

Introduction to density functional theory

Mini course on DFT for PhD
February-March 2026

LECTURE 3

- 1. metals**
- 2. post-processing**
- 3. forces & structural optimization**
- 4. energy barriers**

- 1. metals**
2. post-processing
3. forces & structural optimization
4. energy barriers

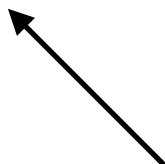
Brillouin zone sampling

We wrote:

$$n(\mathbf{r}) = \sum_i |\psi_i(\mathbf{r})|^2$$

but actually we have to calculate:

$$n(\mathbf{r}) = \sum_{\mathbf{k}} \sum_i |\psi_{\mathbf{k},i}(\mathbf{r})|^2$$

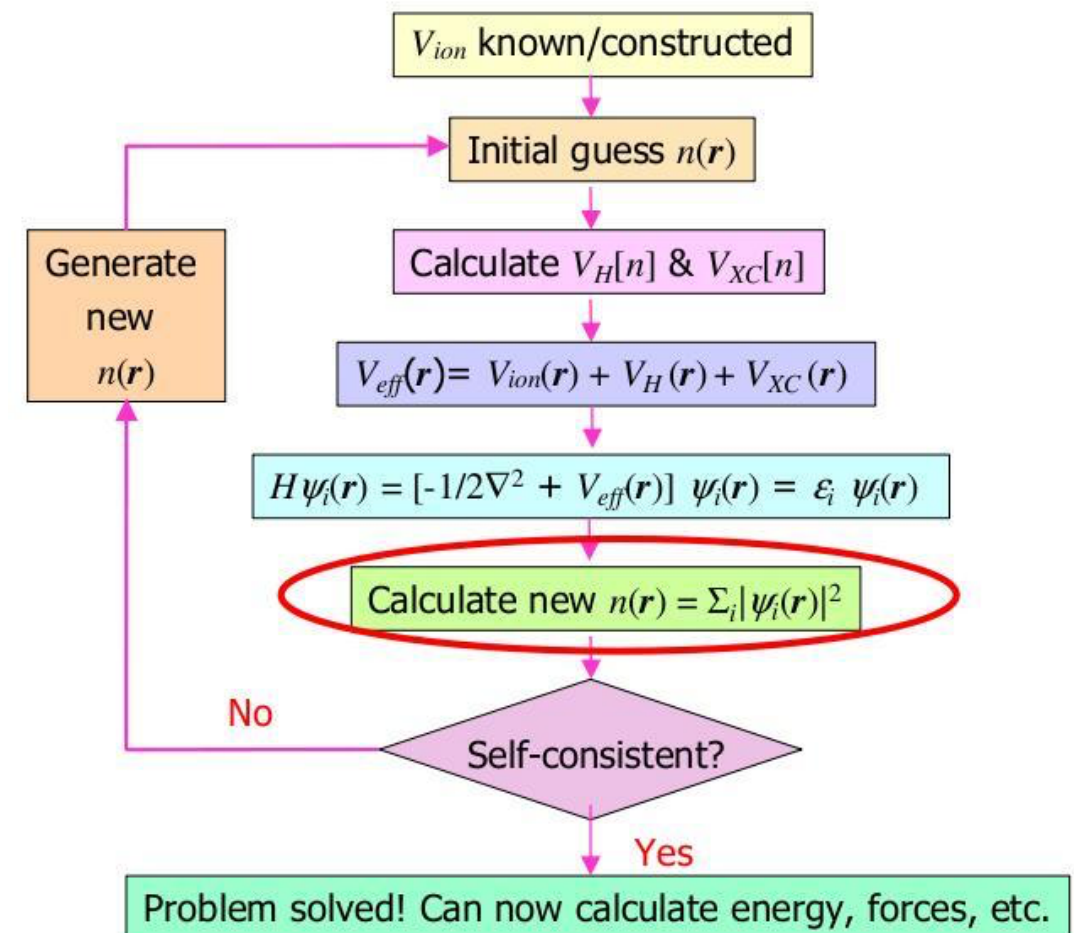
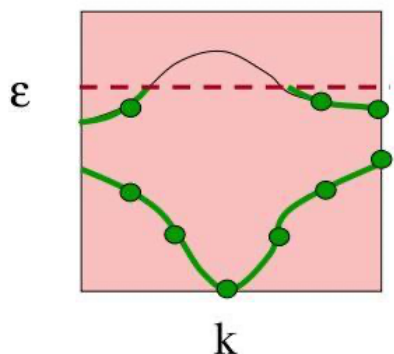


where the $\{\mathbf{k}\}$ s are inside
the first Brillouin zone; the
finer is the $\mathbf{k}$ -mesh, the
more precise is the
description of $\psi \Rightarrow$ **we
already spoke about
convergence test!**

More on $\mathbf{k}$ points and Brillouin zone sampling

$$n(\mathbf{r}) = \sum_{\mathbf{k}} \sum_i |\psi_{\mathbf{k},i}(\mathbf{r})|^2$$

- The calculation of the charge density (and of many other quantities) requires sums over all $\mathbf{k}$ -points in the Brillouin Zone (BZ); in practice, some form of *BZ sampling* is needed. Convergence wrt $\mathbf{k}$ -point sampling *must be tested*!
- For insulators in large supercells, amorphous systems, liquids, molecules, sampling with Γ ($\mathbf{k} = 0$) only is fine. For other insulators, a small number of $\mathbf{k}$ -points is usually sufficient.



- For metals, a very fine sampling of the *Fermi surface*, together with some *broadening*, or *smearing*, technique, is needed. One could in principle use Fermi-Dirac occupations at finite T , but this would require either very high T or too fine sampling

How many bands?

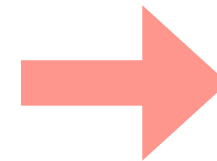
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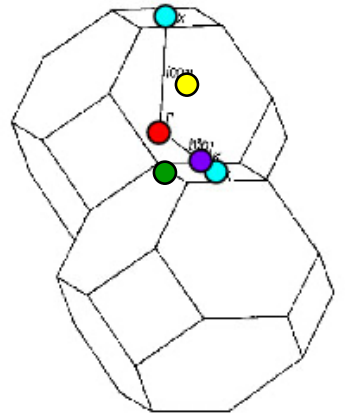
$$n(\mathbf{r}) = \sum_{\mathbf{k}} \sum_i |\psi_{\mathbf{k},i}(\mathbf{r})|^2 f_{i,\mathbf{k}}$$

$f_{i,\mathbf{k}}$ is not just 0 or 1:
 $\sum_i$ include more states, also
with fractional occupation

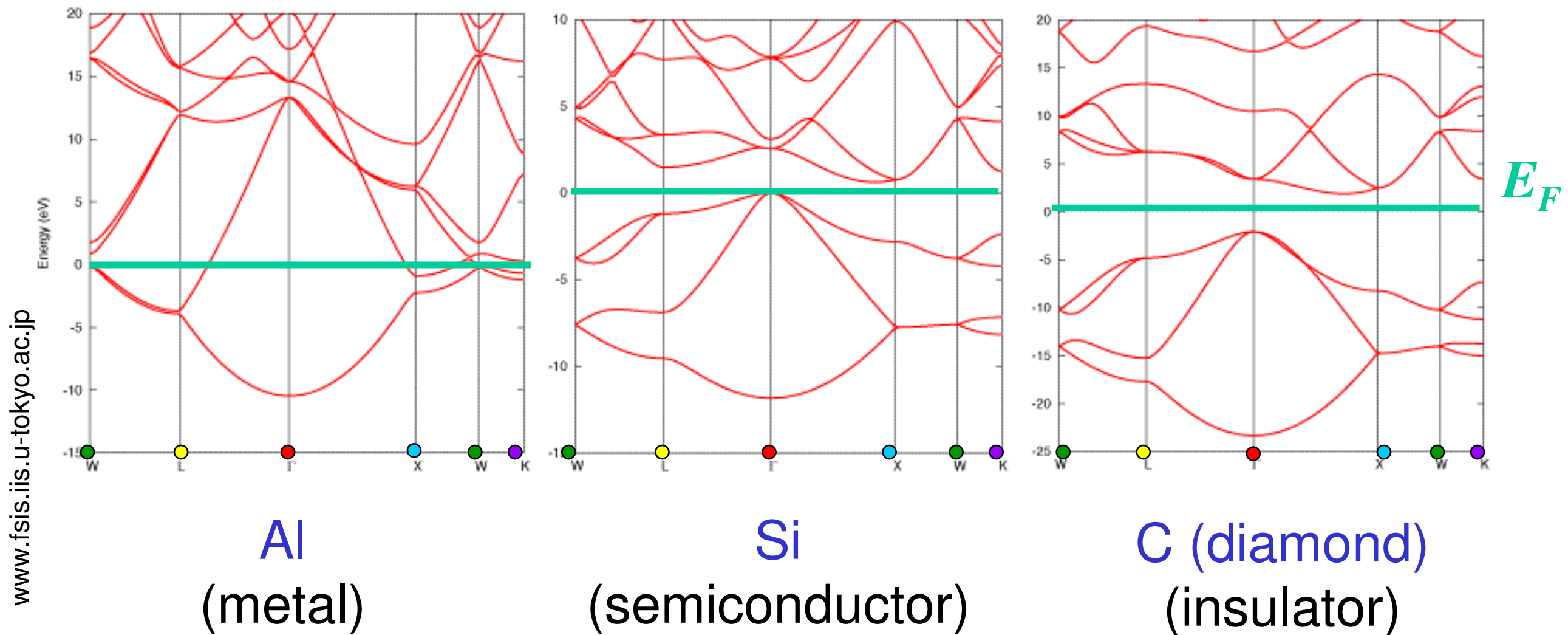


i is given by
nbnd parameter:
typically +20% of
the number of
bands if they
were fully
occupied, but we
can increase it

Band Structure



- “Band structure” (graph of ϵ_n vs. $\mathbf{k}$):
what states are available for electrons.
- At $T=0$, all states that lie below/above Fermi level are occupied/empty.



HANDS-ON: compare different band structures

1. metals
- 2. post-processing**
3. forces & structural optimization
4. energy barriers

Post-processing!

