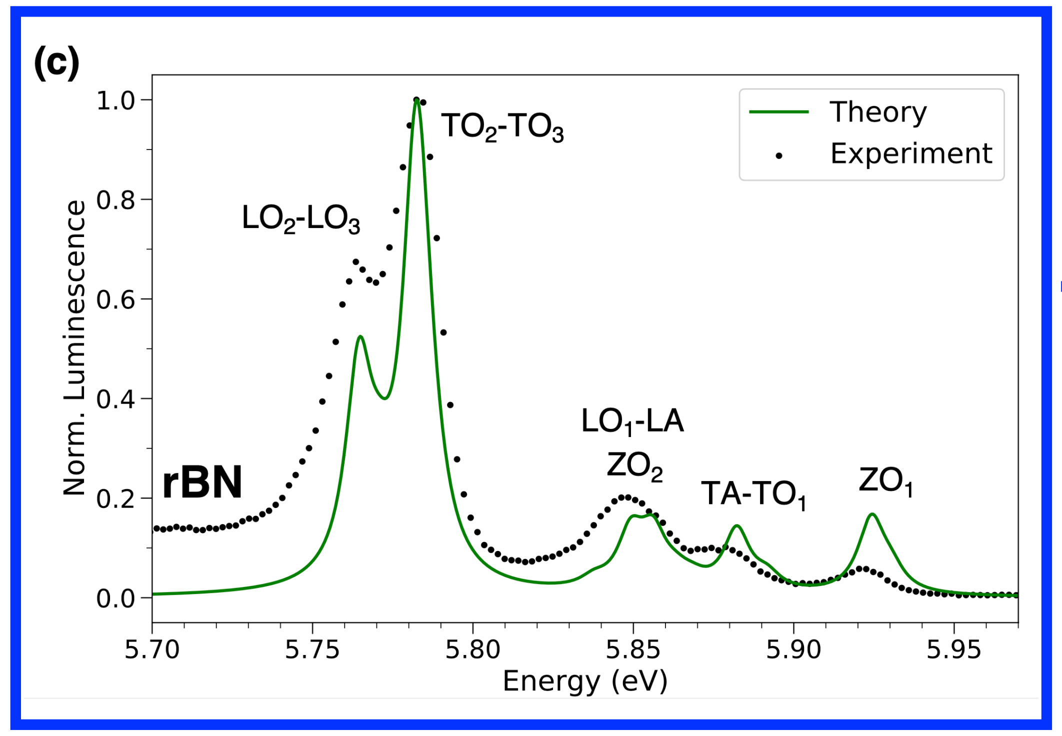

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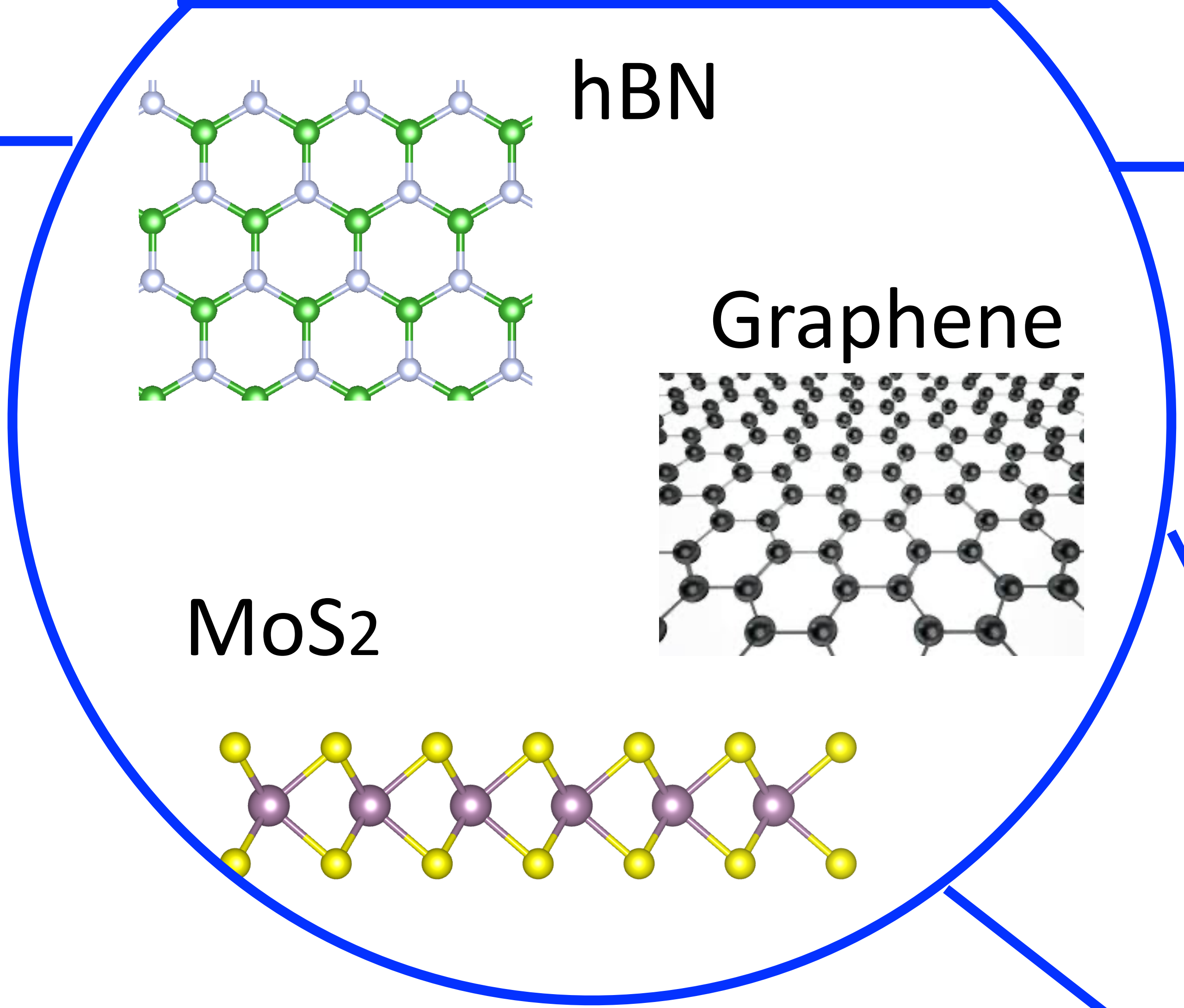

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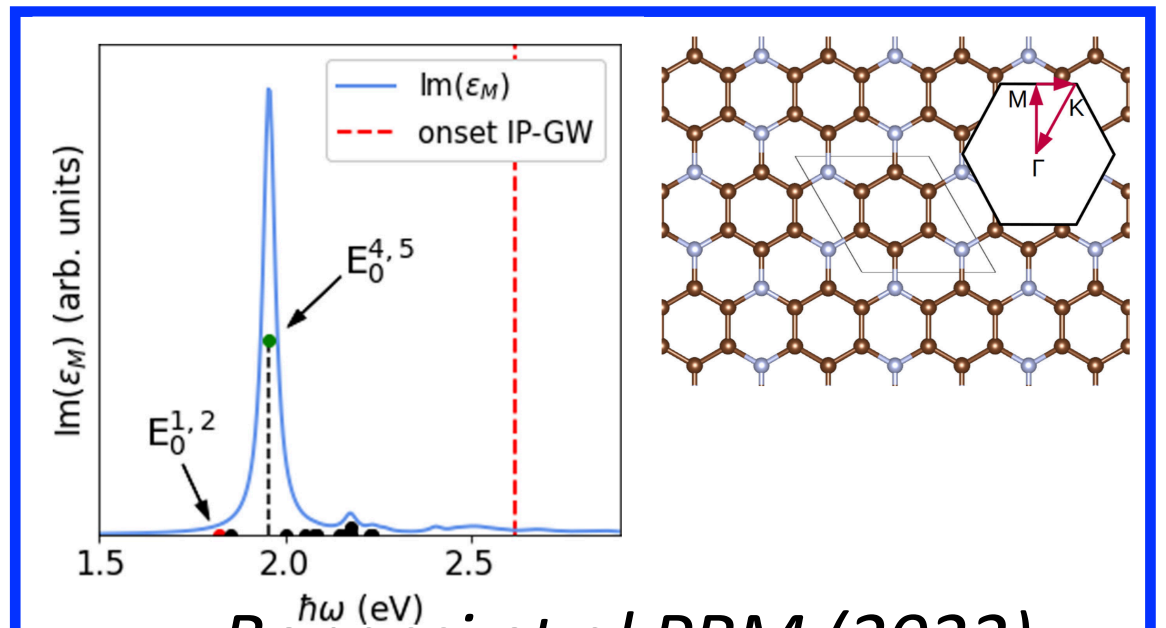

Bonacci et al PRM (2022)

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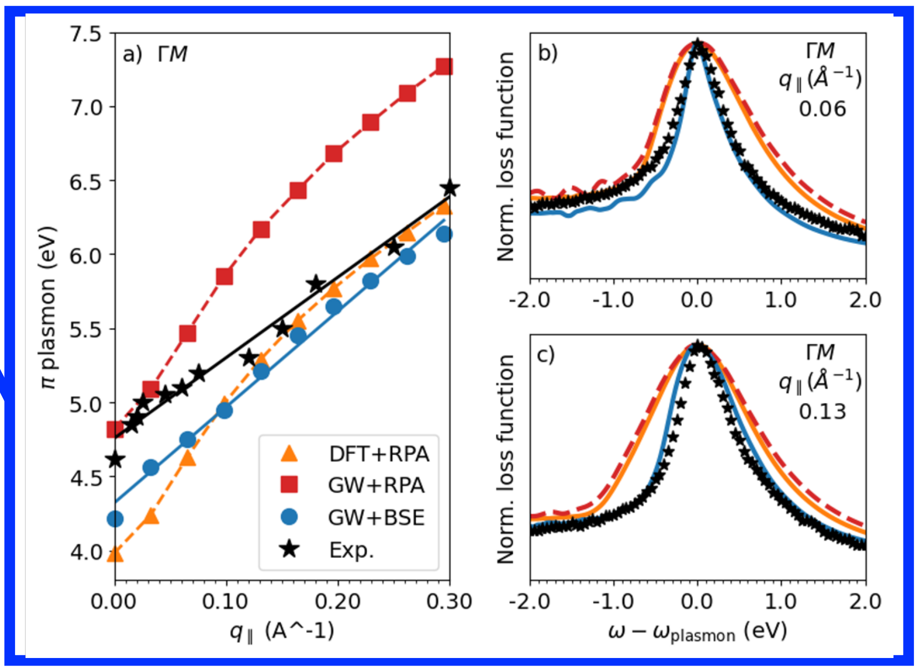

