Many-Body Perturbation Theory:
(1) The GW Approximation

Michael Rohlfing

Fachbereich Physik
Universität Osnabrück

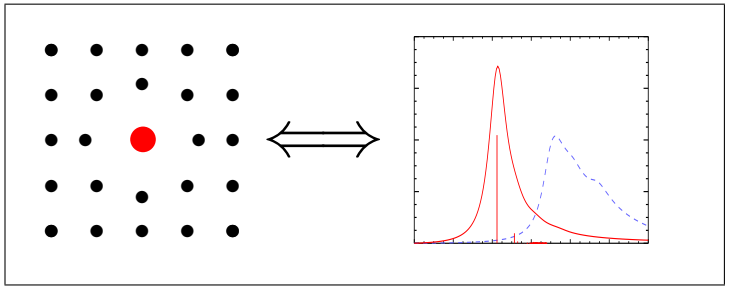
MASP, June 29, 2012

- Motivation
- Excited states: electrons, holes
- Equation of motion
- Approximations and tricks
- Examples

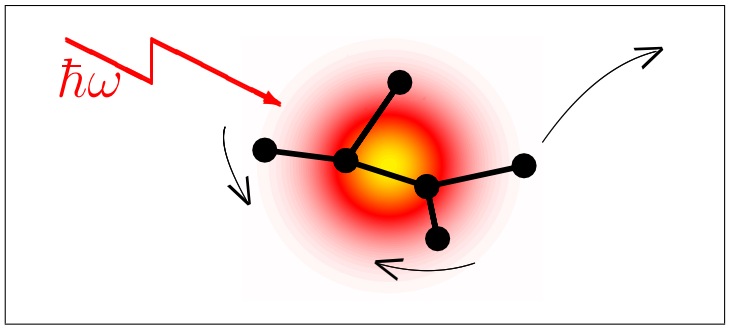
Relevance of excited electronic states

- Spectroscopy:
  - Electrons: Photoemission / Inverse PE / Tunneling spectroscopy
  - Light / Electron-hole pairs: Absorption / Emission / Reflectivity

- Characterisation of systems:
  - Geometric Structure
  - Defects / interfaces / ...
  - Macroscopic signature of microscopic details



- Short-time dynamics:
  - Electrons (femtoseconds)
  - Atomic structure (picoseconds)



- Technological relevance / Materials science:
  - Optoelectronics / Molecular electronics / Photovoltaics
  - Manipulation of bonds / Photochemistry

Density-Functional Theory: from 1960's until today

1950's/60's: Energy of electronic systems (homogeneous electron gas, inhomogeneous systems), including many-body effects (exchange, correlation)

Hohenberg, Kohn, Sham and others 1960's: interrelation between wave function, potential, energy, single-particle density $\rho(\mathbf{r}) = \int |\Psi(\mathbf{r}, \mathbf{r}_2, .., \mathbf{r}_N)|^2 d^3r_2 ... d^3r_N$, "single-particle orbitals" $\psi_n(\mathbf{r})$ and "single-particle energies" ϵ_n
$\Longrightarrow$ Intuitive understanding via effective single-particle quantum mechanics

Technical issues (1970's-today):
Pseudopotentials, basis sets, iterations, geometry optimization, molecular dynamics, ...

Approximation of Exchange+Correlation (1970's-today):
Local-density approximation (LDA), Generalized gradient approximation (GGA), "Hybrid functionals" (including Hartree-Fock exchange) PBE0-BLYP-B3LYP-HSE-... , ...

Today: 50-100 codes + 100-1000 developers + 1000-10000 users
Total energy $E_{tot}[\mathrm{R}]$, Geometric structure, vibrations, chemical reactions, ...
Physics + Chemistry
SIESTA, VASP, ABINIT, CRYSTAL, GAUSSIAN, TURBOMOLE, ...
Interpretation of ϵ_n as "single-particle energies" without formal justification

DFT = "ground-state method": not suited for electronic excitation processes

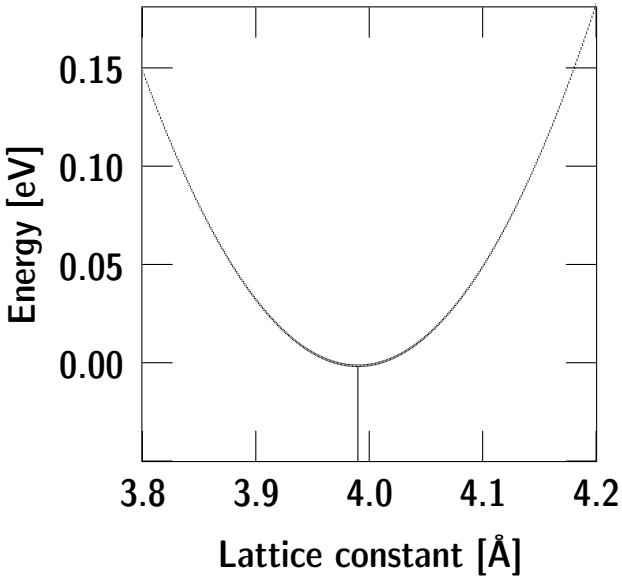
Density-Functional Theory (DFT)

[Hohenberg, Kohn, Sham (1964)]

- Atomic postions $\{\mathbf{R}\}$, Electron density $\rho(\mathbf{r})$
- $\mathsf{E}_{\mathsf{tot}}[\mathbf{R},\rho] = \mathsf{E}_{\mathsf{kin}}[\rho] + \mathsf{E}_{\mathsf{Coul}}[\rho] + \mathsf{E}_{\mathsf{xc}}[\rho] + \mathsf{E}_{\mathsf{ext,e}}[\mathbf{R},\rho] + \mathsf{E}_{\mathsf{nucl,nucl}}$

$\mathsf{E}_{\mathsf{kin}}$	kinetic energy of the electrons
$\mathsf{E}_{\mathsf{Coul}}[\rho]$	classical Coulomb energy of the electrons
$\mathsf{E}_{\mathsf{xc}}[\rho]$	Exchange-correlation functional
	(Local-density approx., gradient corrections)
$\mathsf{E}_{\mathsf{ext,e}}$	Nucl.-electron interaction (+ ext. fields)
$\mathsf{E}_{\mathsf{nucl,nucl}}$	Nucl-Nucl interaction

Aluminium: $\mathsf{E}_{\mathsf{tot}}(\mathsf{a}_{\mathsf{latt}})$



- Optimize $\mathsf{E}_{\mathsf{tot}}[\mathbf{R},\rho]$ w.r.t. $\rho(\mathbf{r}) = \sum |\psi_{\mathsf{m}}^{\mathsf{DFT}}(\mathbf{r})|^2$

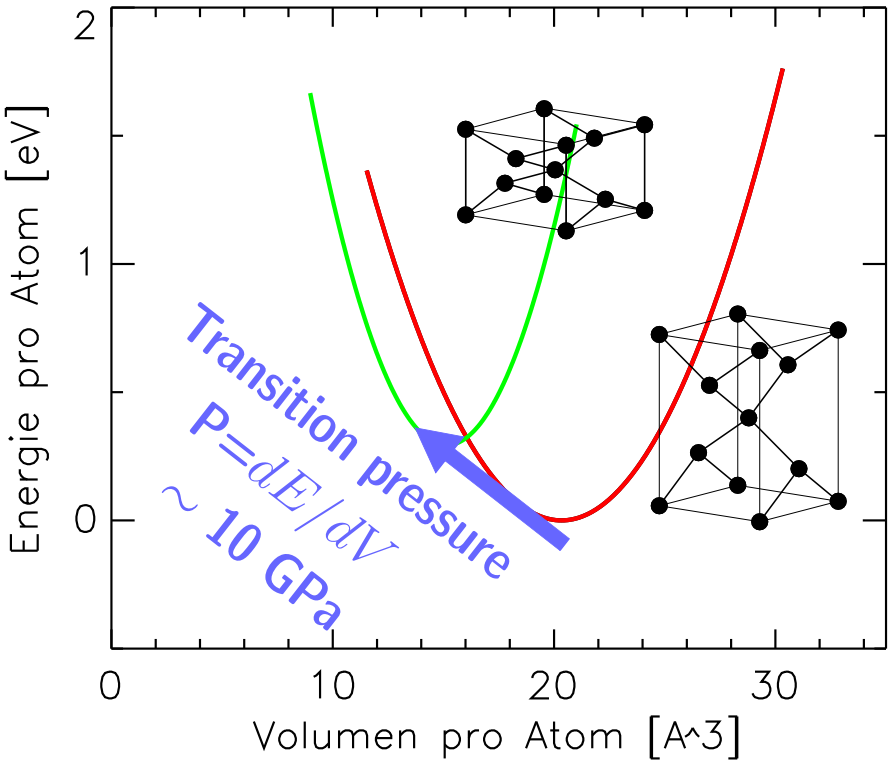
$\Longrightarrow$ Kohn-Sham equations: $$\left(\frac{p^2}{2m} + V_{\mathsf{Coul}}^{[\rho]}(\mathbf{r}) + V_{\mathsf{xc}}^{[\rho]}(\mathbf{r}) + V_{\mathsf{ext,e}}(\mathbf{r})\right)\psi_{\mathsf{m}}^{\mathsf{DFT}}(\mathbf{r}) = \epsilon_{\mathsf{m}}^{\mathsf{DFT}}\psi_{\mathsf{m}}^{\mathsf{DFT}}(\mathbf{r})$$

$\Longrightarrow$ Total energy $\mathsf{E}_{\mathsf{tot}}[\mathbf{R}]$ and forces $\partial \mathsf{E}_{\mathsf{tot}}/\partial R_{i\alpha}$ $\longleftrightarrow$ Geometry, bonds, phonons, ...