Once we get the self-consistent potential, we “freeze” it and we can calculate many electronic properties
by even more accurate accurately sampling of the Brillouin zone

Electronic structure

- Charge densities (and charge transfer, magnetic moments ...)
- Band gap
- Band dispersion $E(\mathbf{k})$
- Density of states and projection on atoms or orbitals
- $\mathbf{k}$ -resolved projection on atoms or orbitals
- Individual Kohn-Sham orbitals

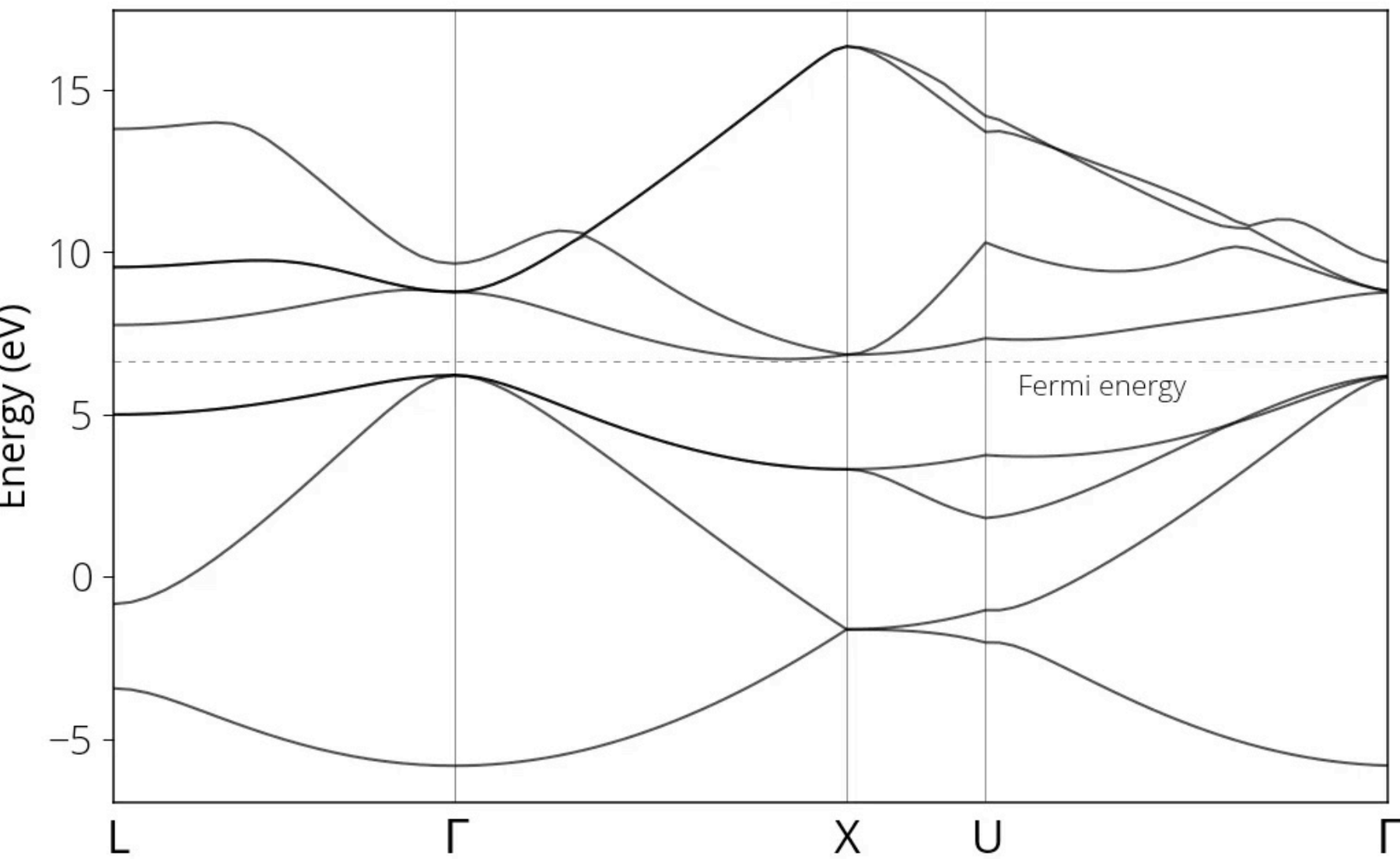
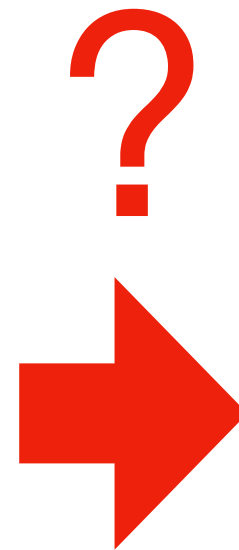


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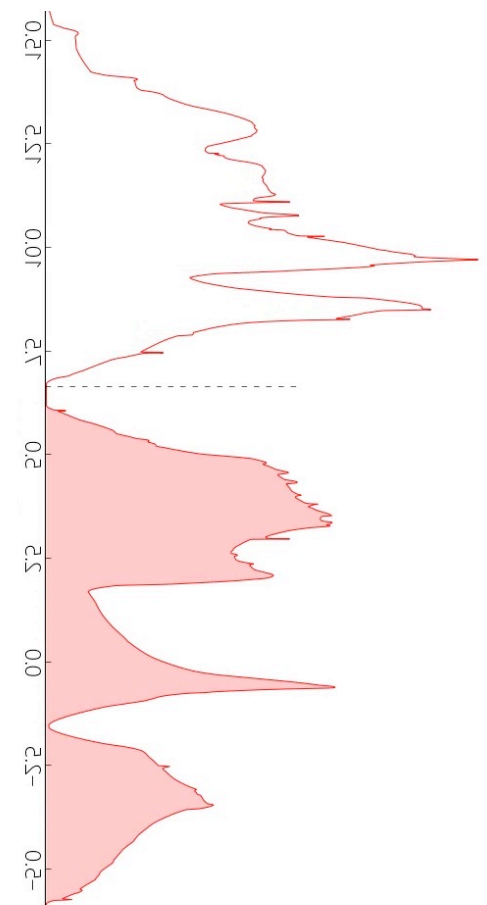
this lecture

- bands



density of states

- DOS

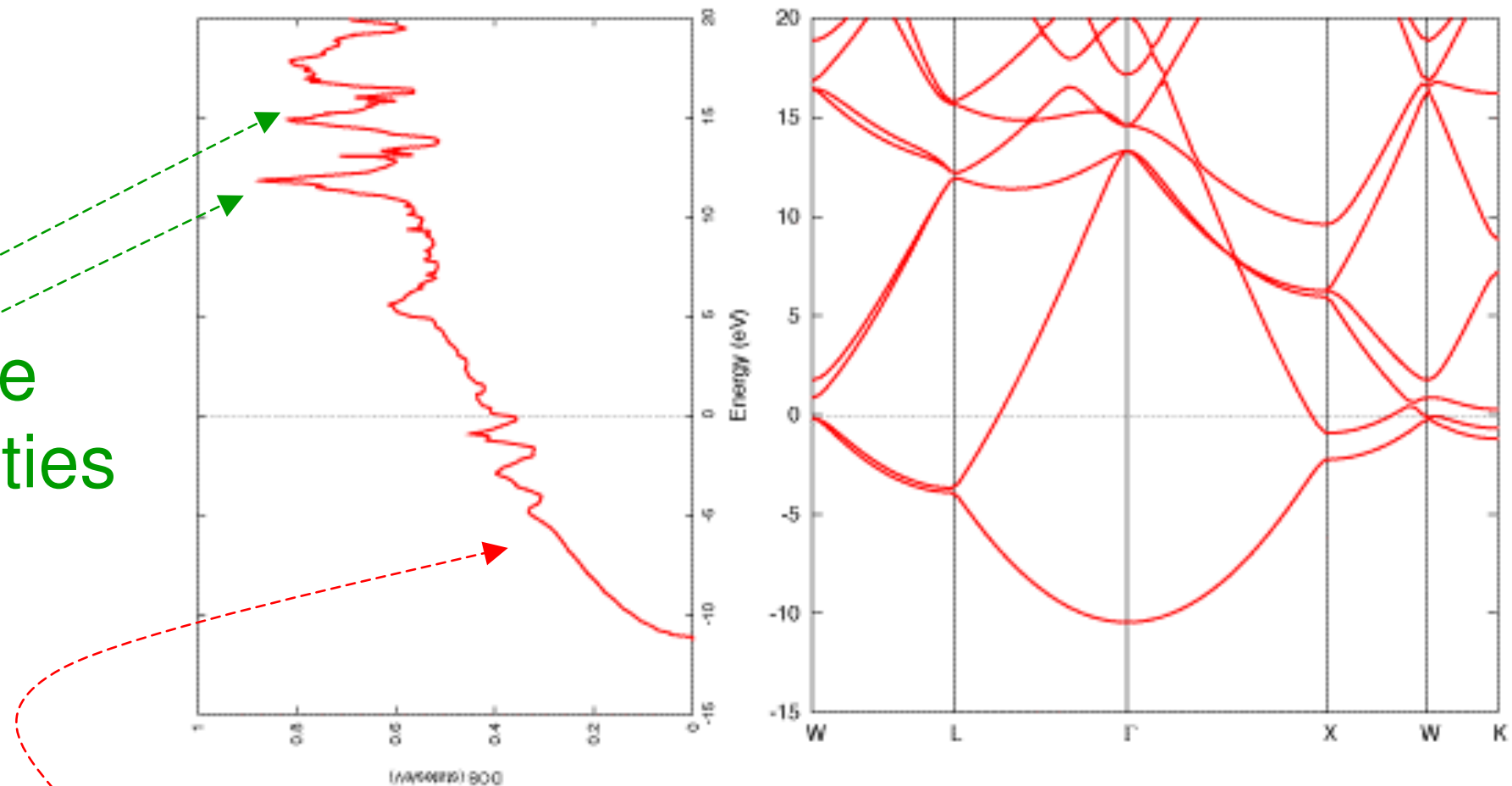


Density of States

- $g(E)dE$: Number of states available in the energy range E to $E+dE$

e.g.,
for Al:

Van Hove
Singularities



Density of States
("sideways"!)