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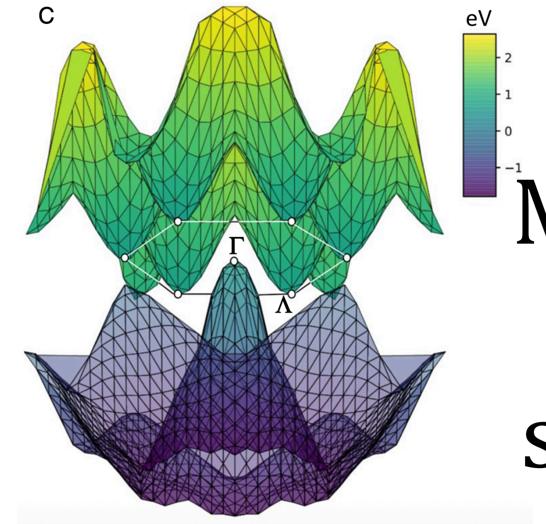

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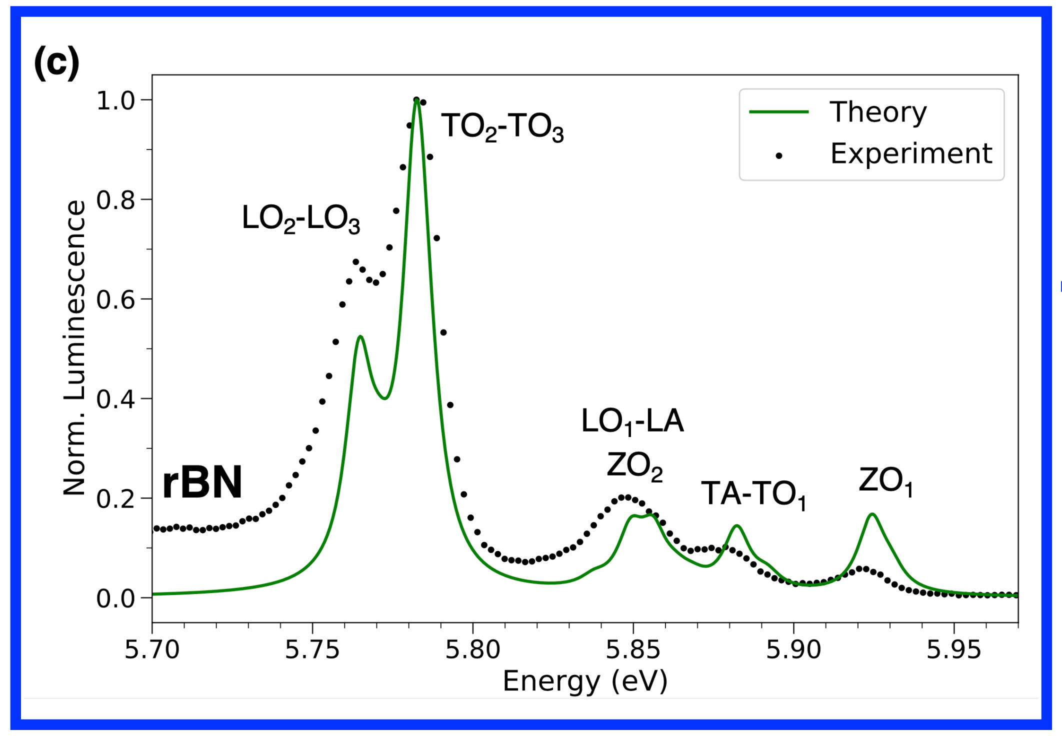

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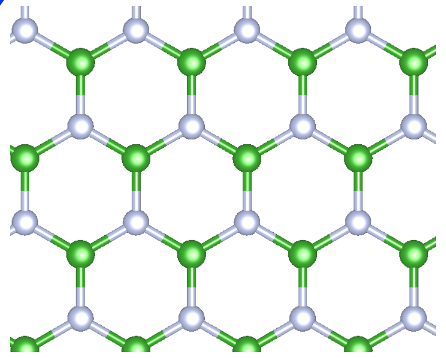

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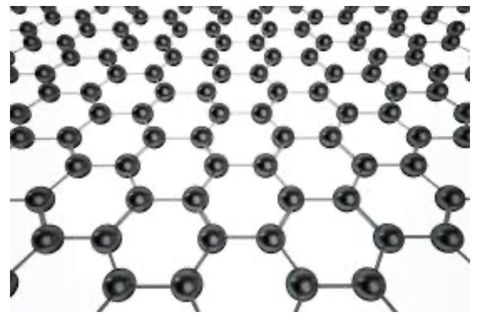
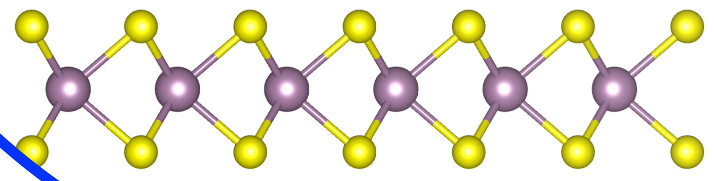


MoS_2



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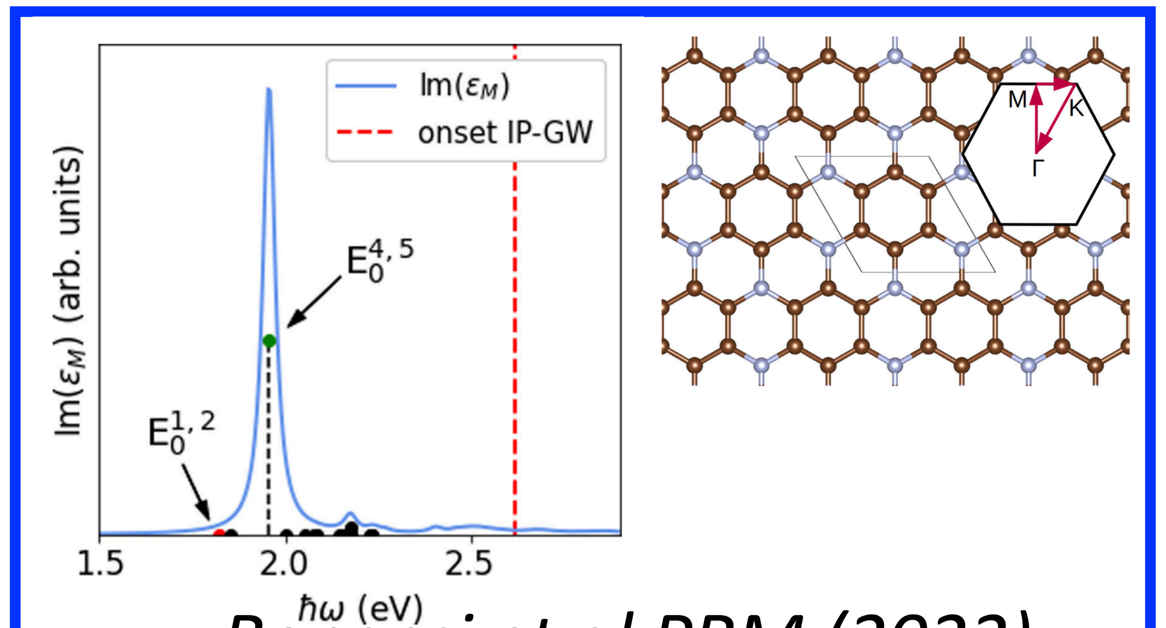

Bonacci et al PRM (2022)

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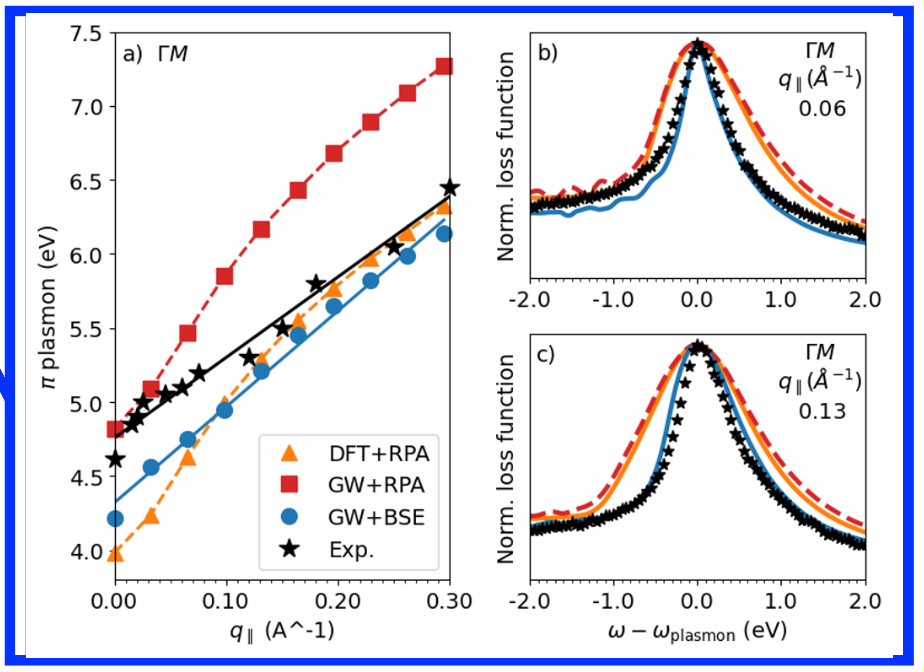