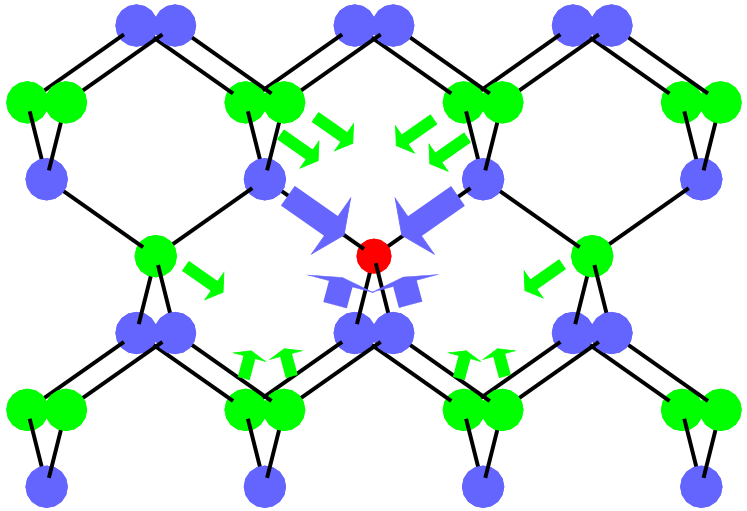
"Wave functions" $|\psi_m^{\mathsf{DFT}}\rangle$, "Band-structure energies" $\epsilon_m^{\mathsf{DFT}}$ (often not really reliable...)

DFT for bulk systems

Phase transition of silicon under pressure:
Diamond → β-Sn



N in GaAs: Forces on atoms



• Ga • As • N

Ga (1.Nb.): 2.0 eV/Å

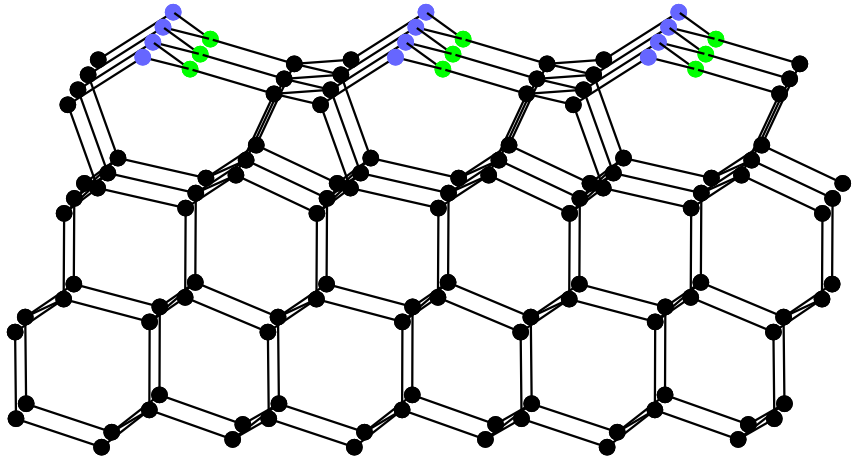
As (2.Nb.): 0.1 eV/Å

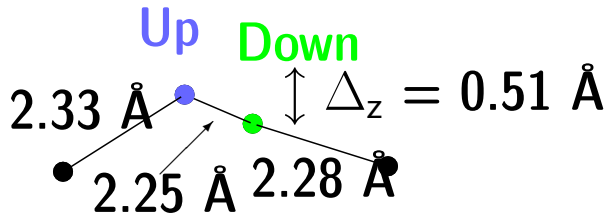
$\Longrightarrow$ **Relaxations at defect**

Surfaces geometries from DFT

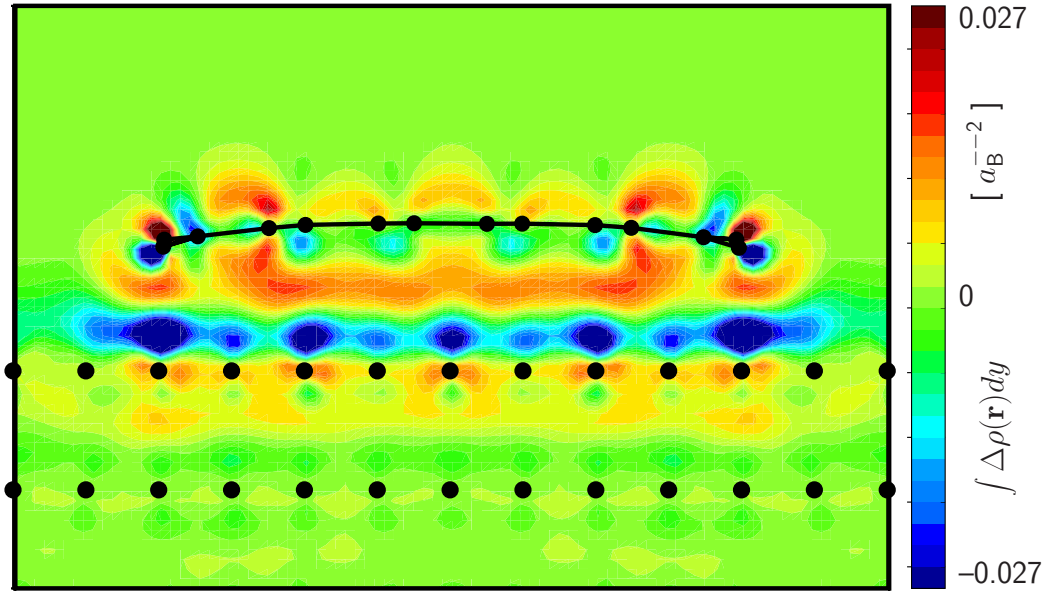
Si(111)-(2×1) surface: π-bonded chains

K.C. Pandey, Phys. Rev. Lett. 49, 223 (1982)





Adsorbed molecules: PTCDA on Ag(111)



Change of charge density during adsorption:

Red: charge accumulation

Blue: charge depletion

Many-Body Perturbation Theory: from 1960's until today

Key Idea of Many-Body Perturbation Theory:

- $H^{(0)}$ (including simplified el.-el. interac.) $\Longrightarrow \quad G_1^{(0)}(E) = (E - H^{(0)})^{-1}$ (exact)
- plus rest of electron-electron interaction (= "perturbation"):

  $\Longrightarrow G_1(E) = G_1^{(0)}(E) + G_1^{(0)}(E)\,\Sigma(E)\,G_1(E)$

  $\Sigma(E)$ = Self-energy operator (=single-particle signature of remaining interaction)

1950's/60's: Spectra of electronic systems (homogeneous electron gas)
[Hedin and others, 1960's]

"Forgotten" (success of DFT; computational effort), "recovered" due to DFT band-gap problem.

Band structure of bulk semiconductors (1980's): Hybertsen, Louie, Godby, Schlüter, Sham, ..

Surfaces, nanostructures (1980's/90's)

Optical spectra (1990's/2000's): Onida, Reining, Benedict, Shirley, Rohlfing, Louie, ...

Technical issues (1980's-today):

Basis sets, frequency integration, eigenvalue decomposition, self consistency, ...

Today: 10-20 codes + 30-50 developers + 50-100 users

Band structures + optical excitations

Crystals, surfaces, molecules, polymers, ...