www.fsis.iis.u-tokyo.ac.jp

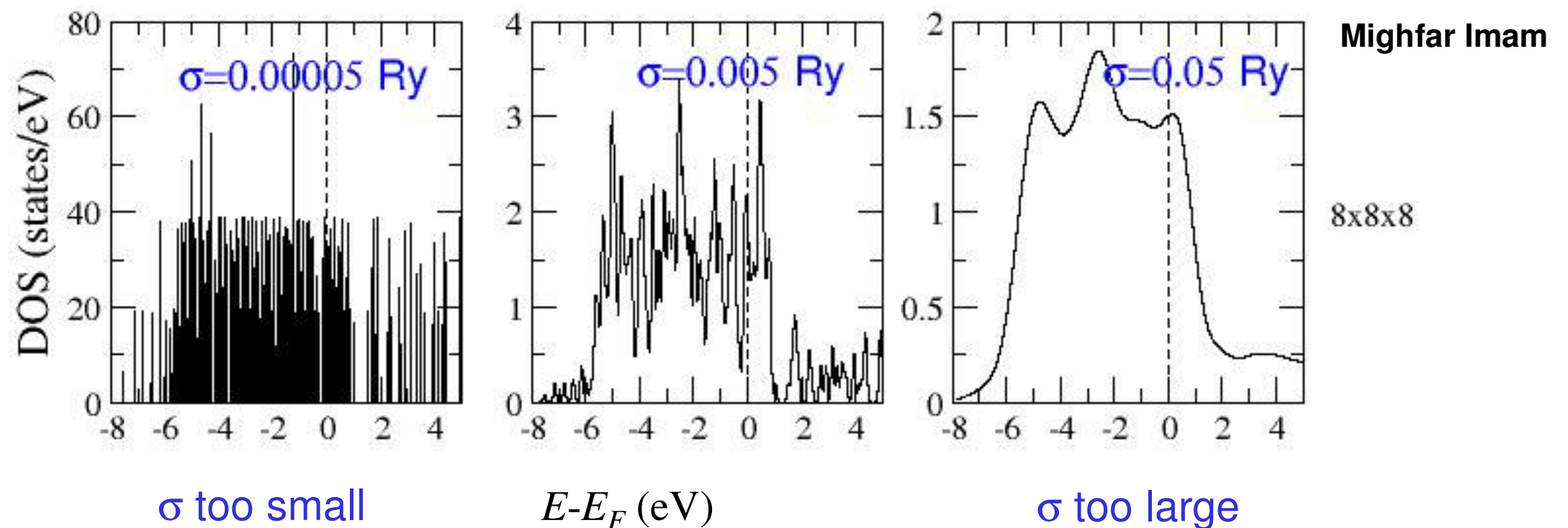


Calculating the Density of States in Practice

$$g(E) = \frac{1}{N_k} \sum_{n, \mathbf{k} \in BZ} \delta(E - \varepsilon_{n\mathbf{k}})$$

- Obtain $\varepsilon_{n\mathbf{k}}$ on a grid of $\mathbf{k}$ in the BZ.
- Approximate δ fn. by smeared-out function (gaussian) with a width σ .

e.g., for bulk rhodium:

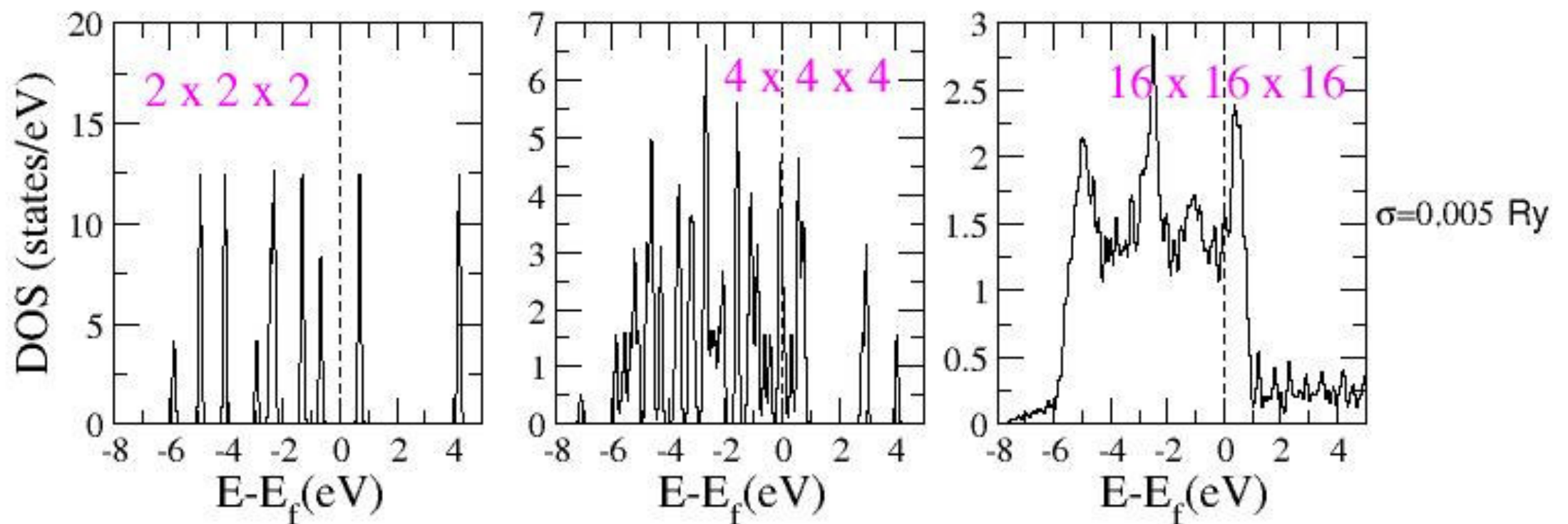


Calculating the Density of States in Practice

$$g(E) = \frac{1}{N_k} \sum_{n, \mathbf{k} \in BZ} \delta(E - \varepsilon_{n\mathbf{k}})$$

- Obtain $\varepsilon_{n\mathbf{k}}$ on a grid of $\mathbf{k}$ in the BZ;
- Approximate δ -fn. by smeared out function (e.g., gaussian).
- Need a very fine **grid in k-space** to get sharp features ok.

e.g., for bulk rhodium:

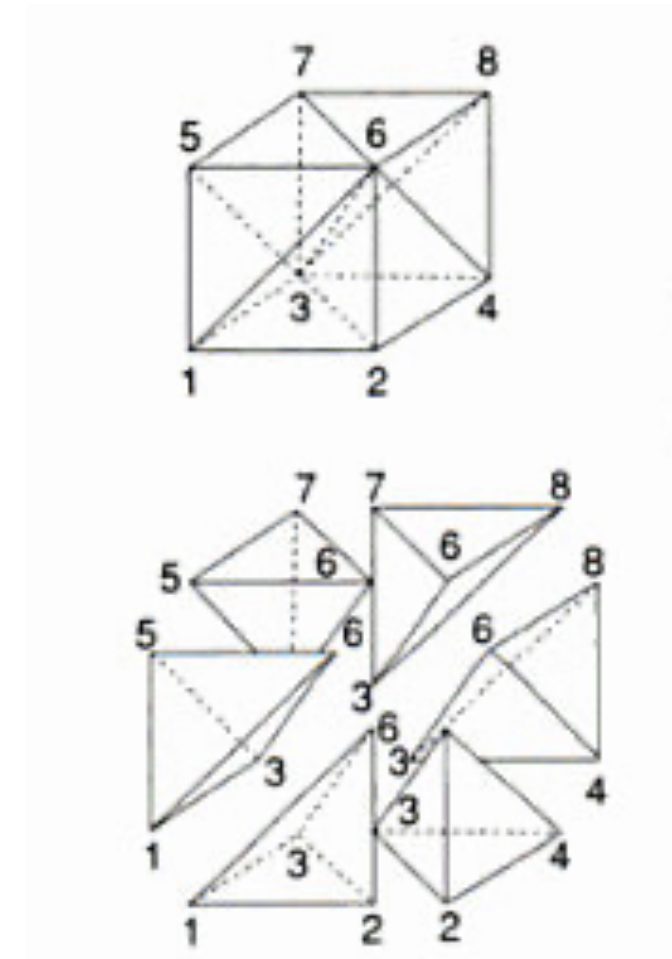


Mighfar Imam



Interpolating between k-points

- In order to get sharp features in the DOS (e.g., van Hove singularities) correctly, use a method that interpolates between k-points.
- e.g., the **Linear Tetrahedron method**.
- Tetrahedra can be used to fill all space for any grid.
- Linear interpolation between values at vertices.