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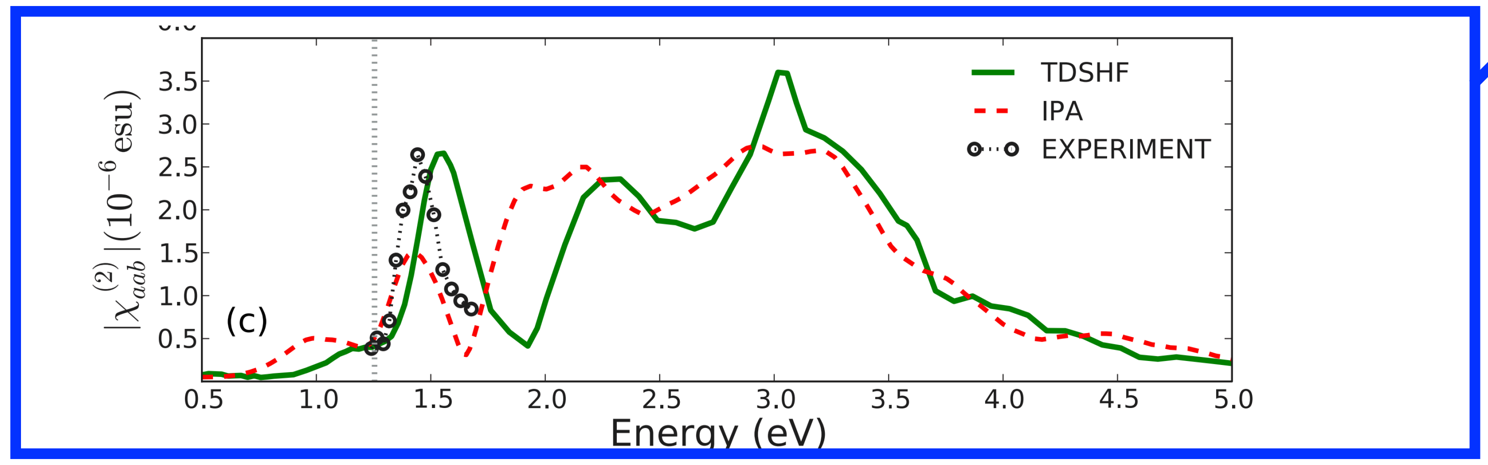
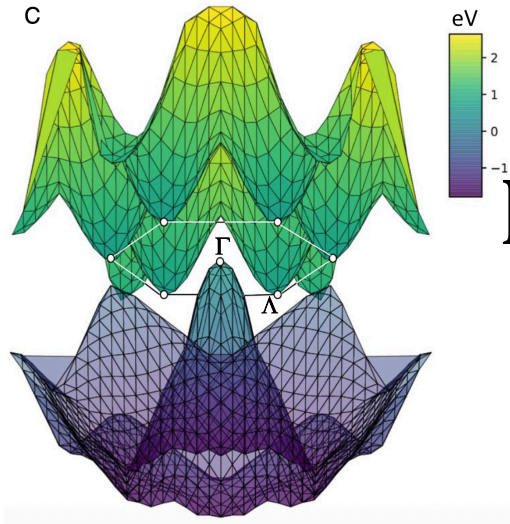
High-harmonic generation



*PRB **89**, 081102(R) (2014)*

Photoemission/quasiparticles



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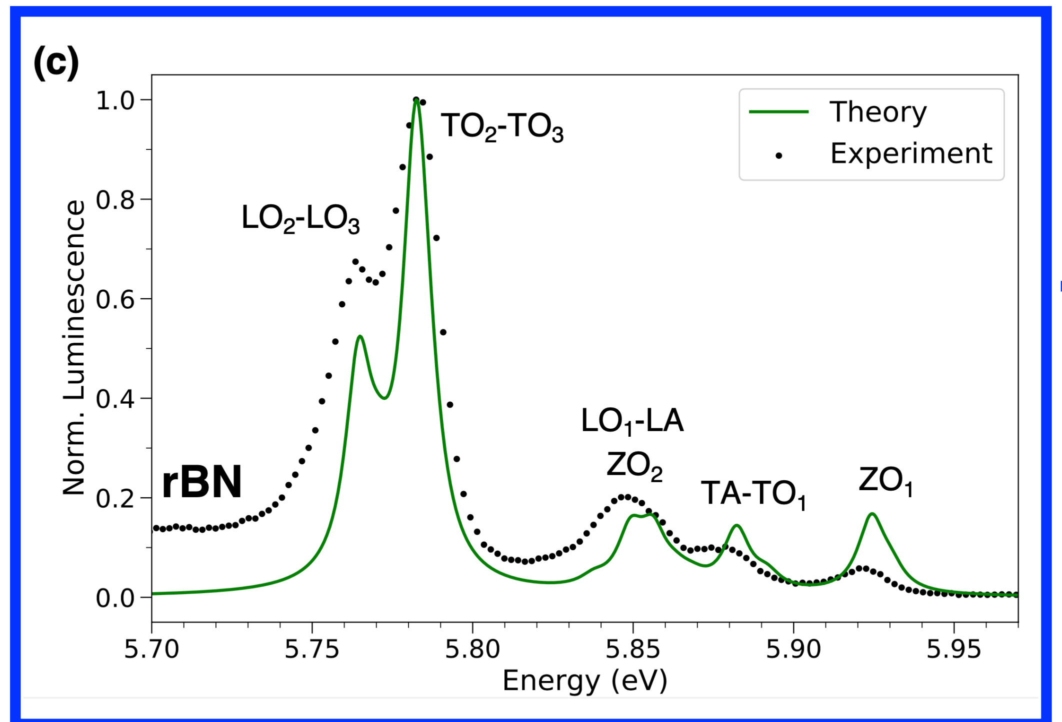

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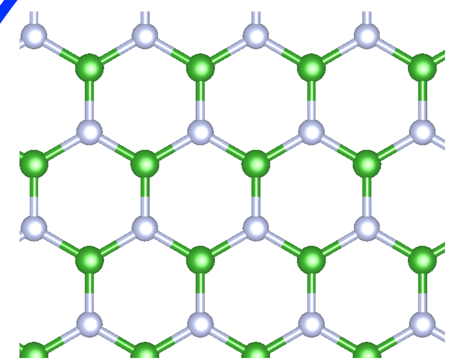
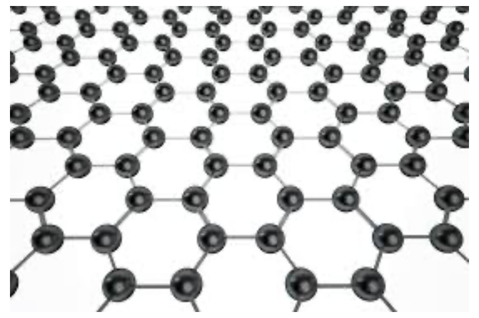
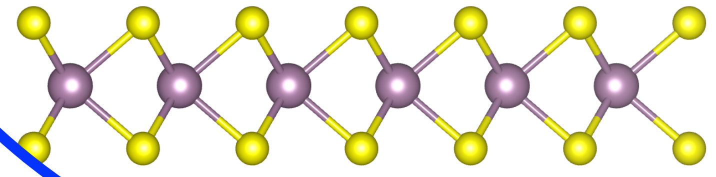


Graphene



MoS_2



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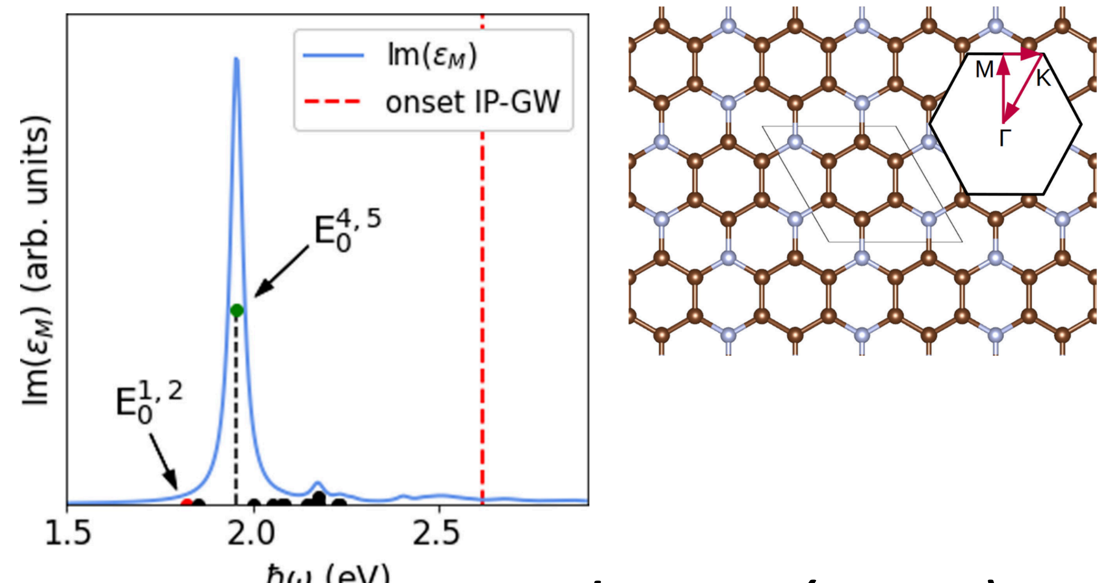
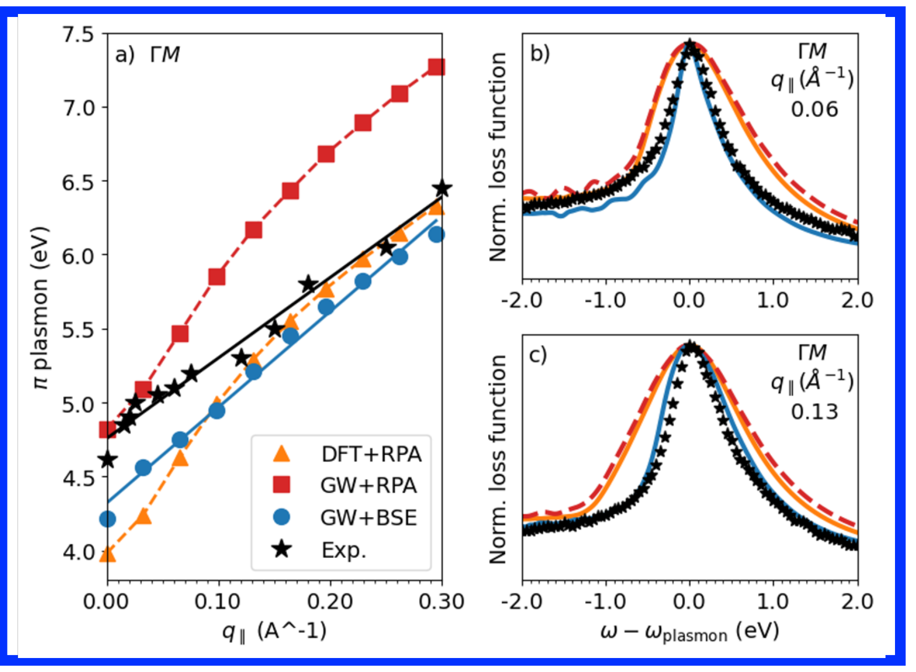