States of a many-electron system

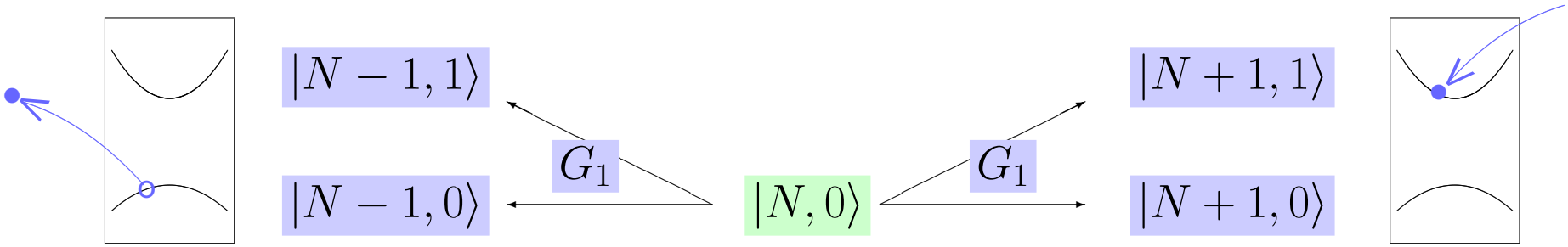
N **Electrons**

$$|N, 0\rangle$$

1. **Ground state** $|N, 0\rangle$ **:** **Density-functional theory** $\Longrightarrow$ **Geometry**

States of a many-electron system

$N-1$ **Electrons** N **Electrons** $N+1$ **Electrons**



G_1 = **Single-particle Green function**

1. **Ground state** $|N,0\rangle$: **Density-functional theory** $\Longrightarrow$ **Geometry**

Many-body perturbation theory:

2. $|N,0\rangle \rightarrow |N\pm 1,m\rangle$: $G_1(\mathbf{x}t,\mathbf{x}'t') = -i\left\langle N,0\left|T\left(\psi(\mathbf{x},t)\psi^+(\mathbf{x}',t')\right)\right|N,0\right\rangle$

(Propagation of electron or hole between $(\mathbf{x},t)$ **and** $(\mathbf{x}',t')$ **)**

Hedin's equations

[L. Hedin, Phys. Rev. 139, A796 (1965), L. Hedin and S. Lundqvist, Sol.St.Phys. 23, 1 (1969).]

- **EOM of G_1:** $\left\{i\frac{\partial}{\partial t}+\nabla^2-V_{\rm ext}(\mathbf{r})-V_{\rm Coul}(\mathbf{r})\right\}G_1(\mathbf{x}t,\mathbf{x}'t')+i\int\frac{e^2}{|\mathbf{r}-\mathbf{r}''|}G_2(\mathbf{x}''t,\mathbf{x}''t,\mathbf{x}t,\mathbf{x}'t')d\mathbf{x}''=\delta(\mathbf{x},\mathbf{x}')\delta(t,t')$
- **Decoupling by self-energy operator Σ:**

$$\{\partial_t+\nabla^2-V_{\rm ext+Coul}(\mathbf{r})\}G_1(12)-\int\Sigma(13)G_1(32)d(3)=\delta(12)$$
$$\Sigma(12) = i\int W(1^+3)G_1(14)\Gamma(42;3)d(34)$$
$$W(12) = \int\epsilon^{-1}(13)v(32)d(3)$$
$$\epsilon(12) = \delta(12)+\int v(13)\chi_0(32)d(3)$$
$$\chi_0(12) = -i\int G_1(23)G_1(42)\Gamma(34;1)d(34)$$
$$\Gamma(12;3)=\delta(12)\delta(13)+\int\frac{\delta\Sigma(12)}{\delta G_1(45)}G_1(46)G_1(75)\Gamma(67;3)d(4567)$$

Σ = Self energy
W = Screened Coulomb interaction
ϵ = Dielectric function
χ_0 = Polarizability
G_1 = Single-particle Green function
Γ = Vertex function
(1) = ($\mathbf{r}_1$,σ_1,t_1) Position/Spin/Time

"GW approximation":
$\Gamma(12;3)=\delta(12)\delta(13)$

$\Longrightarrow$

$$\{\partial_t+\nabla^2-V_{\rm ext+Coul}(\mathbf{r})\}G_1(12)-\int\Sigma(13)G_1(32)d(3)=\delta(12)$$
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$$\chi_0(12) = -iG_1(21)G_1(12)$$

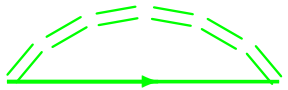
Physical significance of Σ:

- **in vacuum:** χ_0=0, ϵ=1, ϵ^{-1}=1, W=v

  $\Longrightarrow \Sigma = iG_1 v$ **Exchange (Fock) operator / Hartree-Fock theory**

- **in matter:** Dielectric polarizability $\chi_0 \Longrightarrow$ "W<v" **(weaker)**

  $\Longrightarrow \Sigma = iG_1 W$ **"Screened Exchange"**



- **Nomenclature:**

  $\Sigma = iG_1 v + iG_1(W - v)$ = **"Exchange" + "Correlation"**

[L.

• EOM

• Decou

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Σ

W

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χ_0

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$\delta(t,t')$

$\Gamma(12;3) = \delta(12)\delta(13) + \int \frac{\delta\Sigma(12)}{\delta G_1(45)} G_1(46) G_1(\quad 5)\Gamma(67;3) d(4567)$

1 = Vertex function

(1) = ($\mathbf{r}_1$,σ_1,t_1) Position/Spin/Time

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$\Gamma(12;3) = \delta(12)\delta(13)$

$\Longrightarrow$

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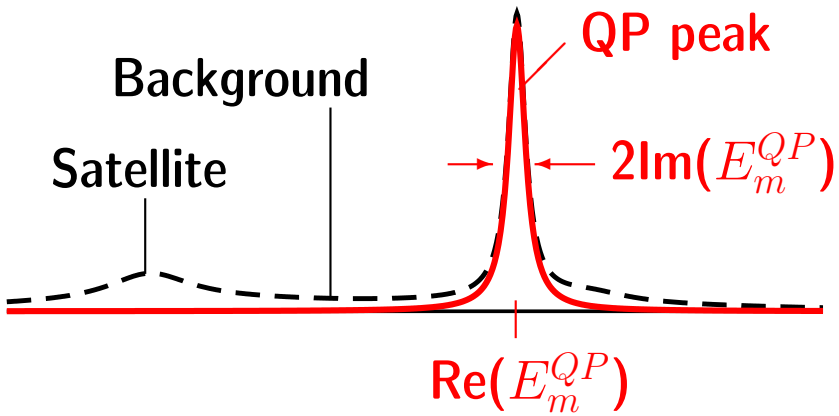
Some pragmatic issues

- **Time homogeneity:** $G_1(t,t') = G_1(t-t')$ **; Fourier transform to energy:** $G_1(E)$, $\Sigma(E)$ **etc.**

- **"Quasiparticle (QP) approximation":**
  Ignore background, satellites, etc. in $G_1(E)$

$$\Longrightarrow G_1(\mathbf{x},\mathbf{x}',E) = \sum_m \frac{\phi_m^{QP}(\mathbf{x})(\phi_m^{QP}(\mathbf{x}'))^*}{E - E_m^{QP} \pm i0^+}$$



Re(E_m^{QP}) = QP band-structure energy,
Im(E_m^{QP}) = spectral width, 1/Im(E_m^{QP}) = lifetime

- **EOM:** $\{-\nabla^2 + V_{\rm ext}(\mathbf{r}) + V_{\rm Coul}(\mathbf{r})\}\phi_m^{QP}(\mathbf{x}) + \int \Sigma(\mathbf{x},\mathbf{x}',E_m^{QP})\phi_m^{QP}(\mathbf{x}')d\mathbf{x} = E_m^{QP}\phi_m^{QP}(\mathbf{x})$

- **Self-consistency problem similar to DFT, Hartree-Fock, etc.**
  $\Longrightarrow$ **either iterate, or use another method as starting point, e.g. DFT:**