Blochl, Jepsen & Andersen

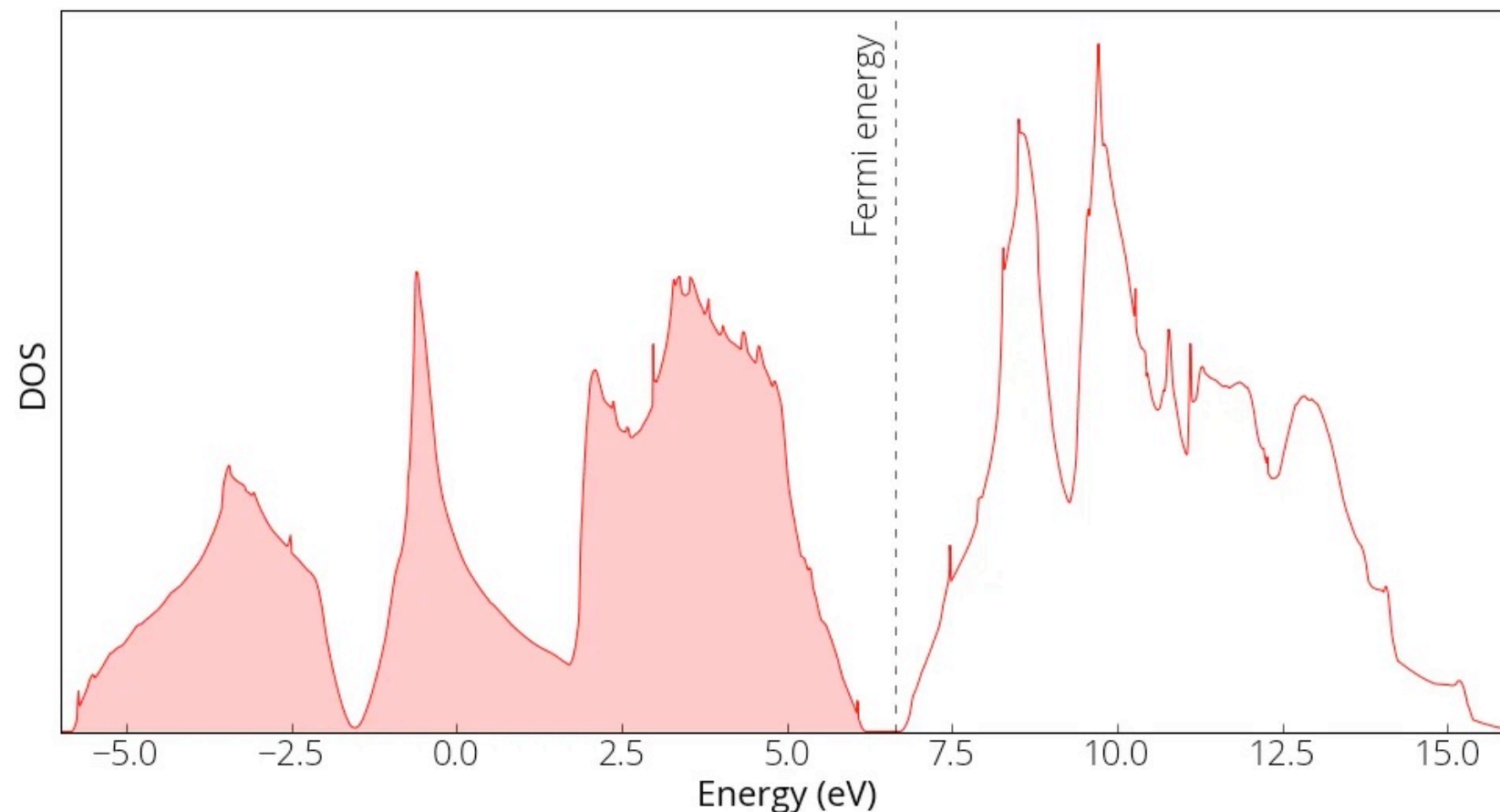


Electronic structure

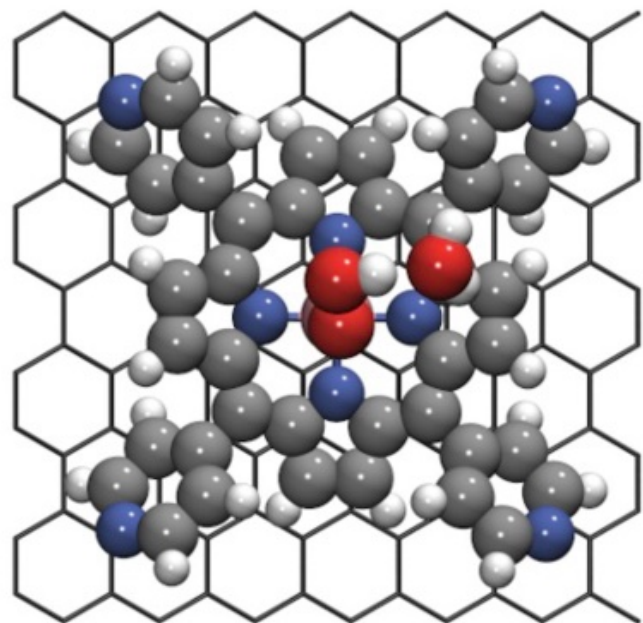
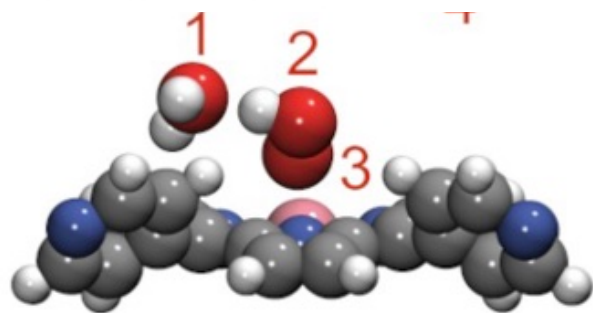
(projected density of states)

- pDOS

which is the contribution from each individual atoms and/or each of their orbital contributions?



O₂H-H₂O/Co/TPyP/GR system

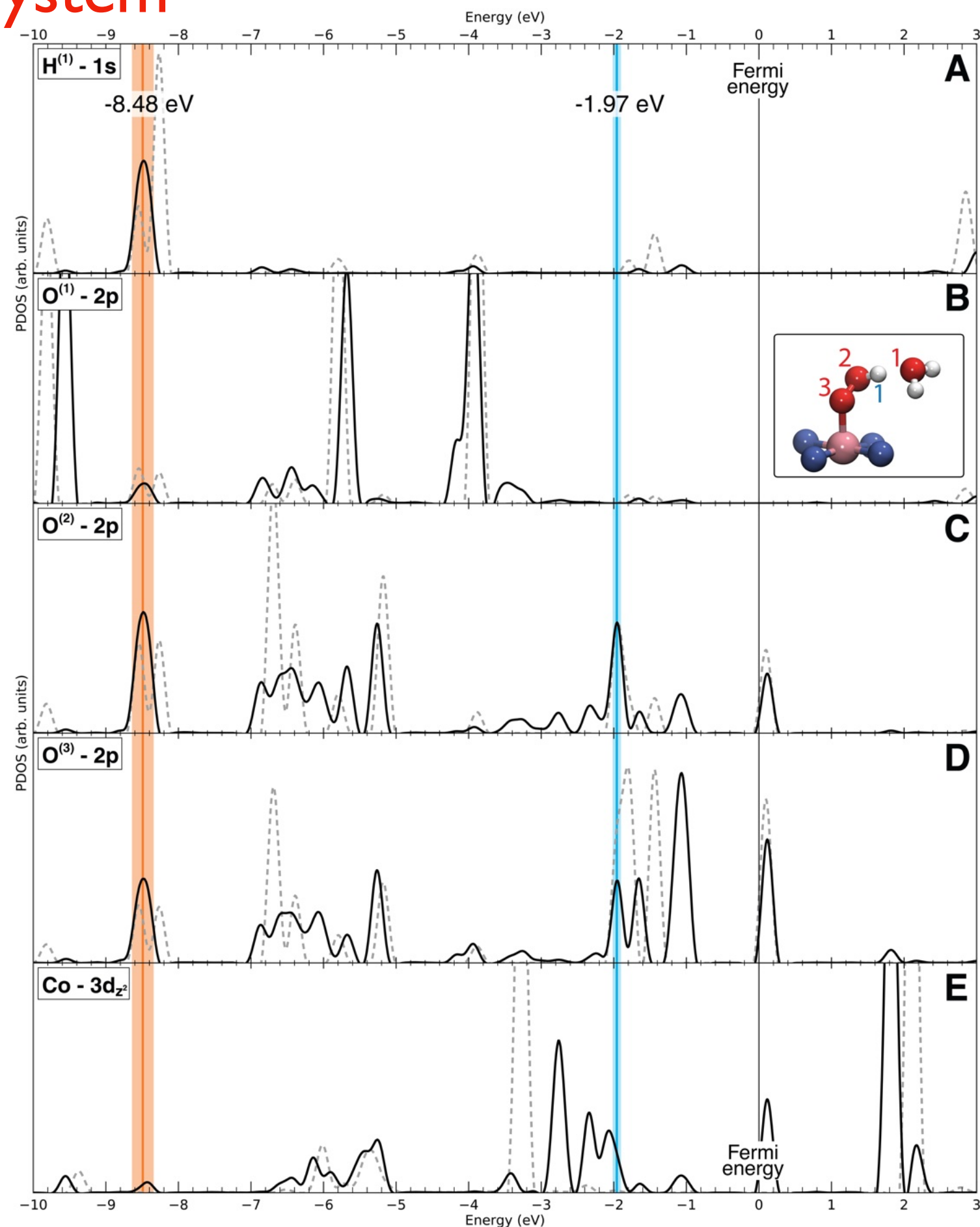


PDOS in

———— bound system

- - - - - separate constituents

Blue and orange vertical stripes:
energy ranges characterized by
the superposition of Co 3d_{z²}
and O 2p contributions in the
bound configuration



Electronic structure

(projected density of states)

- pDOS

1) *SCF calculation (**pw.x**) => calculate the crystalline potential V in $\mathcal{H}$*

2) *NSCF calculations (**pw.x**) => reads/uses the ground state electron density, Hartree, exchange and correlation potentials obtained in the SCF cycle to calculate $E(k)$ on a denser grid of k points (automatic ok).*

3) *use **projwfc.x** => obtain many files:*

{filpdos}.pdos_atm#N(X)_wfc#M(l), where N is atom number, X is atom symbol, M is wfc number, and l=s, p, d, f one file for each atomic wavefunction => one file for each angular momentum l => LDOS(E) is the contribution from the given l

Projecting $\psi(\mathbf{r})$ onto atoms and orbitals

Consider $\{\phi_\alpha(\mathbf{r})\}$ **orthogonalized atomic wavefunctions**:

$$\mathcal{H}^{atomic}\phi_\alpha(\mathbf{r}) = \epsilon_\alpha\phi_\alpha(\mathbf{r}) \quad \text{with} \quad \langle\phi_\alpha|\phi_\beta\rangle = \delta_{\alpha\beta}$$

We can build a sum of atomic wfc with different centers and modulated by a phase factor; it has the properties of a Bloch function (“Bloch sum”):

$$\psi_{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{R}} \sum_{\alpha} b_{\alpha} \phi_{\alpha}(\mathbf{r} - \mathbf{R}) e^{i\mathbf{k} \cdot \mathbf{R}}$$

The Bloch function that we have numerically obtained from the Kohn-Sham hamiltonian has some resemblance to that.

The coefficients b_{α} specify the contribution of each orbital to ψ

Projecting $\psi(\mathbf{r})$ onto atoms and orbitals

Therefore, if the total DoS is:

$$DoS(E) \propto \int_{\mathcal{B.Z.}} d\mathbf{k} \delta(E(\mathbf{k}) - E)$$

we could consider the projection of the DoS onto a specific orbital α :

$$PDoS(\alpha, E) = \int_{\mathcal{B.Z.}} d\mathbf{k} |\langle \psi_{\mathbf{k}} | \phi_{\alpha} \rangle|^2 \delta(E(\mathbf{k}) - E)$$

This will depend on the b_{α} coefficients

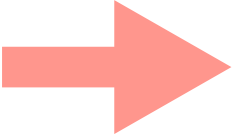
Projecting $\psi(r)$ onto atoms and orbitals