Bonacci et al PRM (2022)

EELS/IXS



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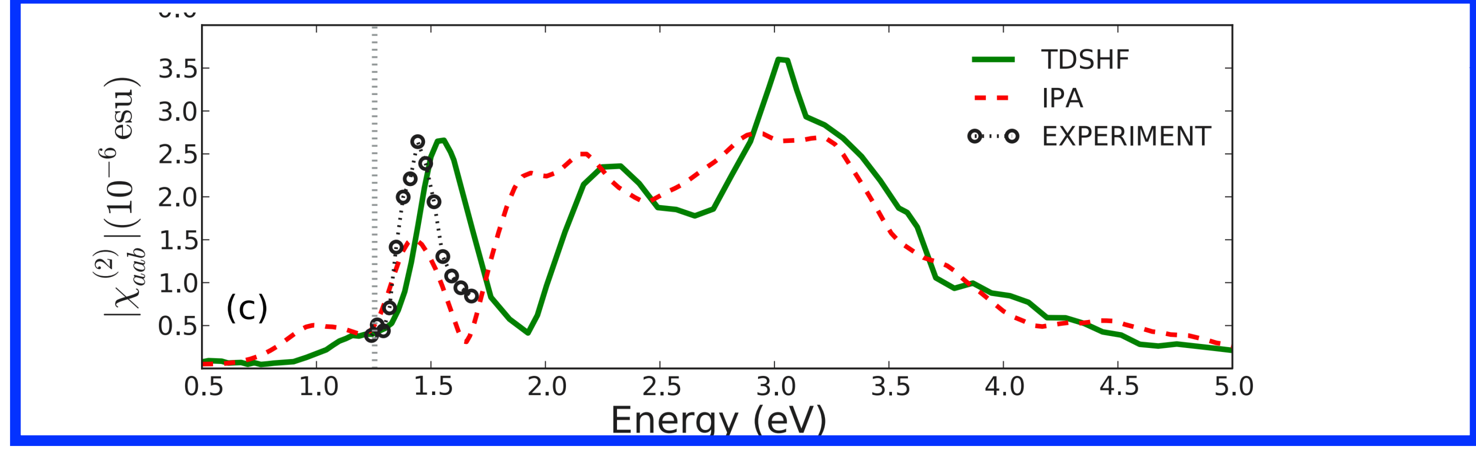
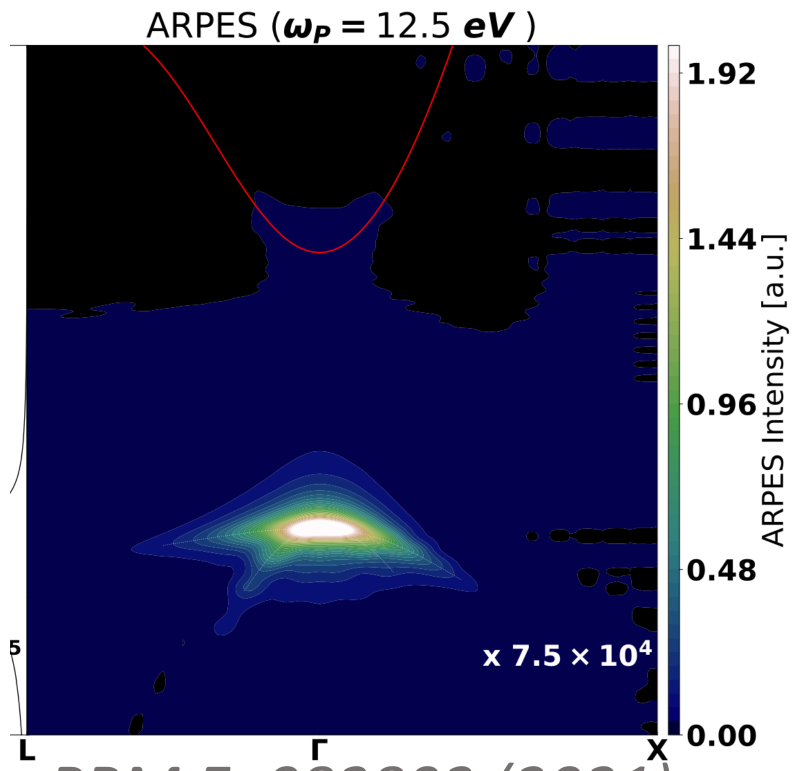


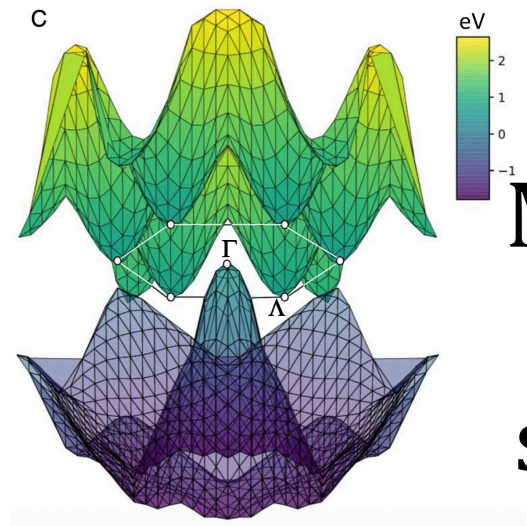
PRB **89**, 081102(R) (2014)

Time-resolved spectra



*PRM **5**, 083803 (2021)*

Photoemission/quasiparticles



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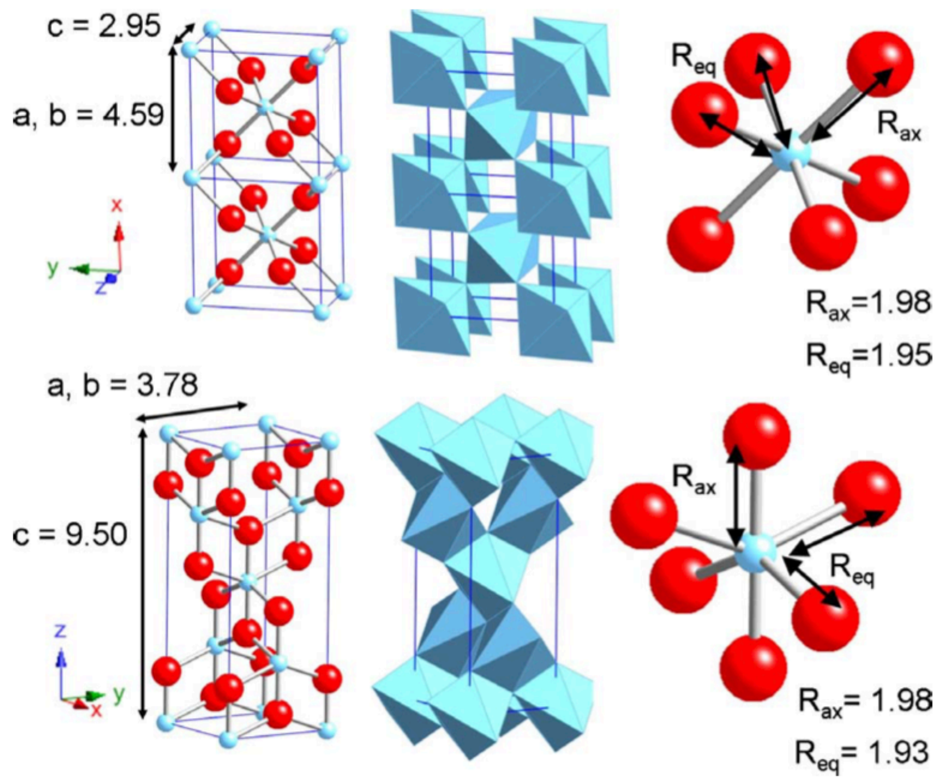
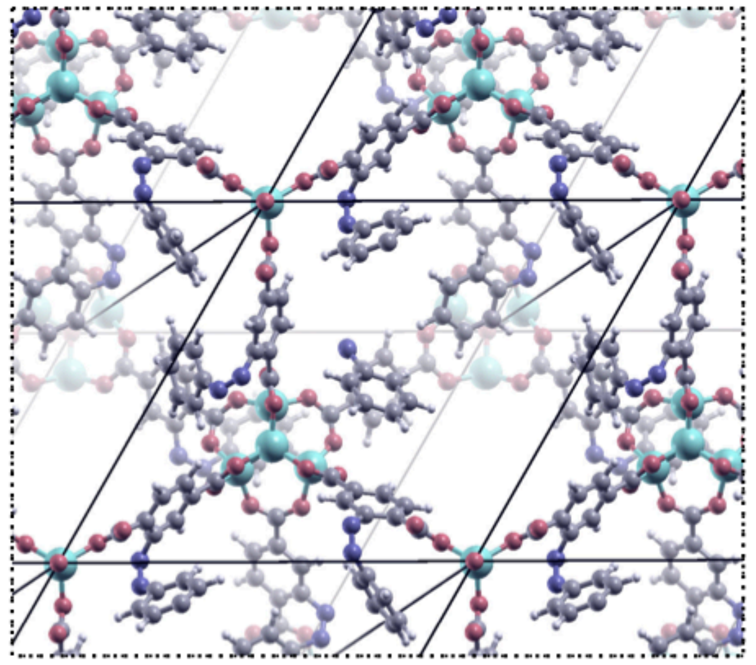
Which systems you can deal with:



L. Chiodo et al. Phys. Rev. B (2010)

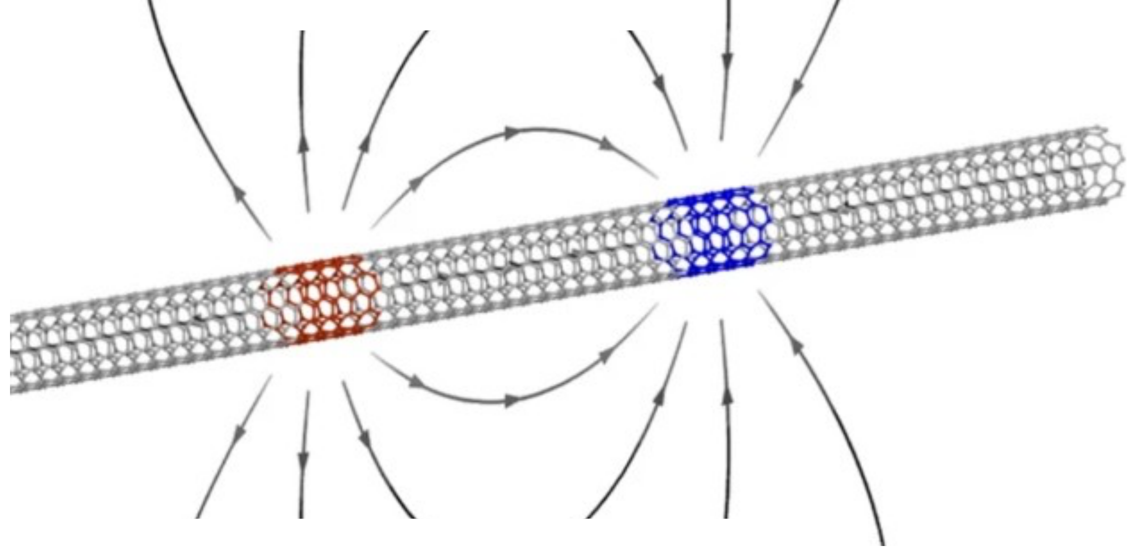
MOFs



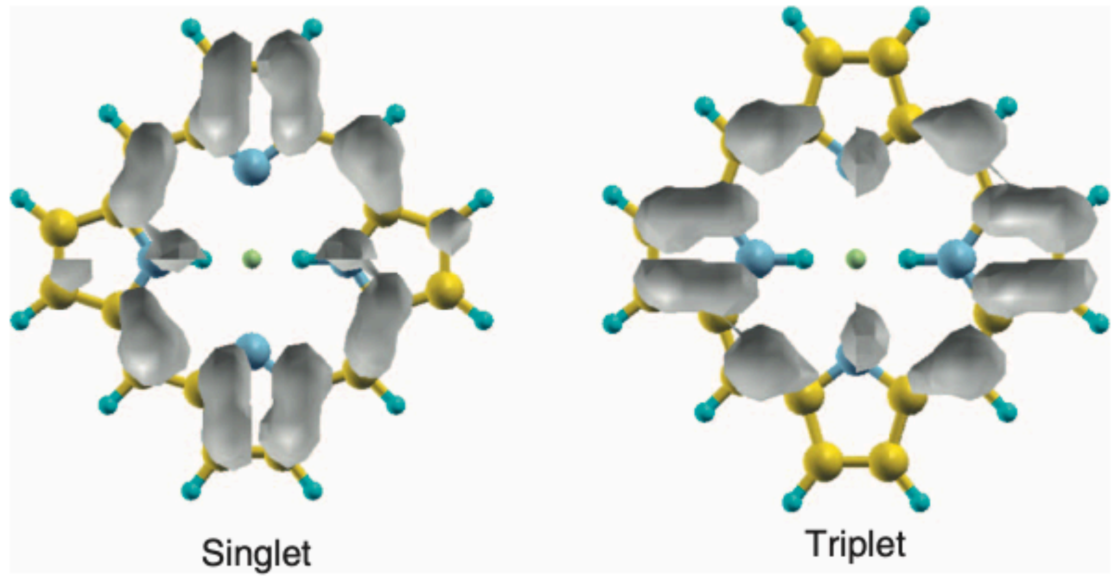
f-PCN-123

A. Rajan et al J. Phys. Chem. Lett. (2021)

Nanostructures

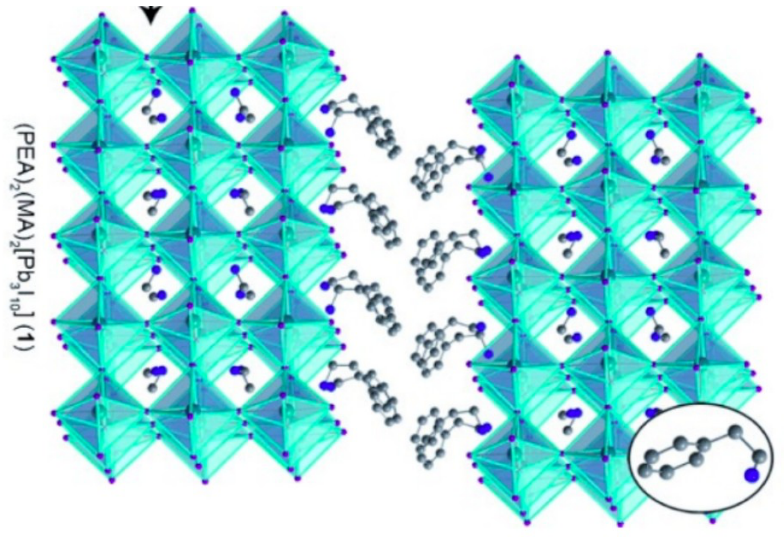


C. Attaccalite et a, Phys. Rev. B 95, 125403 (2017)
D. Varsano, D. Sangalli et al. Nature Comm. 8, 1461 (2017)



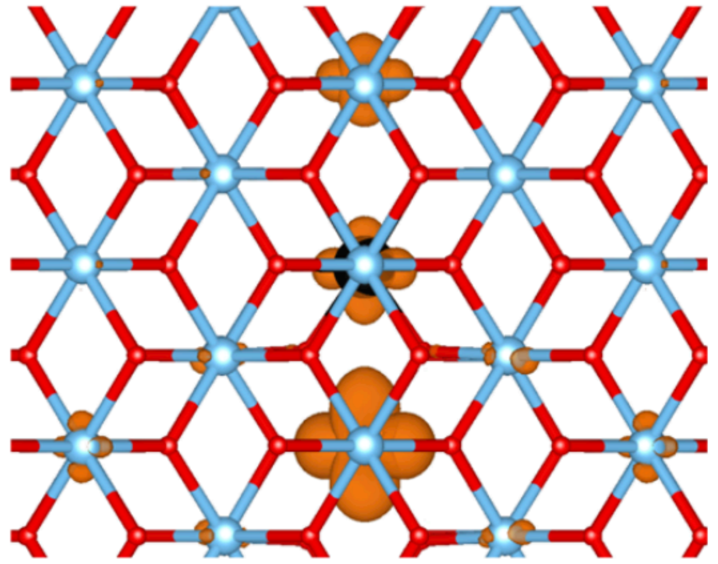
M. Palummo et al *J. Chem. Phys.* (2009)

hybrid organic inorganic halide Perovskites



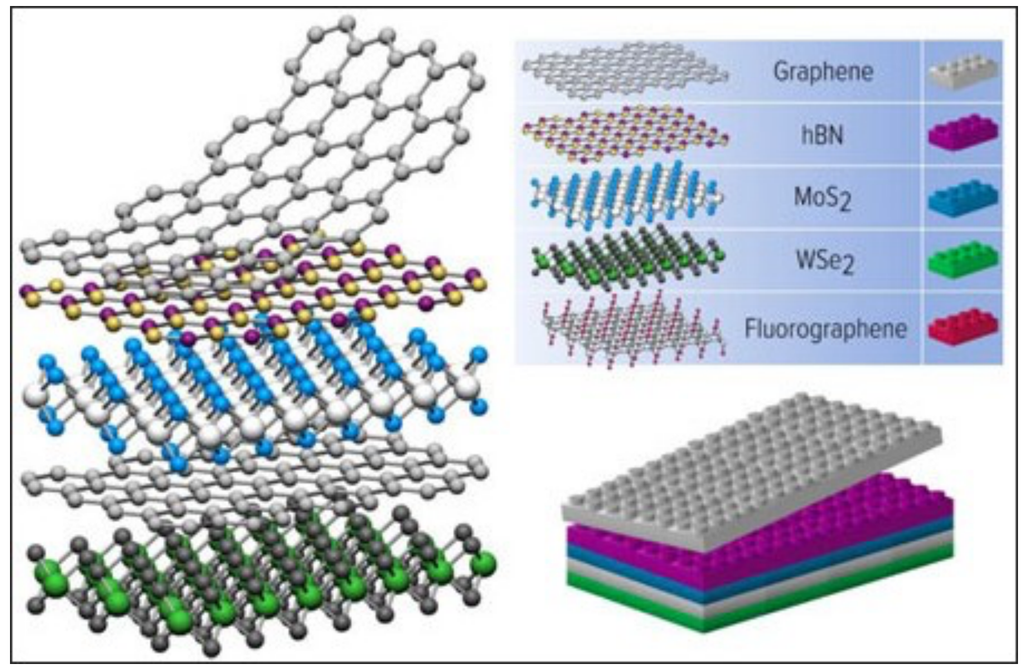
M. Palummo et al. ACS Energy Letter (2020)

(b) TiO_2:Nb_{Ti}

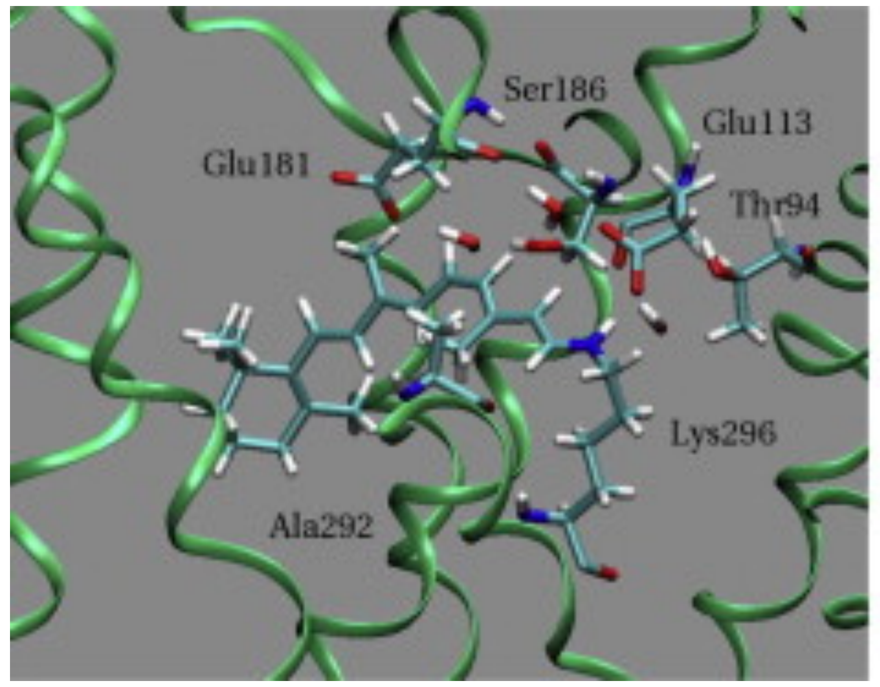


M. Atambo et al. Phys. Rev. Mat (2019)

2D materials and heterostructures



A Molina-Sánchez et al. Nano Lett. (2017)