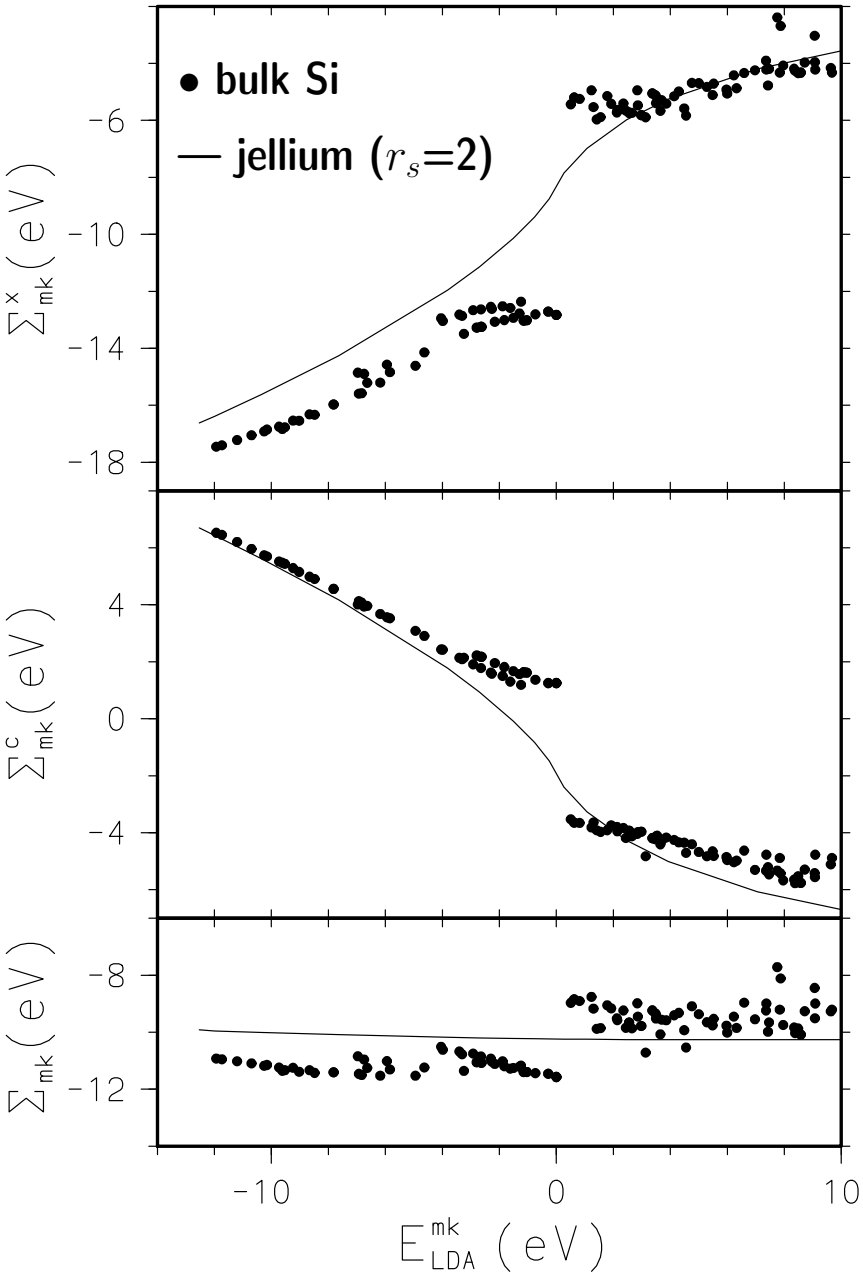
$$\phi_m^{DFT}(\mathbf{x}),\ E_m^{DFT} \Longrightarrow G_1^{DFT} \Longrightarrow \chi_0,\ \epsilon,\ W,\ \Sigma(E)$$

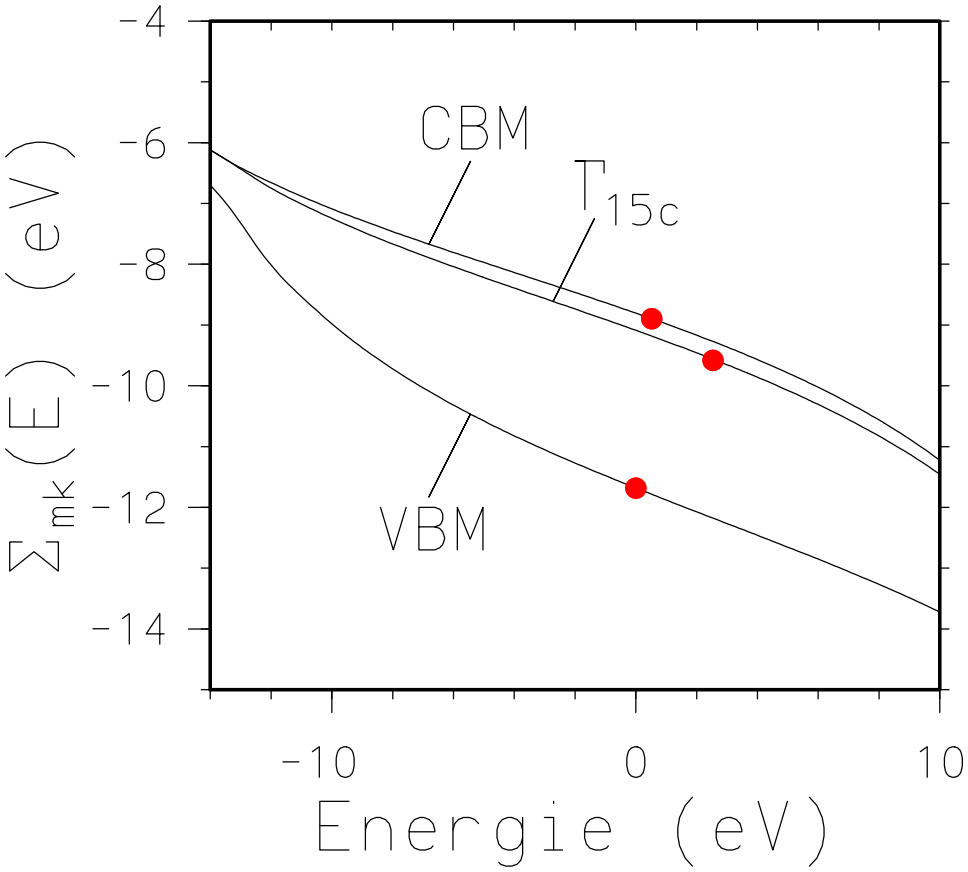
$\Longrightarrow$ **Perturbation** ($\Sigma(E) - V_{xc}^{DFT}$)**:**

$$\{\hat{H}^{DFT} + \underbrace{(\Sigma(E_m^{QP}) - V_{xc}^{DFT})}\}\,|\phi_m^{QP}\rangle = E_m^{QP}|\phi_m^{QP}\rangle$$

"QP correction to DFT"