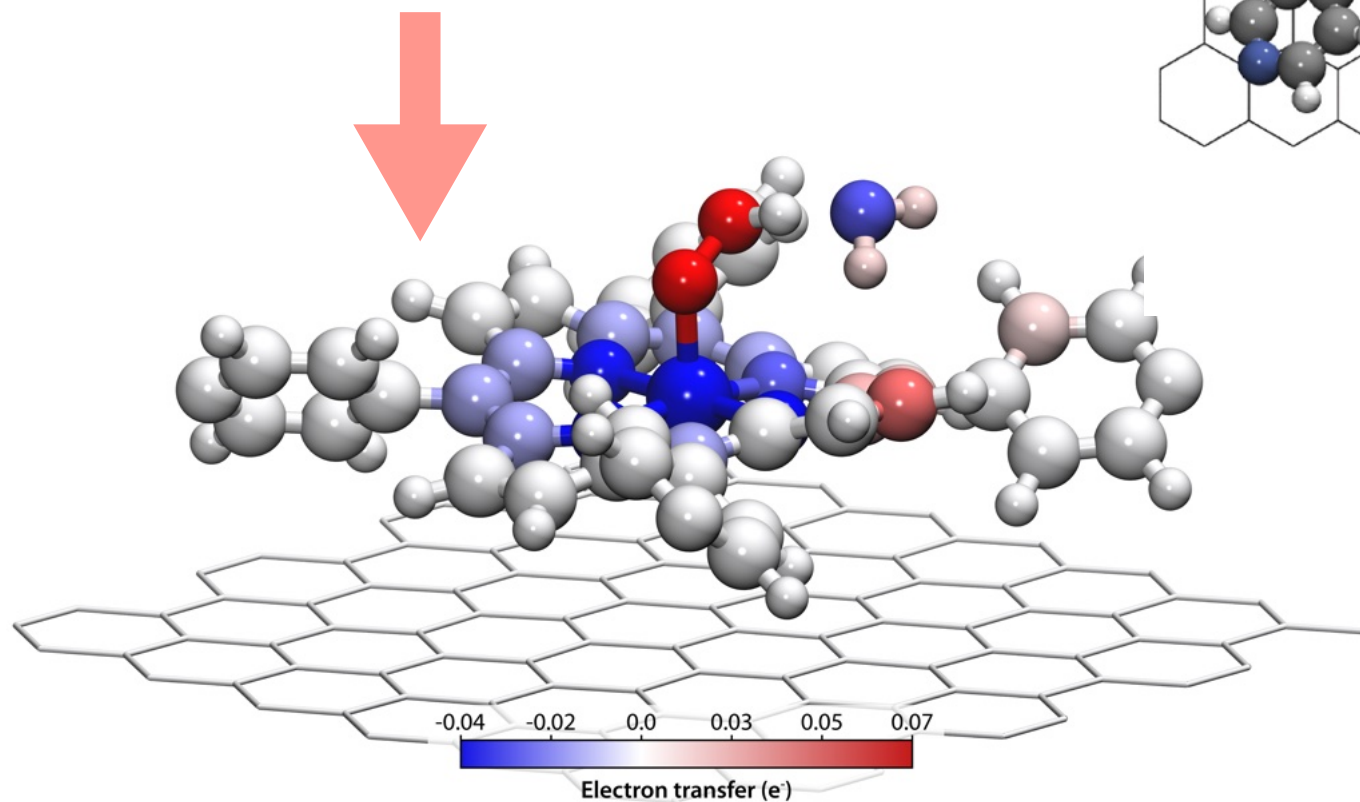
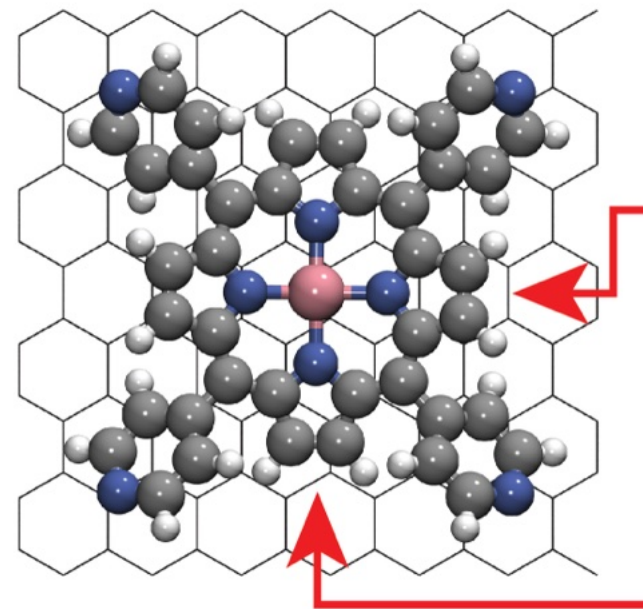
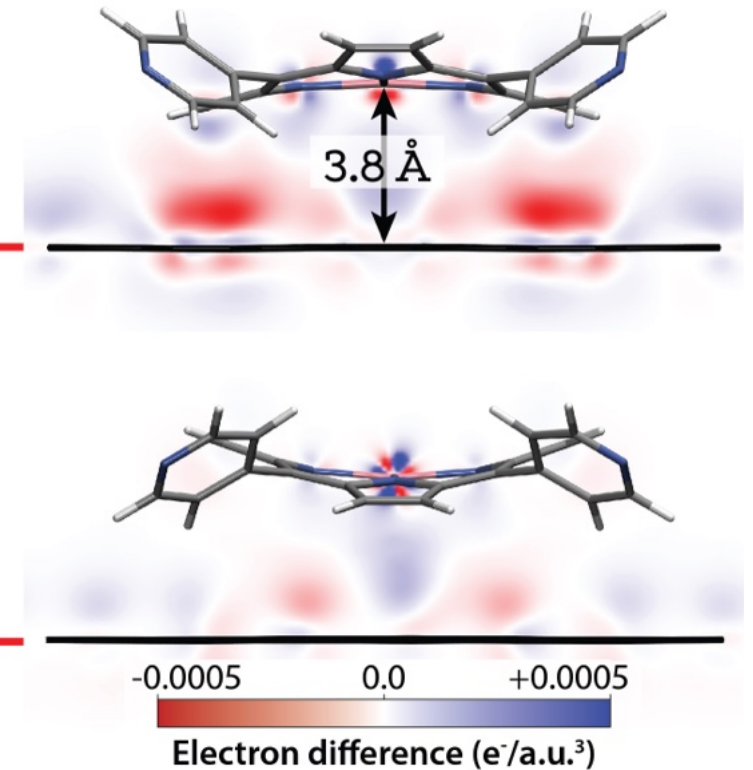
The $\phi_\alpha(\mathbf{r} - \mathbf{R})$ centered on the different $\mathbf{R}$ are not fully orthonormal (overlap between neighboring atoms is not exactly zero)

The projection is not “perfect”...

There is some charge density missing
 (“spilling parameter” estimated in % of the total charge density)

Charge density

- 3D, 2D, 1D plots of $n(\mathbf{r})$
- individual
- differences 
- Löwdin charges



Charge redistribution in the $\text{O}_2\text{H-H}_2\text{O}/\text{CoTPyP}/\text{GR}$ system upon bonding of the $\text{O}_2\text{H-H}_2\text{O}$ complex to the CoTPyP/GR

1. metals
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Forces on the atoms - I

Forces on atoms are the derivatives of the total energy wrt atomic positions. The *Hellmann-Feynman theorem* tells us that forces are the expectation value of the derivative of the external potential only:

$$\mathbf{F}_\mu = -\frac{\partial E}{\partial \mathbf{R}_\mu} = -\sum_i f_i \langle \psi_i | \frac{\partial V}{\partial \mathbf{R}_\mu} | \psi_i \rangle = -\int n(\mathbf{r}) \frac{\partial V}{\partial \mathbf{R}_\mu} d\mathbf{r}$$

This last “=” in particular is
valid only for *local* potentials,

The calculation of the Hellmann-Feynman forces is **in principle** straightforward

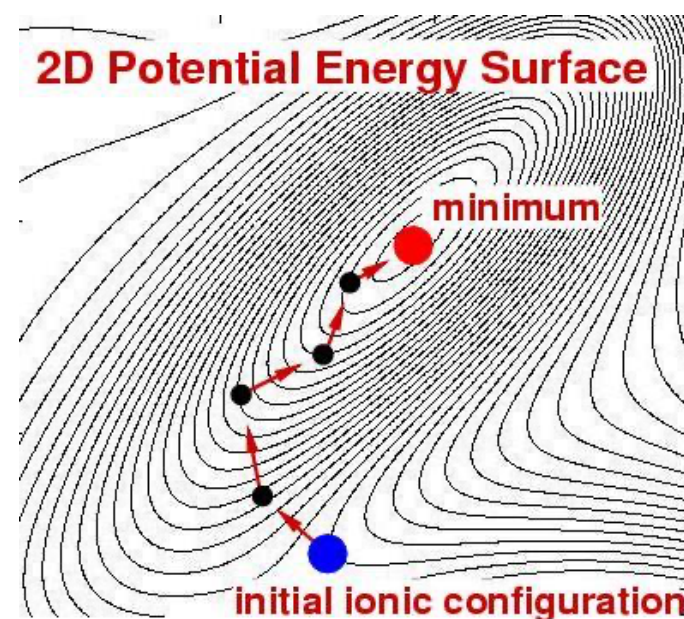
**forces are derivatives of the energy =>
convergence is more difficult!**

(in general: convergence of integrated quantities is much easier)

Structural Optimization and Molecular Dynamics

Within the *Born-Oppenheimer*, or *adiabatic* approximation, the total energy as a function of atomic positions, or *Potential Energy Surface* (PES), determines the behaviour of nuclei.

The *global* ground state can be found by minimizing the function $E(\mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_N)$, depending upon the $3N$ atomic coordinates for a system of N atoms. This is a “standard” mathematical problem: finding the minimum of a function, knowing its derivatives, that is, the Hellmann-Feynman forces (in the picture, a cartoon of a PES in two dimensions with the path to the minimum).



Once forces are calculated, one can perform not only structural optimization (also known as “relaxation”), but also *molecular dynamics*. If a classical behaviour of the nuclei is assumed, all the machinery of classical MD can be recycled, with forces calculated from *first principles*.

Quasi-Newton algorithms for structural optimization

The BFGS (Broyden-Fletcher-Goldfarb-Shanno) algorithm is the workhorse for structural minimization at fixed cell

Close to an equilibrium point $\vec{X}^{(eq)}$, for which $\nabla E(\vec{X}^{(eq)}) = 0$ holds, a quadratic form is assumed for the function $E(\vec{X})$ (H is the Hessian matrix):

$$E(\vec{X}) \simeq E(\vec{X}^{(eq)}) + \frac{1}{2}(\vec{X} - \vec{X}^{(eq)})^T H (\vec{X} - \vec{X}^{(eq)})$$

$\vec{X}$: atomic positions

$\vec{g}$: forces on atoms

Given two points $\vec{X}_1$ and $\vec{X}_0$ and corresponding gradients $\vec{g} = \nabla E(\vec{X})$, this means $\vec{g}_1 - \vec{g}_0 = H(\vec{X}_1 - \vec{X}_0)$, that is, $\vec{g}_1 = 0$ if $\vec{X}_1 = \vec{X}_0 - H^{-1}\vec{g}_0$ (*Newton-Raphson step*).

Practical algorithm: a sequence of calculations at positions $\vec{X}_i$

$$\vec{X}_{i+1} = \vec{X}_i + T_k^L \frac{\vec{s}_k^{NR}}{|\vec{s}_k^{NR}|}, \quad \vec{s}_k^{NR} = -H_k^{-1} \vec{g}_k$$

incremental
displacements
according to the
forces

where T_k^L is called "trust radius".

Forces on the atoms - II

Namelist: &CONTROL

calculation	CHARACTER
-------------	-----------

<i>Default:</i>	'scf'
-----------------	-------

A string describing the task to be performed. Options are:

'scf'

'nscf'

'bands'

'relax'

'md'

'vc-relax'

'vc-md'

(vc = variable-cell).

Forces on the atoms - II

calculation = 'relax'

&CONTROL

[calculation](#) | [title](#) | [verbosity](#) | [restart](#) | [mode](#) | [wf_collect](#) | [nstep](#) | [iprint](#) | [tstress](#) | [tprnfor](#) | [dt](#) | [outdir](#) | [wfcdir](#) | [prefix](#) | [lkpoint_dir](#) | [max_seconds](#) | [etot_conv_thr](#) | [forc_conv_thr](#) | [disk_io](#) | [pseudo_dir](#) | [tefield](#) | [dipfield](#) | [lelfield](#) | [nberrycyc](#) | [lorbm](#) | [lberry](#) | [gdir](#) | [nppstr](#) | [gate](#) | [twochem](#) | [lfcpr](#) | [trism](#)

etot_conv_thr	REAL
Default:	1.0D-4

Convergence threshold on total energy (a.u) for ionic minimization: the convergence criterion is satisfied when the total energy changes less than [etot_conv_thr](#) between two consecutive scf steps. Note that [etot_conv_thr](#) is extensive, like the total energy.
See also [forc_conv_thr](#) – both criteria must be satisfied

forc_conv_thr	REAL
Default:	1.0D-3

Convergence threshold on forces (a.u) for ionic minimization: the convergence criterion is satisfied when all components of all forces are smaller than [forc_conv_thr](#).
See also [etot_conv_thr](#) – both criteria must be satisfied

Forces = 0

(and stress or pressure = 0 if the calculations are well converged
w.r.t. kinetic energy cutoff)

are enough to identify the equilibrium structure?