D. Varsano et al. J. Phys. Condens. Matter (2017)

Take Home Messages:

Even at G^0W^0 level, several convergence parameter and approximations have to be carefully checked: (integration BZ, number of unoccupied states, convergence of the screening ….)

$$\left[\frac{-\nabla^2}{2}+v^s(r)\right]\psi_{nk}(r)=\epsilon_{nk}\psi_{nk}(r)$$

$$\hat{H}_0(\mathbf{r})f_s(\mathbf{r}) + \int \Sigma(\mathbf{r},\mathbf{r}';\epsilon_s)f_s(\mathbf{r}')d^3\mathbf{r}' = \epsilon_s f_s(\mathbf{r})$$

courtesy M. Van Setten

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$$\hat{H}_0(\mathbf{r})f_s(\mathbf{r})+\int\Sigma(\mathbf{r},\mathbf{r}';\epsilon_s)f_s(\mathbf{r}')d^3\mathbf{r}'=\epsilon_s f_s(\mathbf{r})$$

DFT:

pseudopotential

k-point mesh / energy cutoff

smearing

Functional choice

DFT babysitting problem

courtesy M. Van Setten

Take Home Messages:

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GW:

- **N^4 scaling**
- Converge more parameters: **number of empty bands** and **dielectric cutoff** .
- Test **k-point sampling** and **frequency treatment**
- Mind **starting point dependence**.

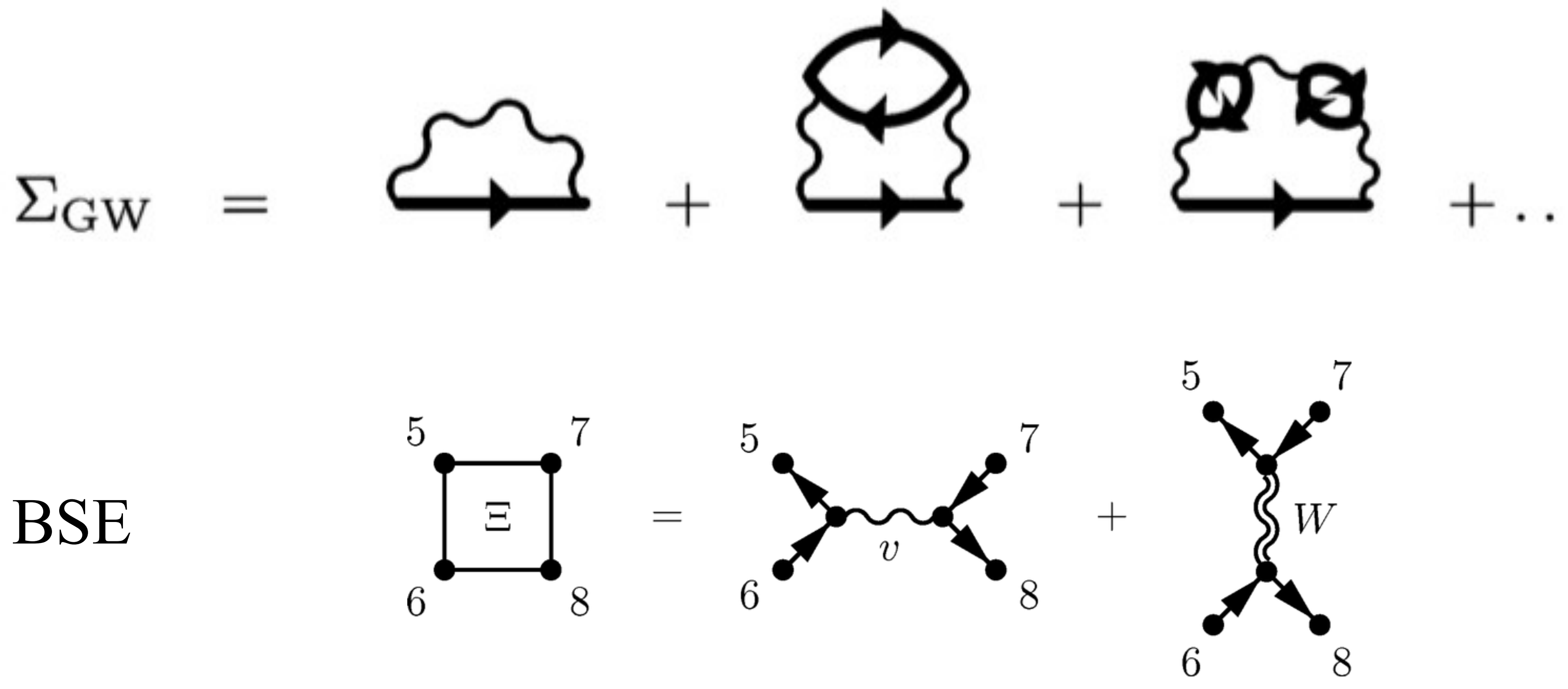
GW babysitting problem

courtesy M. Van Setten

High Throughput MBPT:

Starting point: A DFT calculation:

$$\left[\frac{-\nabla^2}{2}+v^s(r)\right]\psi_{nk}(r)=\epsilon_{nk}\psi_{nk}(r)$$



- **N⁴ scaling**
- Converge **more parameters**
- **No "safe" convergence parameters** for all calculations.
- **No "safe" computational settings** (#cpu's, memory, time)

courtesy M. Van Setten

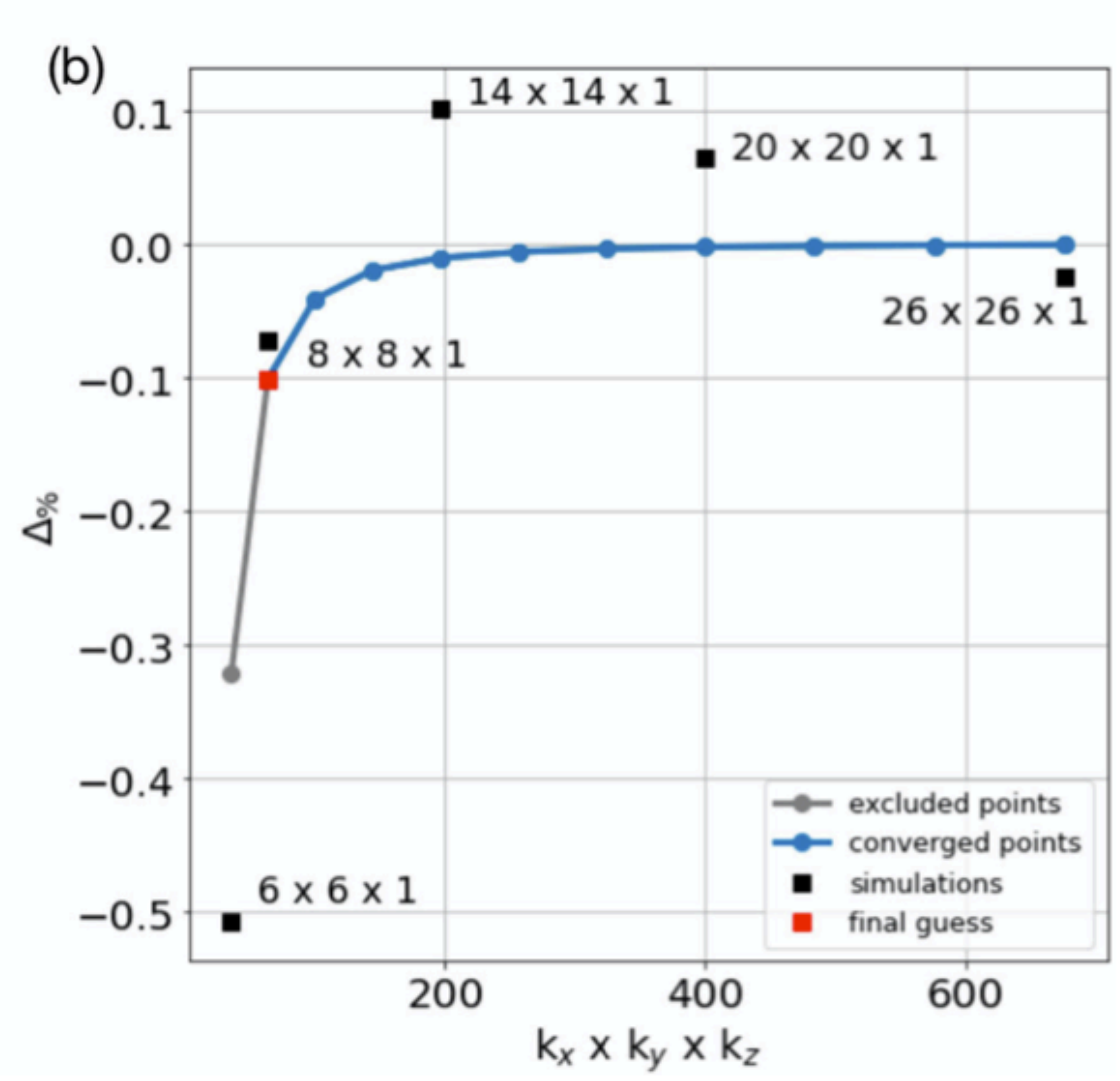
High Throughput MBPT:

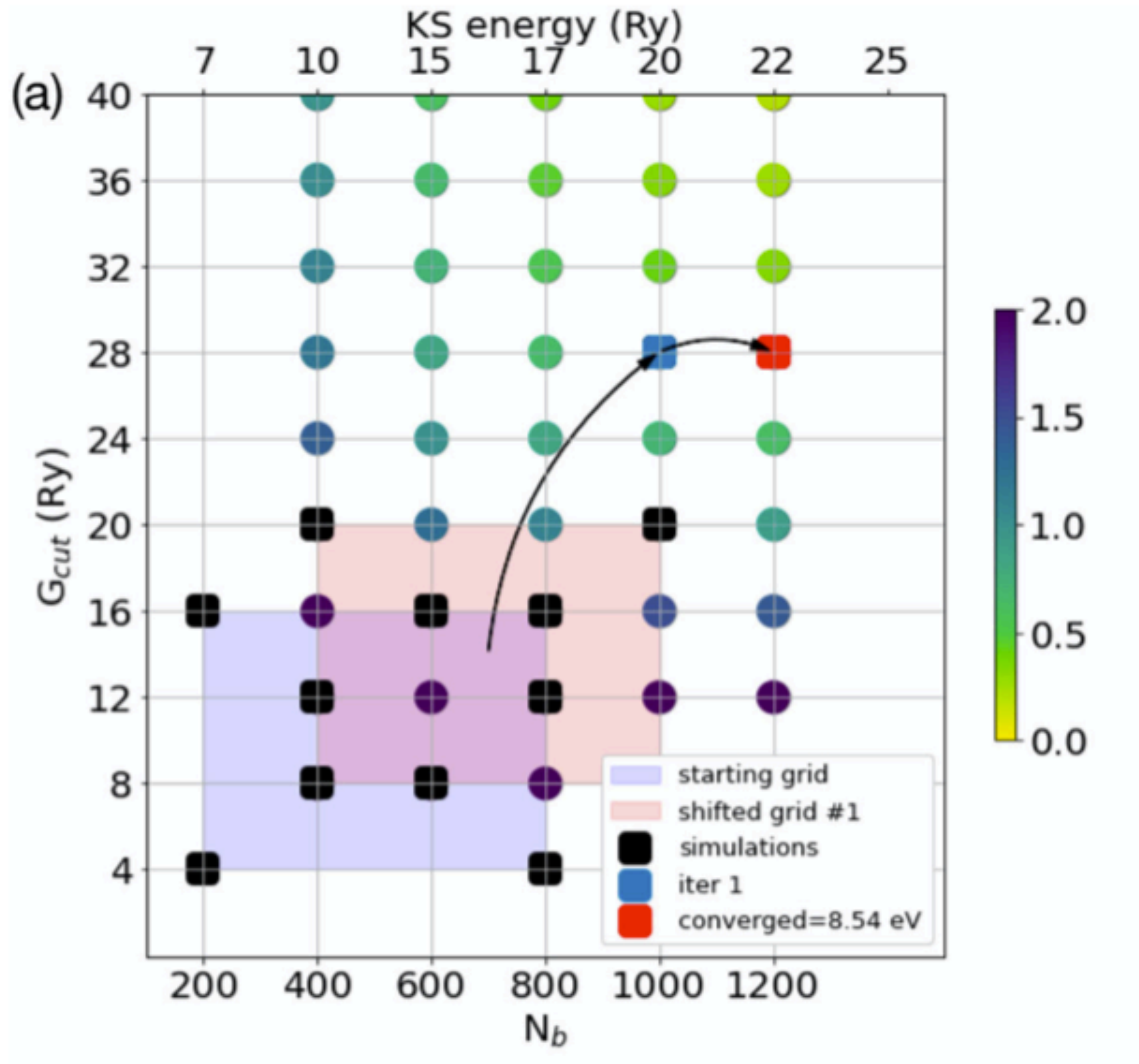
npj Comput Materials **9**, 74 (2023)

Towards high-throughput many-body perturbation theory: efficient algorithms and automated workflows

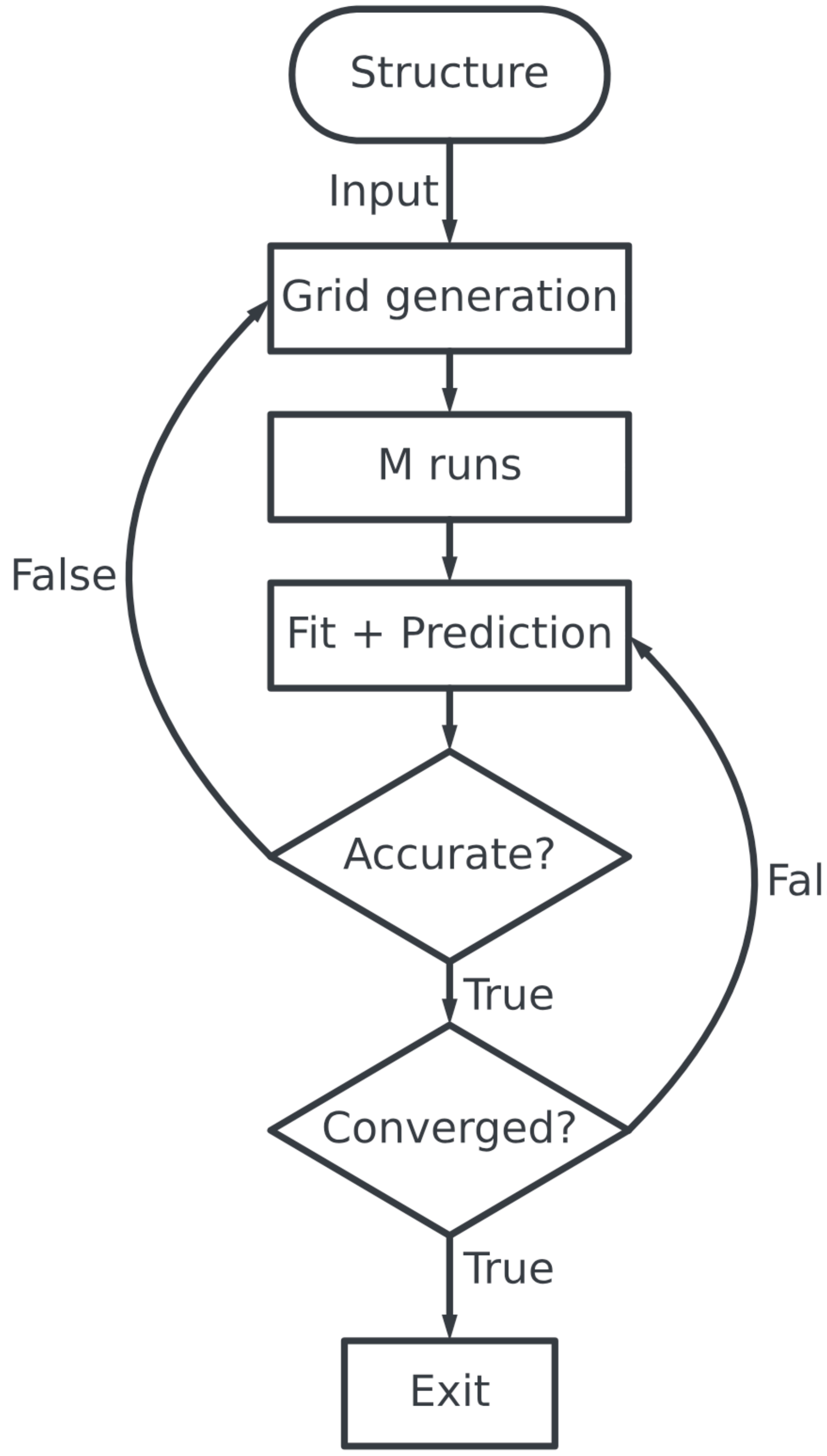
Miki Bonacci[1,2✉], Junfeng Qiao[3], Nicola Spallanzani[2], Antimo Marrazzo[4], Giovanni Pizzi[3,5], Elisa Molinari[1,2], Daniele Varsano[2], Andrea Ferretti[2] and Deborah Prezzi[2]

- Algorithms for **automatic convergence** of many-body perturbation theory methods
- **efficient sampling** in multi-dimensional parameter space
- combines yambo workflows with the AiiDA automation engine





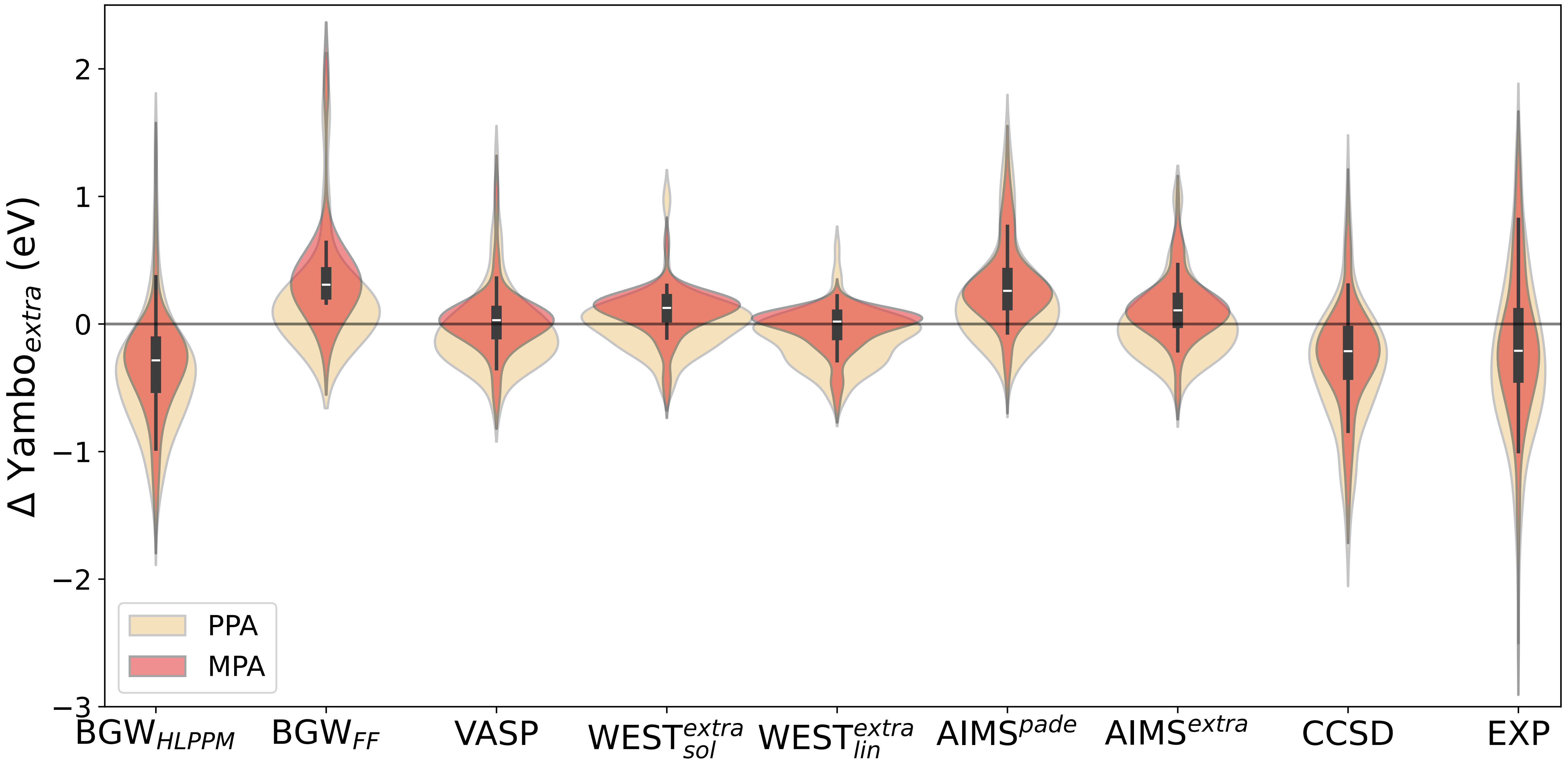
Miki Bonacci
(CNR-Nano, Modena)