Self-energy data



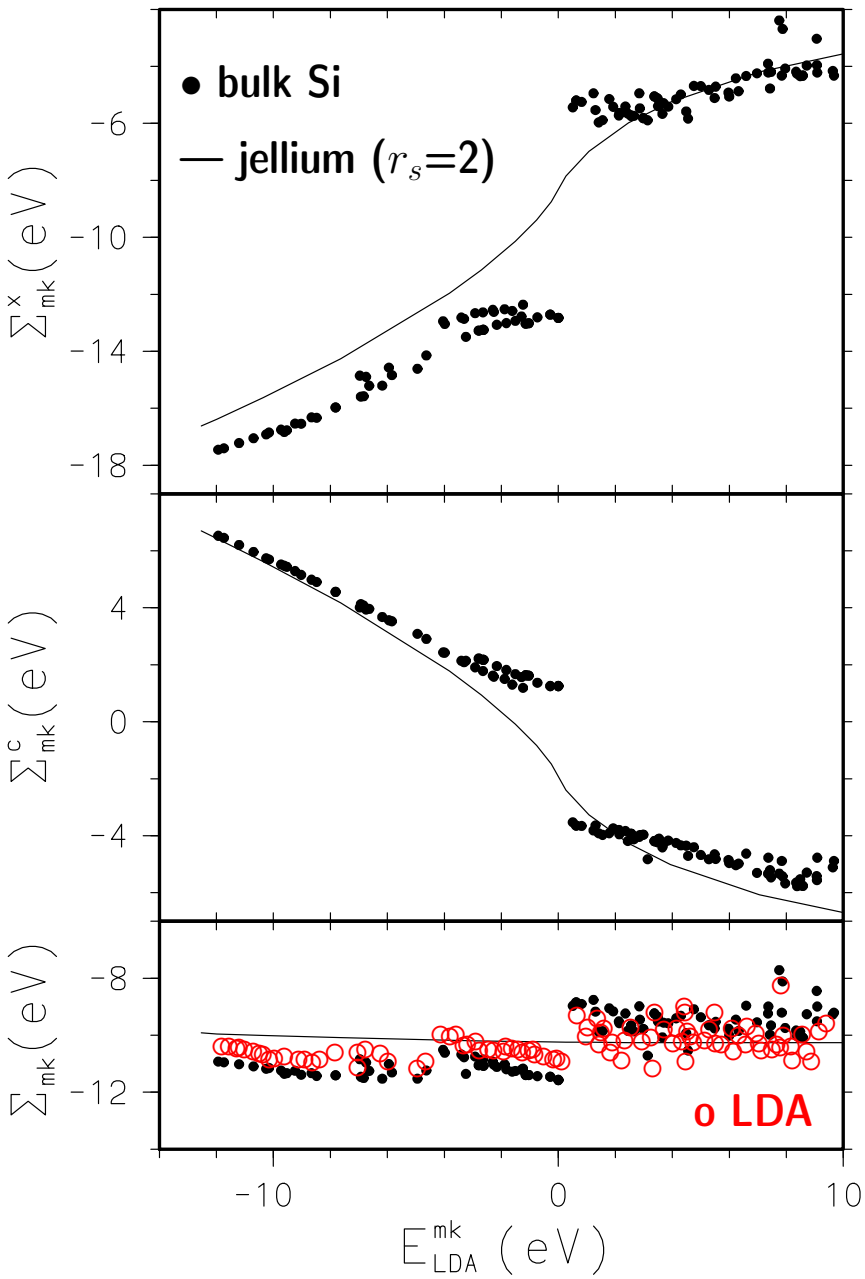


— $\Sigma(E)$

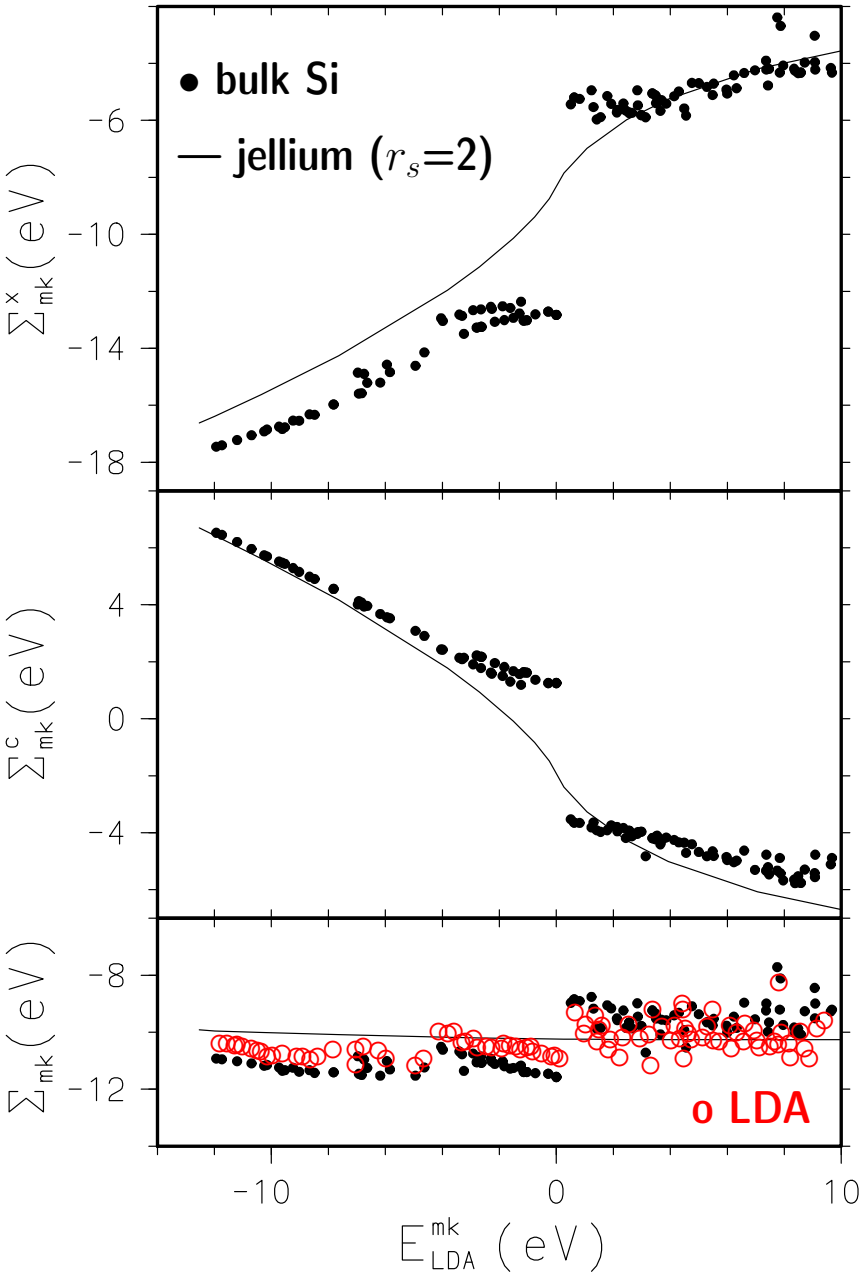
• Solution $E_{m\mathbf{k}}$ of

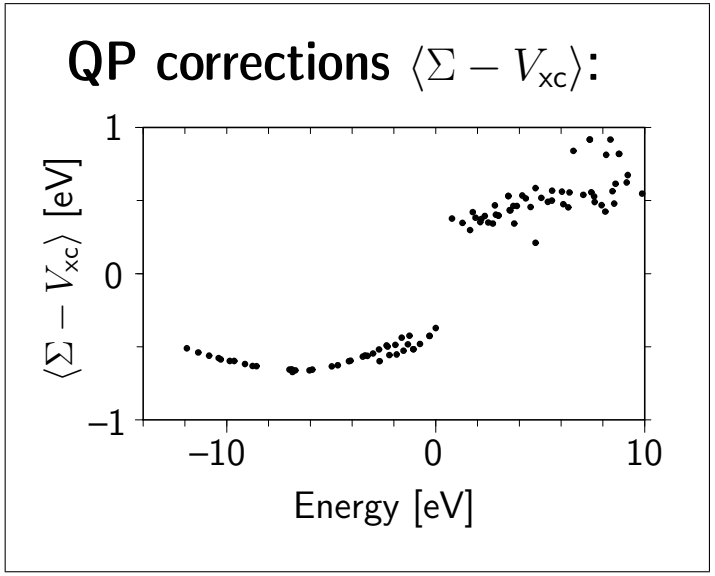
$$(H^{DFT} + \Sigma(E_{m\mathbf{k}}) - V_{xc})|\phi_{m\mathbf{k}}\rangle = E_{m\mathbf{k}}|\phi_{m\mathbf{k}}\rangle$$