Summary (optimization of ionic positions only)

Some important aspects of structural optimization

- Structural optimization may find only the closest minimum: it cannot overcome potential barriers, so it may be trapped into a local minimum.
- Structural optimization does not break crystal symmetry, at least in principle (numerical noise may occasionally break the symmetry).
- Structural optimization uses both energies and forces to locate the minima along search directions. Discrepancies between those values, due to insufficient scf convergence, will lead to bad convergence of the BFGS algorithm or even to errors. Remember that the error on forces is *linear* in the self-consistency error, while the error on energies is *quadratic* due to its variational character.

Note that in simple crystalline structures *the force on atoms can be zero by symmetry, even if the system is not at equilibrium!*

different crystalline structures for elemental Si:

the minimum of each structure is characterized by zero forces

but this is not enough to determine the equilibrium structure

equilibrium structure =
minimum energy + zero forces

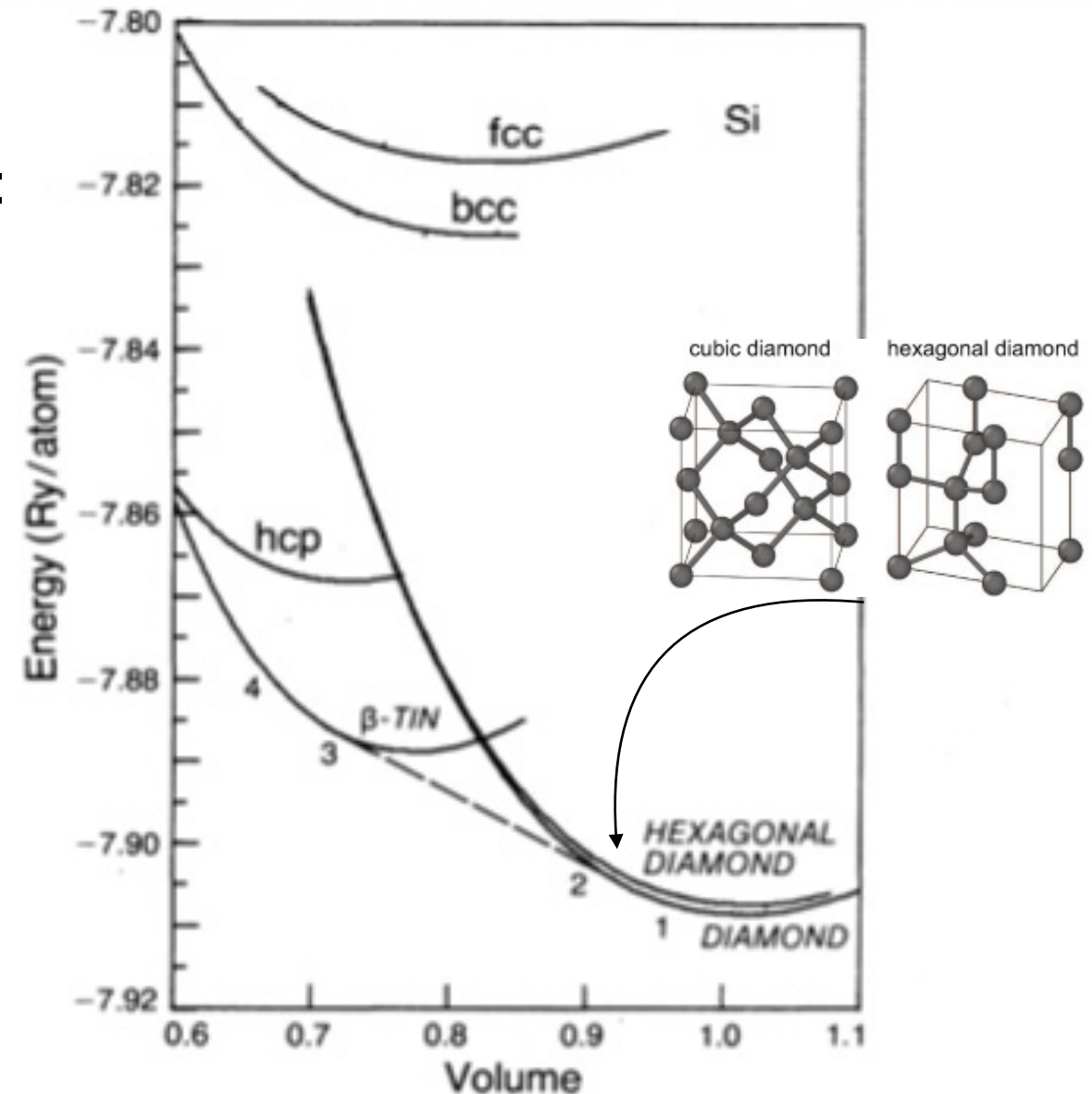


FIG. 1. The diamond, hexagonal diamond, and β -tin, hcp, bcc, and fcc structural energies (in units of Ry/atom) as a function of the atomic volume [normalized to the measured free volume (Ref. 16)] for Si. The dashed line is the common tangent of the energy curves for the diamond and the β -tin structures.

What can I do with “standard” DFT calculations?

- **Ground-state calculations:**

Self-consistent total energies, forces, stresses,
Kohn-Sham orbitals

- **Structural optimization:**

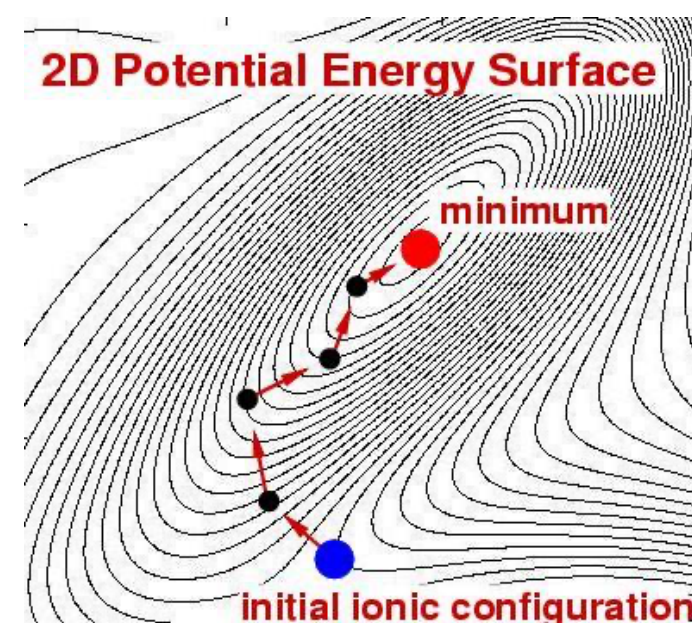
from calculation of forces acting on atoms

- **Molecular Dynamics: Born-Oppenheimer**

Structural Optimization and Molecular Dynamics

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Once forces are calculated, one can perform not only structural optimization, but also *molecular dynamics*. If a classical behaviour of the nuclei is assumed, all the machinery of classical MD can be recycled, with forces calculated from *first principles*.

Courtesy of P Giannozzi

Molecular dynamics

Affording the nuclear motion

Remind: Born-Oppenheimer approximation

$$m \frac{d^2 \vec{r}}{dt^2} = \vec{F}(\vec{r}) \quad \Longrightarrow \quad \mathbf{r}(t), \mathbf{v}(t)$$

Newton eq. of motion , but with **F** calculated from quantum mechanics.

Discretize and iterate!

$$\mathbf{r}(t + \Delta t) = \mathbf{r}(t) + \mathbf{v}(t)\Delta t + (1/2)\mathbf{a}(t)\Delta t^2 + (1/6)\mathbf{b}(t)\Delta t^3 + O(\Delta t^4)$$

$$\mathbf{r}(t - \Delta t) = \mathbf{r}(t) - \mathbf{v}(t)\Delta t + (1/2)\mathbf{a}(t)\Delta t^2 - (1/6)\mathbf{b}(t)\Delta t^3 + O(\Delta t^4)$$

$$\mathbf{r}(t + \Delta t) = 2\mathbf{r}(t) - \mathbf{r}(t - \Delta t) + \mathbf{a}(t)\Delta t^2 + O(\Delta t^4)$$

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HANDS-ON

- **Structural optimization:**
from calculation of forces acting on atoms

last part of theory of today

Other issues...

- from interacting many-body Schr. eq. $\Rightarrow$ non interacting many body Schr. eq. $\Rightarrow$ one electron (Kohn-Sham) Schr. eq.
- functionals: different approximations

Interacting => non interacting system

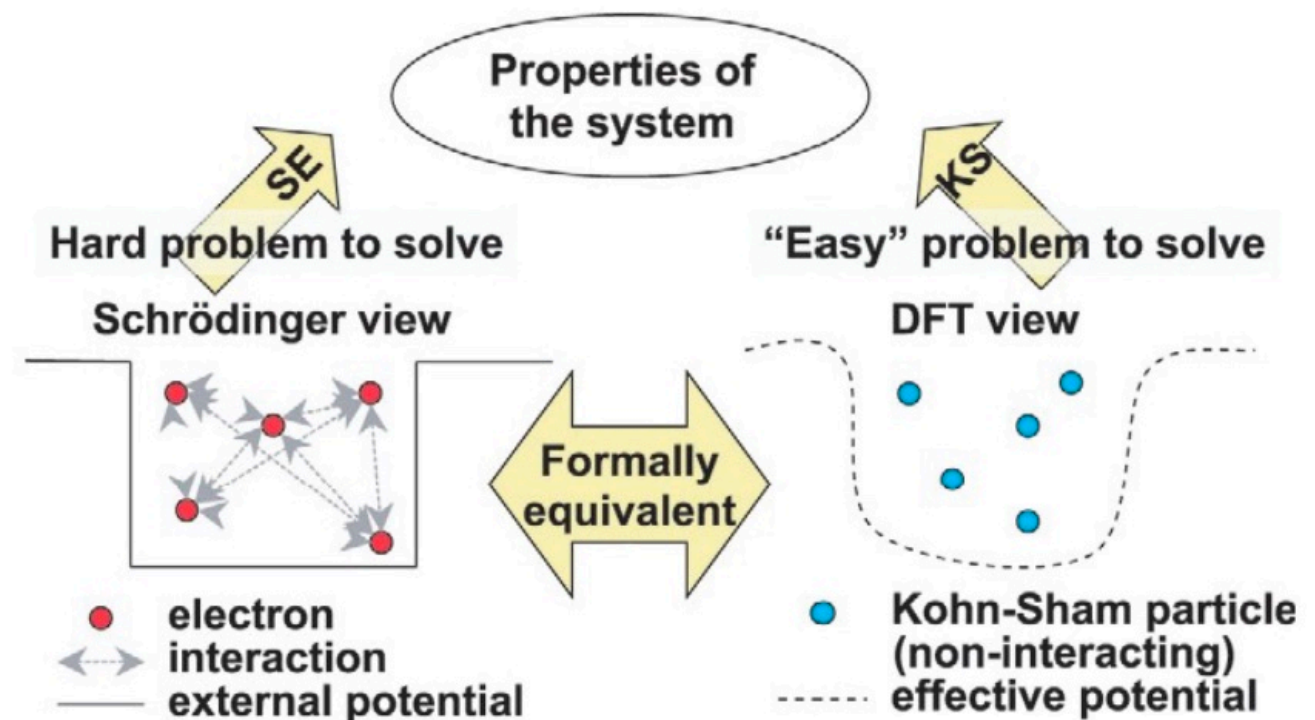
if $n(\mathbf{r})$ is the only relevant variable
we can map the interacting system into a non-interacting one with the same density