High Throughput MBPT and validation:

GW100 Dataset

Miki Bonacci
(CNR-Nano, Modena)



M. Bonacci, D. A. Leon et al JCTC (2026)

ELSEVIER

Computer Physics Communications
Volume 255, October 2020, 107242

Reproducibility in G_0W_0 calculations for solids ☆

Yambo, Abinit and BerkeleyGW calculations on Si, TiO2, ZnO, Au the converged QP energies calculated with the different codes agree within 0.1 eV. Coulomb divergences, dynamical treatment of the screening, PPs, as a major source of discrepancy among different implementations.

T. Rangel, M. Del Ben. D. Varsano et al. Comp. Phys Comm. (2020)

Take Home Messages:

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GW: parameter-free method which provides in most of the case accurate results (QP energies, but also total energies, lifetimes)

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GW: Starting point for absorption spectroscopy - excitonic effects: Bethe-Salpeter (see next lectures)

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G^0W^0 today is feasible for medium size systems: algorithms suitable for HPC computation (also hybrids architectures, GPU cards).

Take Home Messages:

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GW: Many approximations enters in a practical calculations:

- in it's widespread G^0W^0 flavour it is not self-consistent: strong **dependence on the DFT starting point** (specially true for molecules. Start from hybrid DFT?)
- Even in partial self consistent flavour usually **QP wave function assumed to be the same as the initial KS wave function**
- Screening treated at **RPA** level
- Frequency dependence of the screening usually approximated with a **PP model**

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GW successful in the interpretation of spectroscopical properties of many systems but calculations need careful checks and relies on different approximations that can fail.

Useful Links:

Instruction for the tutorials

https://wiki.yambo-code.eu https://yambo-code.github.io/yambo-wiki/

Documentation

- Theory
- Lectures
- Cheatsheets
- Input file variables
- Selected Readings
- Thesis

Cheatsheet

For yambo 5.0

DRIVING THE EXASCALE TRANSITION

(8) Correlation part of self energy: `yambo -gw0 ppa`

$$\Sigma^c_{n\mathbf{k}}(\omega) = \langle n\mathbf{k}|\Sigma^c|n\mathbf{k}\rangle = i\sum_m \int_{BZ}\frac{d\mathbf{q}}{(2\pi)^3}\sum_{\mathbf{G},\mathbf{G}'}\frac{4\pi}{|\mathbf{q}+\mathbf{G}|^2}\rho_{nm}(\mathbf{k},\mathbf{q},\mathbf{G})\rho^*_{nm}(\mathbf{k},\mathbf{q},\mathbf{G}') \times \int d\omega' G^0_{m\mathbf{k}-\mathbf{q}}(\omega-\omega')\epsilon^{-1}_{\mathbf{G}\mathbf{G}'}(\mathbf{q},\omega')$$

```
% GbndRnge
  1 | 50 |
%
```

Bands used in the GW summation
QP energies usually shows slow convergence
Tip: If you are interested in gaps, energy differences converge faster

NGsBlkXp= 100 RL
Response block size
See (9)

```
%QPkrange
  1|  5| 20|  59|
  4|  8| 60|  80|
%
%QPerange (-V qp)
  1| 32| 0.0|-1.0|
%
```

nk, n'k' ranges where GW/Σ_c elements are calculated
first k-point | last k-point | lower band | upper band
This can be split over several lines for multiple groups
Tip: careful use of fewer k-points and bands reduces the calculation time; yambo will interpolate the rest

https://yambo-code.eu/forum

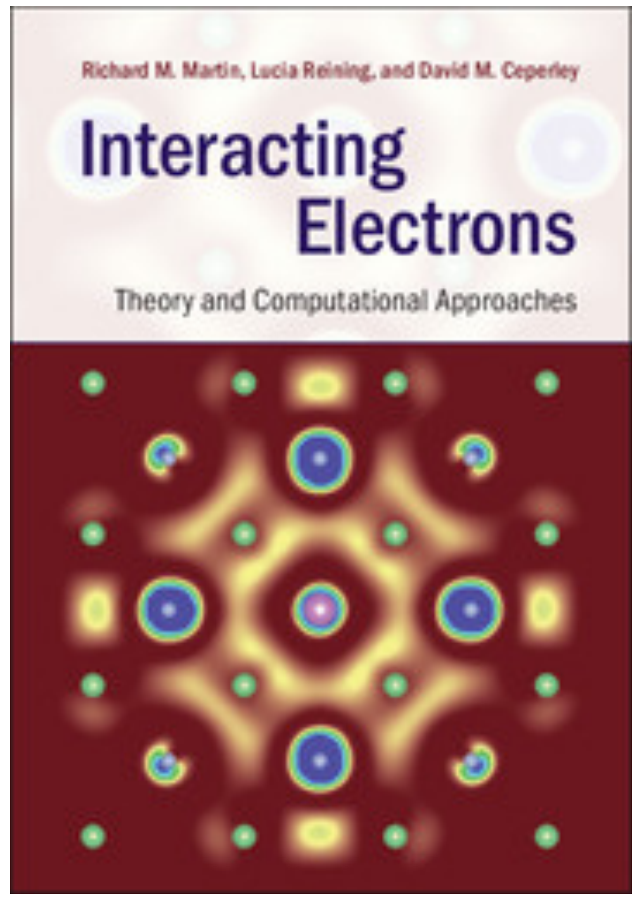
Board index — Last visit w

SUBFORUMS	STATISTICS
Announcements and Job offers A subforum where you can post Announcements and Job offers related with the Yambo code **Moderators:** Davide Sangalli, andrea.ferretti, myrta gruning, andrea marini, Daniele Varsano, Conor Hogan	Topics: 13 Posts: 24
Compilation Having trouble compiling the Yambo source? Using an unusual architecture? Problems with the "configure" script? Problems in GPU architectures? This is the place to look. **Moderators:** Davide Sangalli, andrea.ferretti, myrta gruning, andrea marini, Daniele Varsano, Conor Hogan, Nicola Spallanzani	Topics: 219 Posts: 1499
Importing core databases (a2y, p2y and e2y) Forums dealing with all aspects related to conversion of data from Abinit, PWscf or ETSF-io into the native Yambo core databases. **Moderators:** andrea.ferretti, Conor Hogan **Subforums:** PW, Abinit	Topics: 96 Posts: 513
Running Yambo Yambo can be operated on several different runlevels: here you will find several forums that deal with the specific physical task that you are trying to carry out. **Subforums:** Initialization, Linear Response and Screening in reciprocal space, GW calculations, Bethe Salpeter, Electron-Phonon effects (yambo_ph), Non linear optics (yambo_nl), Real time propagation (yambo_rt), Other issues	Topics: 1100 Posts: 6576
Post Processing (ypp) Anything regarding the post-processing utility (e.g. excitonic wavefunction analysis) is dealt with in this forum. **Moderators:** Davide Sangalli, andrea marini, Daniele Varsano	Topics: 225 Posts: 1265
Yambo-py Post here any question you encounter when running the scripts of the yambo-py suite. Post here problem strictly to the python interface as problem coming from the yambo runs should go in the appropriate subforum. **Moderators:** amolina, palful, mbonacci	Topics: 69 Posts: 219
Technical Issues Various technical topics such as parallelism and efficiency, netCDF problems, the Yambo code structure itself, are posted here. **Moderators:** Davide Sangalli, andrea.ferretti, myrta gruning, andrea marini, Daniele Varsano, Conor Hogan, Nicola Spallanzani	Topics: 110 Posts: 618
Yambo old versions You can find here problems arising when using old releases of Yambo (< 5.0). Issues as parallelization strategy, performance issues and other technical aspects. **Moderators:** Davide Sangalli, andrea.ferretti, myrta gruning, andrea marini, Daniele Varsano, Conor Hogan	Topics: 251 Posts: 1425

WHO IS ONLINE

Suggested reading:

R. Martin, L. Reining, D. Ceperley
Cambridge University Press



Seminal papers:

L. Hedin Phys. Rev. A 139, A796 (1965)

L. Hedin, S. Lundqvist . in Solid State Physics, 23, 1–181 (1970)

Reviews:

D. Golze, M. Dvorak, and P. Rinke Front Chem. 2019; 7: 377. (2019)

Reining, L, WIREs Comput Mol Sci, 8: e1344. (2018)

Aulbur W. G., Jönsson L., Wilkins J. W. in Solid State Physics, Vol. 54, 1–218 (2000)

Aryasetiawan F., Gunnarsson O. The *GW* method. Rep. Prog. Phys. 61:237 (1998)

Yambo code implementation:

A. Marini, C. Hogan, M. Gruning and D. Varsano Comp. Phys. Comm. 180, 1293 (2009)

D. Sangalli et al. J. Phys.: Condens. Matter 31 325902 (2019)

Acknowledgment:

EuroHPC Joint Undertaking

Funded by the European Union

HANAMI

EU-Japan Alliance in HPC

MAX DRIVING THE EXASCALE TRANSITION

MaX (Materials design at the eXascale)

Yambo

The Yambo developers team

Thank you for your attention

Don’t hesitate to ask questions:

after the lectures, coffee breaks, hands-on sessions, anytime