Self-energy data



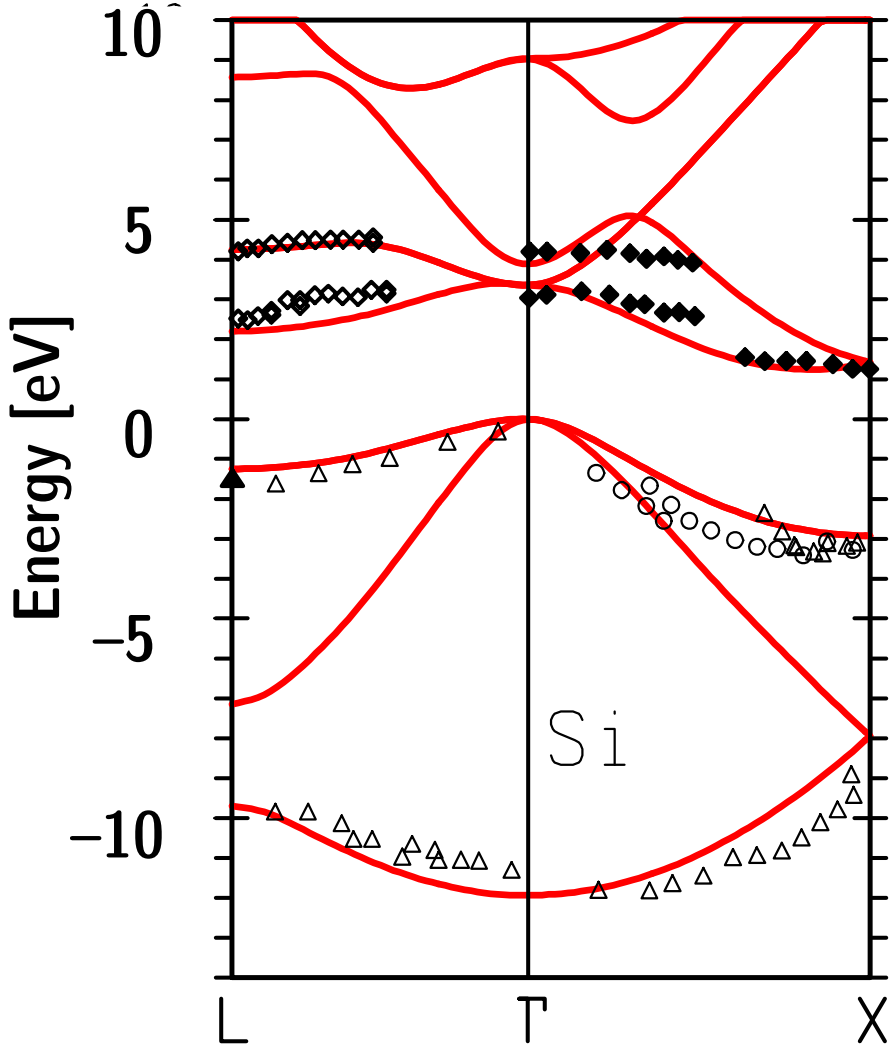
Self-energy data





GW band structure: Bulk crystals

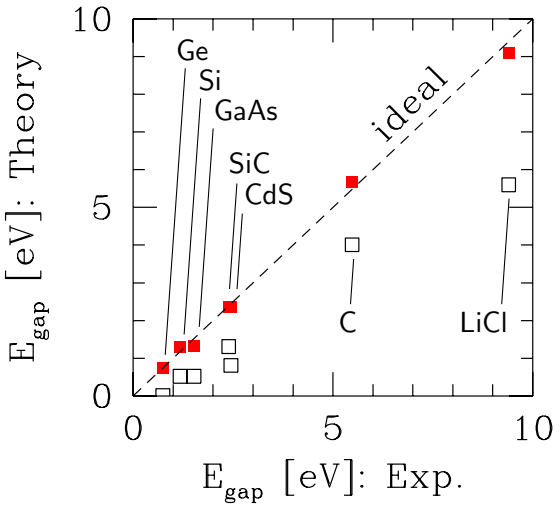
GW band structure of Si:



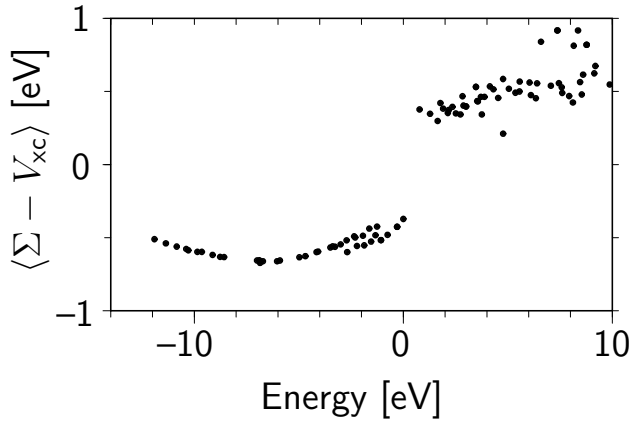
◇□• Exp.: J.E. Ortega and F.J. Himpsel, PRB 47, 2130 (1993)

Semiconductor gap energies:

GWA ■ / LDA □



QP corrections $\langle \Sigma - V_{xc} \rangle$:



GW band structure: Molecules / Clusters

Ionisation energies:

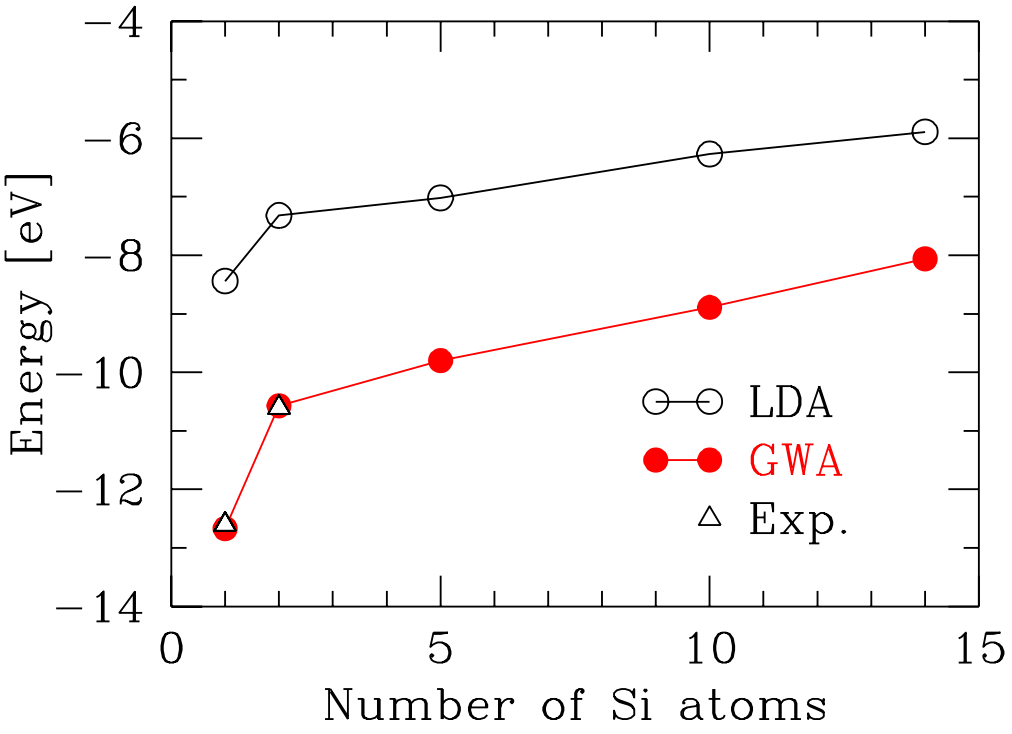
[eV]	LDA[a]	GWA	Exp.[b]
He	15.48	24.68	24.586
Ne	13.06	21.47	21.564
Ar	10.35	15.94	15.759
CO	9.1	14.3	14.01
HCl	8.0	12.6	12.75
CH_4	9.3	12.5	12.99
C_2H_4	6.9	10.4	10.5
Si_2H_6	7.3	10.5	10.6

[a] LDA: $-E_{\text{HOMO}}$

[b] Exp.: Landolt-Börnstein, Vol. I-1;
G. Herzberg, "Molecular Spectra";
U. Itoh et al., JCP 85, 4867 (1986).

Si_mH_n: QP HOMO Energies:

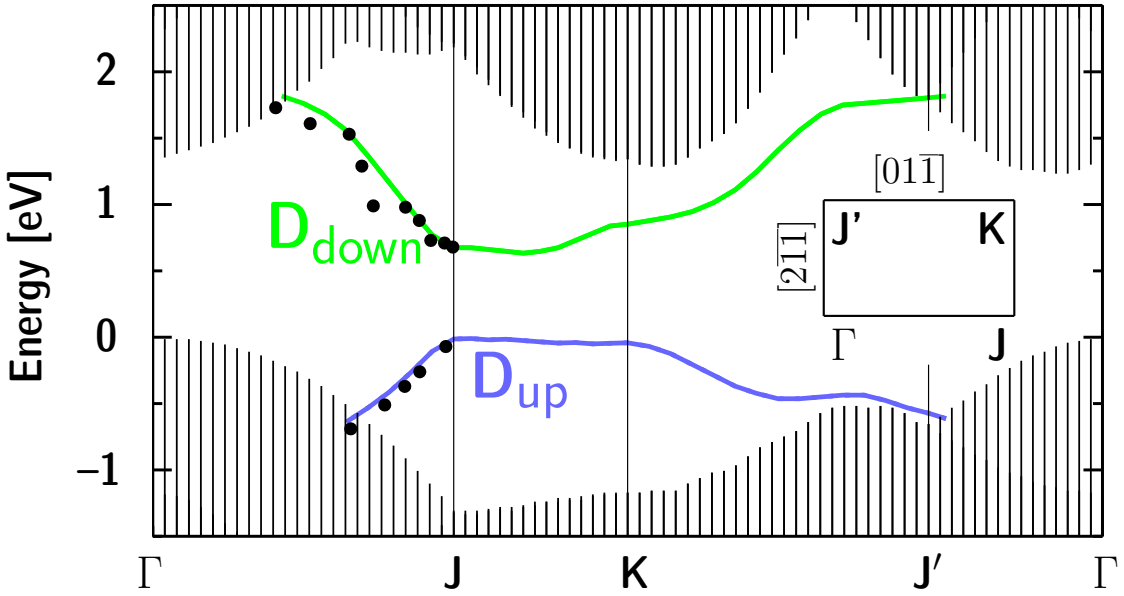
Size dependence / Quantum confinement



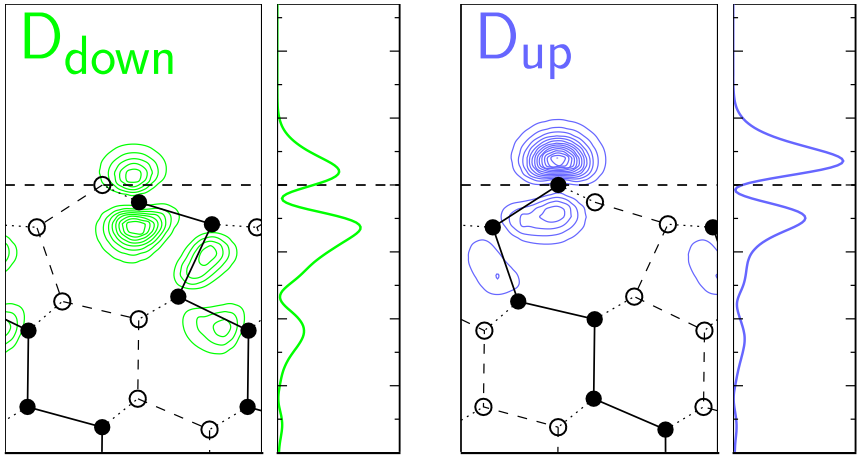
Exp.: U. Itoh et al., JCP 85, 4867 (1986).