- interacting system $\rightarrow$ non interacting system

- $n(\mathbf{r}) \leftrightarrow V_{\text{ext}}(\mathbf{r})$

- $$\left(-\frac{1}{2m_e} \nabla^2 + V_{\text{eff}}(\mathbf{r}; [n(\mathbf{r})]) \right) \psi_i(\mathbf{r}) = \epsilon_i \psi_i(\mathbf{r})$$

also indicated as V_{KS} (Kohn-Sham)



Kohn-Sham equations

=> The system of interacting electrons is mapped onto a **non-interacting electrons having the same density**

For non-interacting electrons:

$$n(\mathbf{r})$$

$$n(\mathbf{r}) = \sum_i |\psi_i(\mathbf{r})|^2$$

(for all the fully occupied orbitals;
otherwise, insert an occupation factor)

← link between $n(\mathbf{r})$ and single-electron wavefunctions

with $\psi_i(\mathbf{r})$ **one-electron** orthonormal orbitals (Kohn-Sham orbitals) satisfying:

say U , from the e-e interaction

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + \underbrace{V(\mathbf{r}) + V_H[n(\mathbf{r})] + V_{xc}[n(\mathbf{r})]}_{= V_{KS}[n(\mathbf{r})]} \right) \psi_i(\mathbf{r}) = \epsilon_i \psi_i(\mathbf{r})$$

V_{ext} : if we do not have
external fields, this is V_{nucl}

HK theorem and functionals

Consequence of the HK theorem:

E is a **functional** $E[n(\mathbf{r})]$ **of** $n(\mathbf{r})$

interacting el.
potential ↓

external
potential ↓

$$E[n(\mathbf{r})] = \langle \Psi | T + U + V | \Psi \rangle = \langle \Psi | T + U | \Psi \rangle + \langle \Psi | V | \Psi \rangle \\ = F[n(\mathbf{r})] + \int n(\mathbf{r}) V(\mathbf{r}) d\mathbf{r}$$

$F[n(\mathbf{r})]$ is a **universal** functional of $n(\mathbf{r})$ (and not of $V(\mathbf{r})$)
(unknown!)

Problem: determine $n(\mathbf{r})$ which minimizes $E[n(\mathbf{r})]$

Kohn-Sham equations (II)

recover the expression for the energy:

$$E[n(\mathbf{r})] = F[n(\mathbf{r})] + \int n(\mathbf{r})V(\mathbf{r})d\mathbf{r}$$

From the mapping on to a non-interacting system:

$$F[n(\mathbf{r})] = T_s[n(\mathbf{r})] + E_H[n(\mathbf{r})] + E_{xc}[n(\mathbf{r})]$$

with:

$$T_s[n(\mathbf{r})] = -\frac{\hbar^2}{2m} \sum_i \int \Psi_i^*(\mathbf{r}) \nabla^2 \Psi_i(\mathbf{r}) d\mathbf{r} \quad \text{kinetic energy of non-interacting electrons}$$

$$E_H[n(\mathbf{r})] = \frac{e^2}{2} \int \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}d\mathbf{r}' \quad \begin{array}{l} \text{Hartree energy:} \\ \text{electrostatic energy of non-interacting electrons} \end{array}$$

$$E_{xc}[n(\mathbf{r})]$$

exchange-correlation energy:

contains all the remaining terms!!! (unknown)

How to solve the one-electron Schr. eq.? (Kohn-Sham)

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) + V_H[n(\mathbf{r})] + V_{xc}[n(\mathbf{r})] \right) \psi_i(\mathbf{r}) = \epsilon_i \psi_i(\mathbf{r})$$

where

- $n(\mathbf{r}) = \sum_i f_i |\psi_i(\mathbf{r})|^2$ is the charge density, f_i are occupation numbers
- V is the nuclear (pseudo-)potential acting on electrons (may be nonlocal)
- $V_H[n]$ is the Hartree potential, $V_H(\mathbf{r}) = e^2 \int \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}'$
- $V_{xc}[n]$ is the exchange-correlation potential.

contains all the remaining terms (UNKNOWN!!!)

How to solve the one-electron Schr. eq.?

The formal derivation of the KS equations is exact, but approximations are necessary for the practical implementation of the theory:

- **how to describe ψ ?** use of **plane-waves** for wavefunction expansion (and **periodic boundary conditions**)
- **how to describe V_{nucl} ?** use of **pseudopotentials**
- **how to perform the integrations?** use of **k-point discrete meshes** for numerical integration in k-space
- **how to describe V_{xc} ?** choice of **approximate exchange-correlation (xc) functionals**



done

The exchange-correlation (xc) functional

Local density approximation for the exchange-correlation energy and potential

Kohn-Sham approximate the **functional** with a **function** of the density:

$$E_{xc}[n(\mathbf{r})] = \int \epsilon(n(\mathbf{r}))n(\mathbf{r})d\mathbf{r}$$

and analogously for the potential:

$$V_{xc}[n] = \mu_{xc}(n(\mathbf{r}))$$

But $\epsilon(n(\mathbf{r}))$ and $\mu_{xc}(n(\mathbf{r}))$ are **unknown** even in case of homogeneous electron gas! Use approximate forms

Local density approximation: successes and failures

- simpler than other approaches (e.g. Hartree-Fock)
- several results of good quality (e.g. structural properties)
- good even in highly inhomogeneous systems such as atoms and molecules
- self-interaction not exactly cancelled
- overbinding (overestimate of cohesive energies ~20% and more; VdW interactions: absent by construction (due to charge fluctuations, not to overlap!) but part of the attractive effect recovered by wrong overestimate of the overlap)
- underestimate of band gap in insulators (up to 50%!)

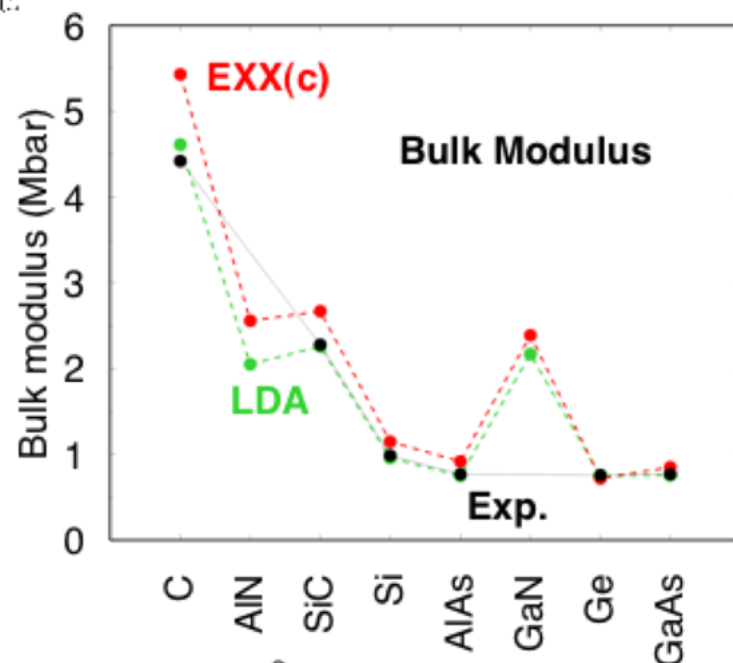
- **several results of good quality (e.g. structural properties)**

- Bulk moduli B to within $\pm 10\%$.

$$B = -V \left. \frac{\partial P}{\partial V} \right|_{V_0} = -V \left. \frac{\partial^2 E}{\partial V^2} \right|_{V_0}$$

V = crystal volume,

$P = \partial E / \partial V$ = pressure.



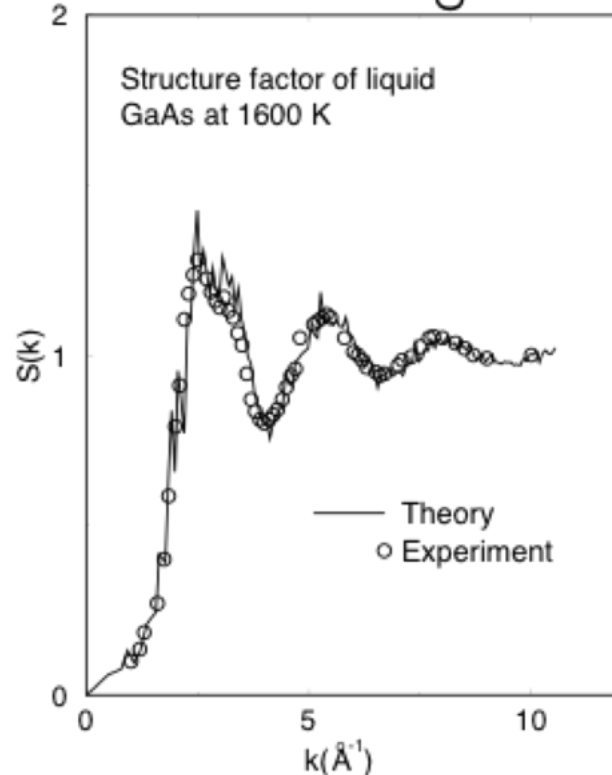
- Structure factor ($\Rightarrow$ pair correlation function) to within a few percent:

$$S(\mathbf{k}) = \frac{1}{N} \langle \rho_{\mathbf{k}} \rho_{-\mathbf{k}} \rangle - N \delta_{\mathbf{k},0}$$