GW band structure: Si(111)-(2×1) Surface

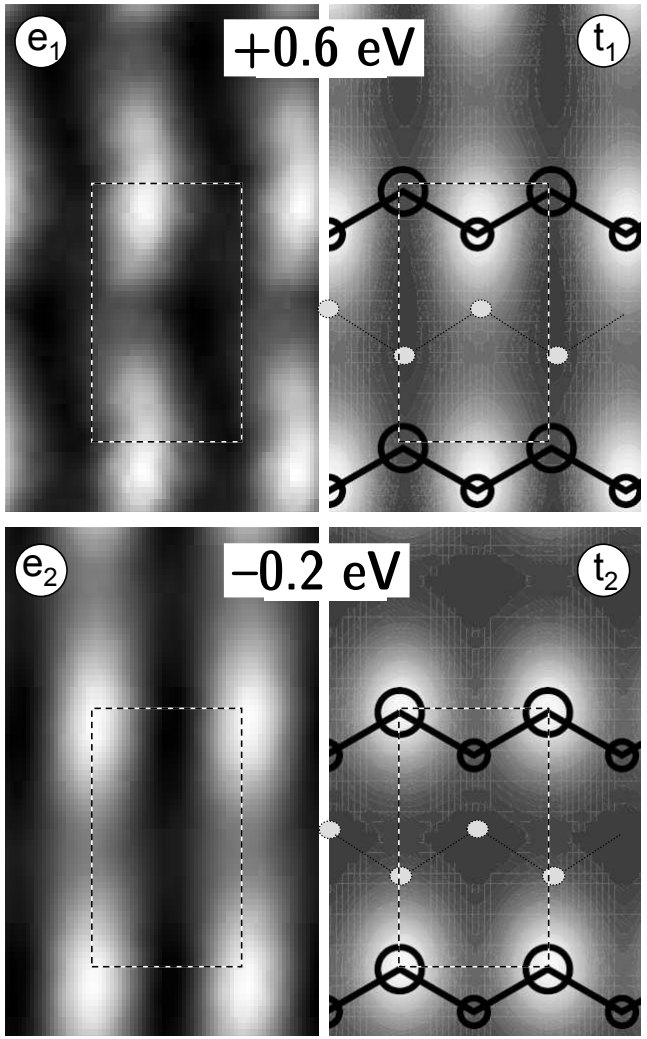
Si(111)-(2×1): Surface band structure:



Exp. (•): Uhrberg et al., Perfetti et al.



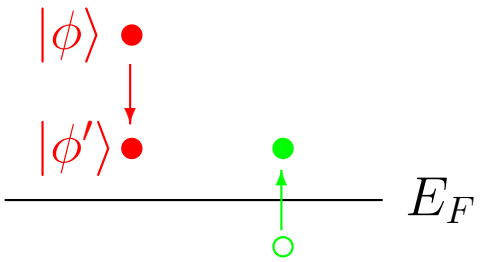
Measured / simulated STM image:



J.Garleff et al., PRB 70, 245424 (2004).

Lifetimes from scattering due to Coulomb-interaction

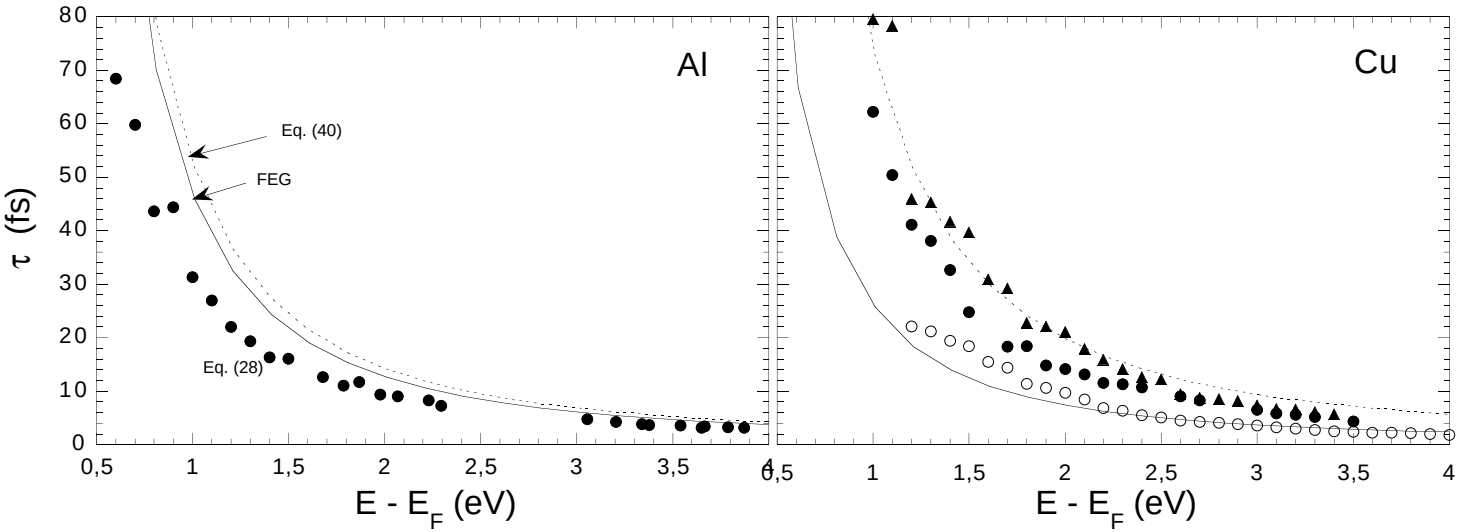
See, e.g., P.M. Echenique et al., Chemical Physics 251, 1 (2000).

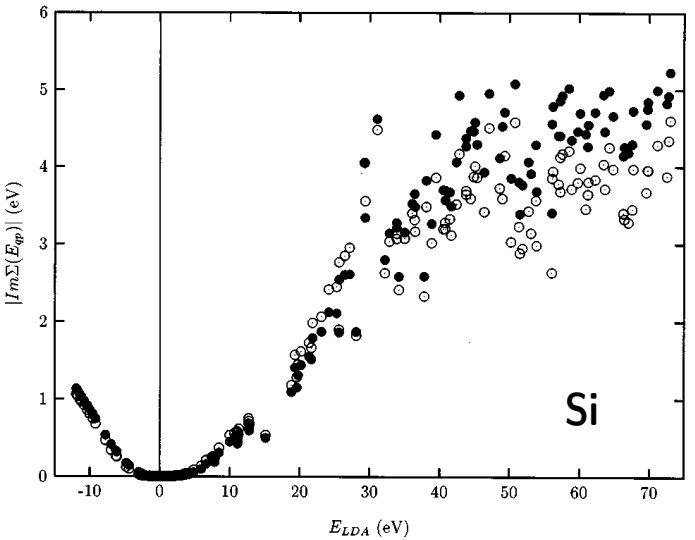


- Scattering of additional electron by other electrons:
  $|\phi\rangle$ at $E \longrightarrow |\phi'\rangle$ at $E'<E$ plus electron-hole pair(s)

  (Conservation of energy + momentum)

- In QP language: "the particle in state $|\phi\rangle$ is gone $\Longrightarrow$ it had a finite lifetime!"
- Coulomb-scattering is included in Σ^{GWA} $\Longrightarrow$ Lifetime = Inverse of Im$\langle\phi|\Sigma^{GWA}|\phi\rangle$
- Two-photon photoemission; finite mean-free path of (high-energy) electrons ; ...





[P.M. Echenique et al., Chemical Physics 251, 1 (2000); A. Fleszar and W. Hanke, PRB 56, 10228 (1997).]