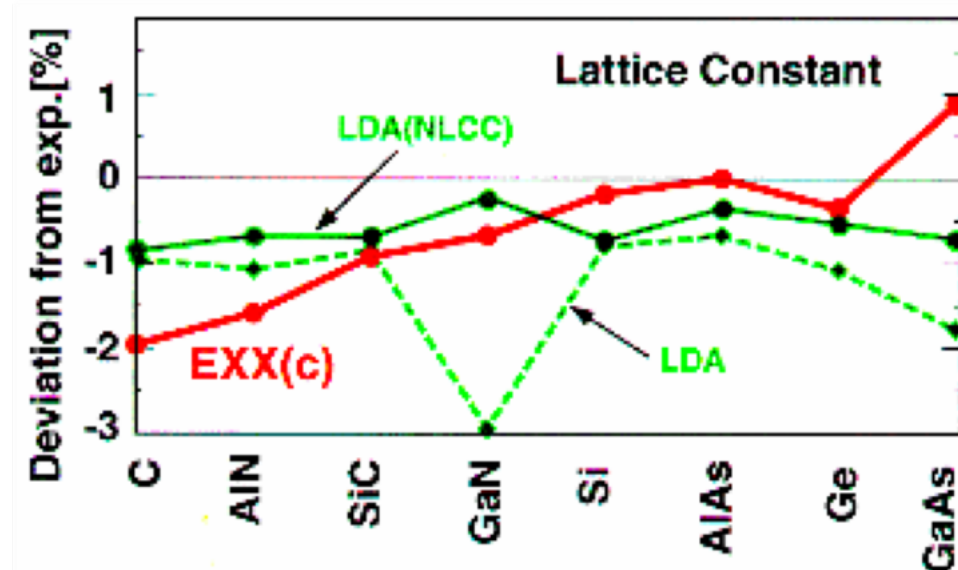
$$\rho(\mathbf{k}) = \sum_{\mathbf{r}} e^{-i\mathbf{k} \cdot \mathbf{R}_{\mathbf{r}}}$$

$\mathbf{R}_{\mathbf{r}}$ = atomic position.

- Phonon frequencies, surface reconstructions, catalysis, ...



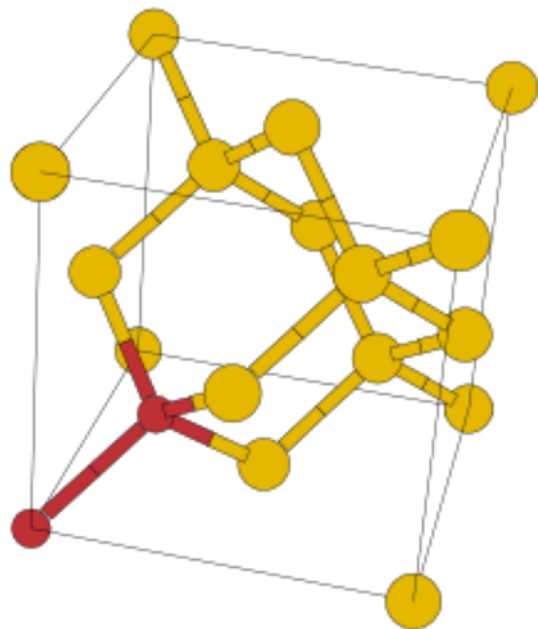
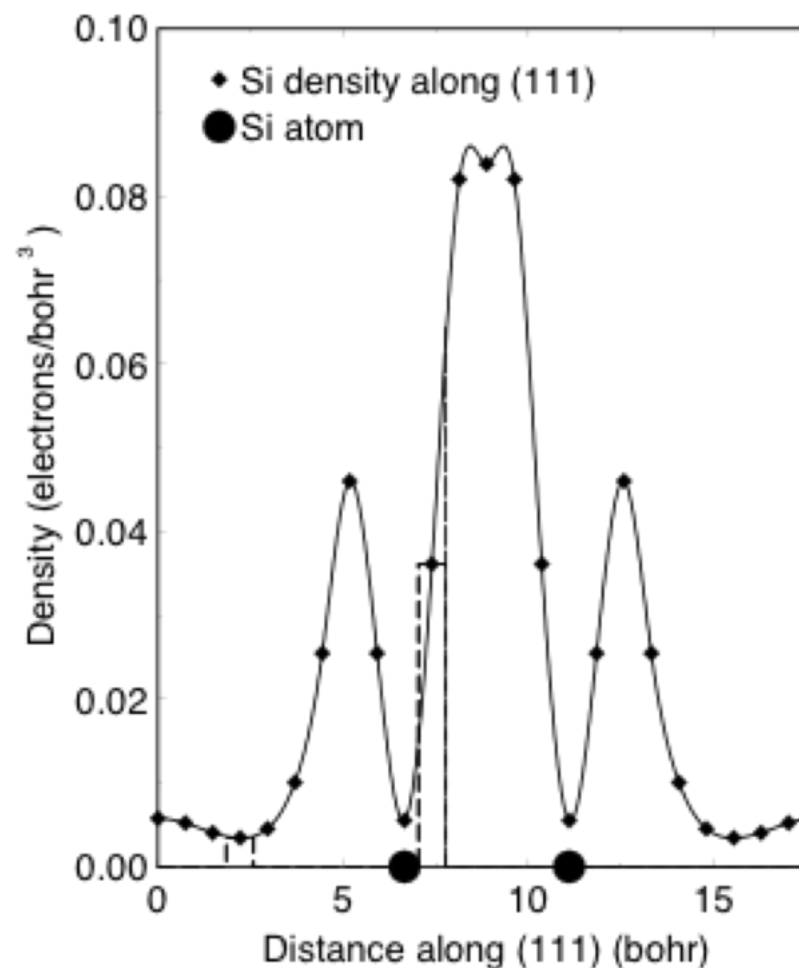
- Lattice constants to within $\pm 1\%$.



LDA(NLCC) = approximate treatment of core electrons.

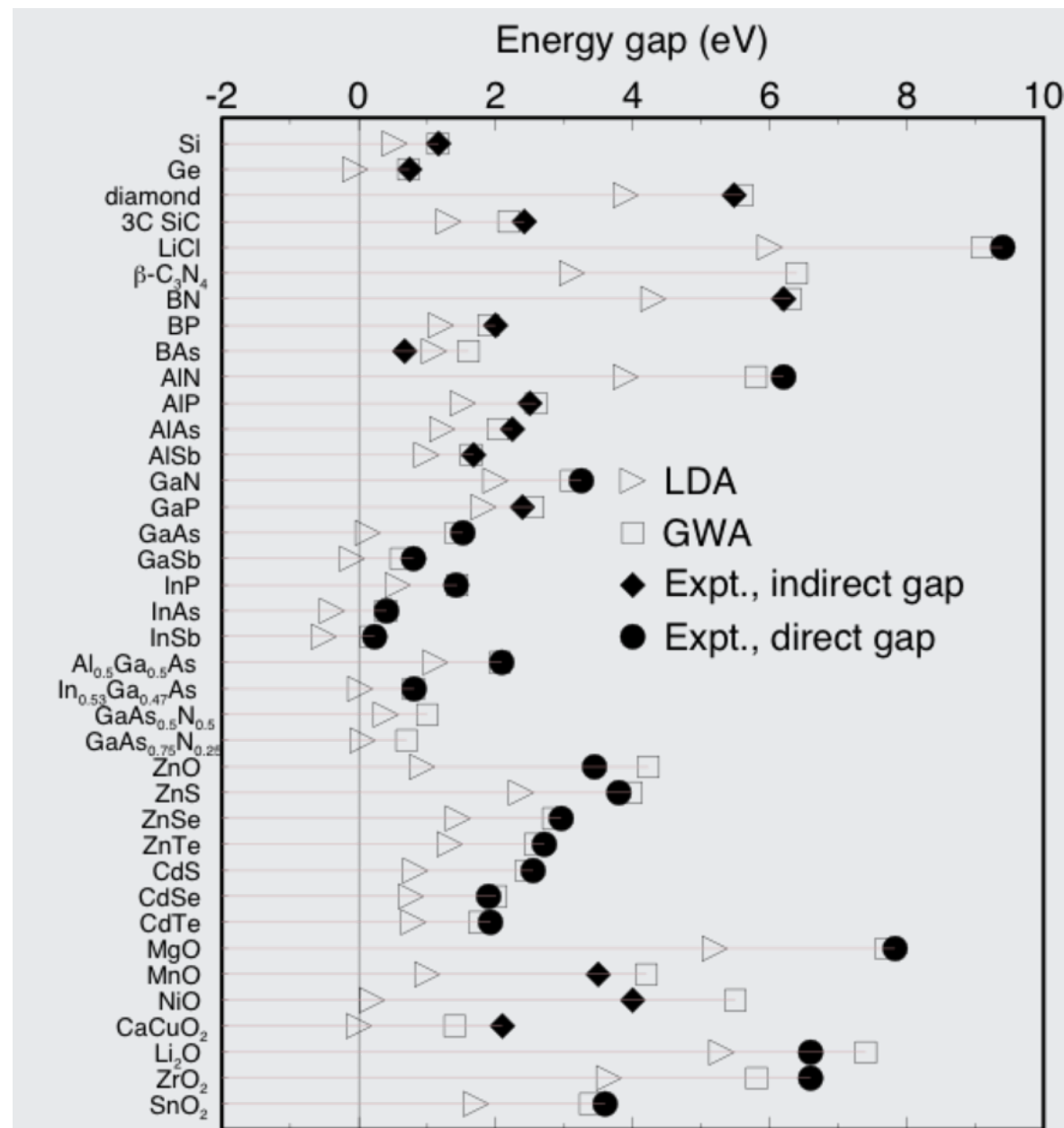
LDA = core electrons not treated.

- good even in highly inhomogeneous systems such as atoms, molecules, non metallic solids...



correct description of not-so-slowly varying density along the chemical bonds

- underestimate of band gap in insulators (up to 50%!)



Other approximations

generalized gradient approximations (GGA)
(and here let's explicitly express the spin dependence)

$$E_{\text{XC}}^{\text{GGA}}[n_{\uparrow}, n_{\downarrow}] = \int \varepsilon_{\text{XC}}(n_{\uparrow}, n_{\downarrow}, \nabla n_{\uparrow}, \nabla n_{\downarrow}) n(\mathbf{r}) \, \text{d}^3 \mathbf{r}.$$

Other approximations

- **LDA (Local Density Approximation):** Relies only on the local electron density at a specific point.
- **GGA (Generalized Gradient Approximation):** Considers the local density and its gradient (density change). Common examples include PBE, BLYP.
- **Meta-GGA:** Includes the Laplacian of the density or the kinetic energy density. Examples: SCAN, TPSS.
- **Hybrid Functionals:** Mixes a portion of exact exchange from Hartree-Fock theory with DFT exchange-correlation.
- ...

Common Functional GGA Types

- **B3LYP:** One of the most popular functionals in chemistry for molecules.
- **PBE:** Standard for solid-state physics calculations.

THE END - III