Dielectric screening within the random-phase approximation

- Key element of many-body perturbation theory: Response function $\chi(\mathbf{r}, \mathbf{r}', \omega)$
- Here: simple notation within classical electrodynamics, without exchange-correlation effects

... charge response to an external perturbing field: $\partial\rho_{ind} = \chi\partial V_{ext}$

... charge response to the total perturbing field, $\partial V = \partial V_{ext} + \partial V_{ind}$: $\partial\rho_{ind} = \chi_0\partial V$

- Relationship with dielectric function $\epsilon(\mathbf{r}, \mathbf{r}', \omega)$: $\epsilon = 1 - v\chi_0$ / $\epsilon^{-1} = 1 + v\chi$

- Approx. evaluation from DFT: $G_1^{(0)}(\mathbf{x}, \mathbf{x}', E) = \sum_{\mathsf{m}} \frac{\psi_{\mathsf{m}}^{\mathsf{DFT}}(\mathbf{x})\psi_{\mathsf{m}}^{\mathsf{DFT}}(\mathbf{x}')^*}{E - E_{\mathsf{m}}^{\mathsf{DFT}} \pm i0^+}$, $\chi_0 = iG_1G_1$
- Dyson equation $\chi = \chi_0 + \chi_0 v\chi$ or, more general: $\chi_\lambda = \chi_0 + \chi_0(\lambda v)\chi_\lambda$ **λ=0...1**
- Screened Coulomb potential $W(\mathbf{r}, \mathbf{r}', \omega)$ between charged particles: $W = \epsilon^{-1}v$
  - $W(\omega) \implies \Sigma = iG_1W$ QP band structure
  - $W(\omega = 0) \implies K^{eh}$; K^{eh} + QP band structure $\rightarrow$ Optical spectrum
  - $\chi_\lambda(iu) \implies$ Correlation energy beyond DFT; Van der Waals interaction etc.

Dielectric screening within the random-phase approximation (2)

- **Explicit expression, e.g. in plane waves:**

$$\chi^{(0)}_{\mathbf{G}\mathbf{G}'}(\mathbf{q},\omega) = 2\frac{1}{V}\sum_{\mathbf{k}}\sum_{\mathrm{m}\in\mathrm{Val}}\sum_{\mathrm{n}\in\mathrm{Con}} M^{\mathrm{mn}}_{\mathbf{G}}(\mathbf{k},\mathbf{q})\left[M^{\mathrm{mn}}_{\mathbf{G}'}(\mathbf{k},\mathbf{q})\right]^* \times\left[\frac{1}{E_{\mathrm{m}\mathbf{k}}-E_{\mathrm{n},\mathbf{k}+\mathbf{q}}-\omega+i0^+}+\frac{1}{E_{\mathrm{m}\mathbf{k}}-E_{\mathrm{n},\mathbf{k}+\mathbf{q}}+\omega+i0^+}\right]$$

  - **Double summation over occupied and empty states: extremely time consuming**
  - **Recent progress in simplification (Galli et al., Reining et al.,...)**

  with matrix elements $M^{\mathrm{mn}}_{\mathbf{G}}(\mathbf{k},\mathbf{q}) = \int \phi^*_{\mathrm{m}\mathbf{k}}(\mathbf{r}) e^{-i(\mathbf{q}+\mathbf{G})\mathbf{r}} \phi_{\mathrm{n},\mathbf{k}+\mathbf{q}}(\mathbf{r}) d^3r$

- $\epsilon_{\mathbf{G}\mathbf{G}'}(\mathbf{q},\omega) = \delta_{\mathbf{G}\mathbf{G}'} - \frac{1}{|\mathbf{q}+\mathbf{G}|}\chi^{(0)}_{\mathbf{G}\mathbf{G}'}(\mathbf{q},\omega)\frac{1}{|\mathbf{q}+\mathbf{G}'|}$

- **After matrix inversion: macroscopic dielectric constant** $\epsilon_M(\mathbf{q},\omega) = [\epsilon_{\mathbf{00}}(\mathbf{q},\omega)]^{-1}$
  e.g. bulk silicon $\epsilon_M(0,0) = 12$, **SiO$_2$** $\epsilon_M(0,0) = 2$

- **Homogeneous system:** $\epsilon_{\mathbf{G}\mathbf{G}'}(\mathbf{q},\omega) \longrightarrow \epsilon(|\mathbf{q}+\mathbf{G}|,\omega)$

- **jellium: Lindhard formula for** $\epsilon(|\mathbf{q}+\mathbf{G}|,\omega)$: $\epsilon(0,\omega\approx 0) = 1-\frac{\omega_P^2}{\omega^2}$ $\epsilon(q\approx 0,0) = 1+\frac{q_{TF}^2}{q^2}$

- **anisotropic non-cubic systems: 3x3 tensor** $\epsilon_M(\mathbf{q},\omega) \longrightarrow \epsilon_{ij}(\mathbf{q},\omega)$ $i,j{=}x,y,z$

Self-energy operator / Numerical issues

- Matrix elements (i.e., between DFT states $|m\mathbf{k}\rangle$ and $|m'\mathbf{k}\rangle$) of self-energy operator:

$$\Sigma_{m,m'}(\mathbf{k},E) = \sum_n \sum_{\mathbf{q},\mathbf{G},\mathbf{G}'} M^{\mathrm{mn}}_{\mathbf{G}}(\mathbf{k},\mathbf{q}) \left[M^{\mathrm{m'n}}_{\mathbf{G}'}(\mathbf{k},\mathbf{q})\right]^* \frac{i}{2\pi}\int d\omega \frac{W_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega)}{E - E_{n\mathbf{k}+\mathbf{q}} - \omega \pm i0^+}$$

- Band summation $\sum_n$ very demanding [about (10-20)$\times$(Number of valence bands)]
  ... can be avoided/circumvented: see, e.g., Reining et al.
- Sum over $\mathbf{G}$, $\mathbf{G}'$ / Representation of χ_0, ϵ etc.:
  ... replace by localized orbitals (Gaussians, numerical orbitals, SIESTA, ...)
  ... mixed basis: localized orbitals PLUS plane waves
  (see, e.g., Blase et al., Rinke+Scheffler, Rohlfing et al., ...)
- Frequency integration $\int d\omega$:
  — numerical integration: Garcia-Gonzalez, Rubio and many others
  — imaginary frequency (or time): Godby, Rinke, Schindlmayr, and others
  — Plasmon-Pole Model for $W(\omega)$: $\int d\omega$ becomes analytic: most authors

$$W(\omega) \to 1 + \frac{A}{(\omega^2 - \Omega^2) \pm i0^+} \quad \Longrightarrow \quad \frac{i}{2\pi}\int d\omega(\ldots) \to -\Theta_{E_n<E_F} \pm \frac{A\Omega}{2(E - E_n \pm \Omega)}$$

Summary: Many-body perturbation theory for $|N,0\rangle \rightarrow |N \pm 1, m\rangle$ / G_1

- $H^{(0)}$ (simplified el.-el. interac., here: DFT) $\Longrightarrow$ $G_1^{(0)}(E) = (E - H^{(0)})^{-1}$ (exact)
- plus rest of electron-electron interaction (= "perturbation"):

$$\Longrightarrow G_1(E) = G_1^{(0)}(E) + G_1^{(0)}(E)\, d\Sigma(E)\, G_1(E) \qquad \text{(Dyson eq.)}$$

$d\Sigma(E) =$ remaining self-energy operator (here: $(\Sigma(E) - V_{xc}^{DFT})$)
(=single-particle signature of remaining interaction)

- Equation of motion for a single quasiparticle (= excited electron / hole):

$$\left\{H^{(0)} + d\Sigma(E_{\mathsf{m}}^{\mathsf{QP}})\right\} \phi_{\mathsf{m}}^{\mathsf{QP}} = E_{\mathsf{m}}^{\mathsf{QP}} \phi_{\mathsf{m}}^{\mathsf{QP}}$$

$\Longrightarrow$ Quasiparticle wave functions $\phi_{\mathsf{m}}^{\mathsf{QP}}(\mathbf{r})$

QP energies $E_{\mathsf{m}}^{\mathsf{QP}} = \mathrm{Re}E_{\mathsf{m}}^{\mathsf{QP}} + i \cdot \mathrm{Im}E_{\mathsf{m}}$

$$\phi_m(t) \sim \exp(i\mathrm{Re}E^{\mathsf{QP}}t) \cdot \exp(-\mathrm{Im}E_m^{\mathsf{QP}}t)$$

$\mathrm{Re}E_{\mathsf{m}}^{\mathsf{QP}}$ = Energy level / Band-structure energy

$\mathrm{Im}E_{\mathsf{m}}^{\mathsf{QP}}$ = Spectral width / Inverse lifetime