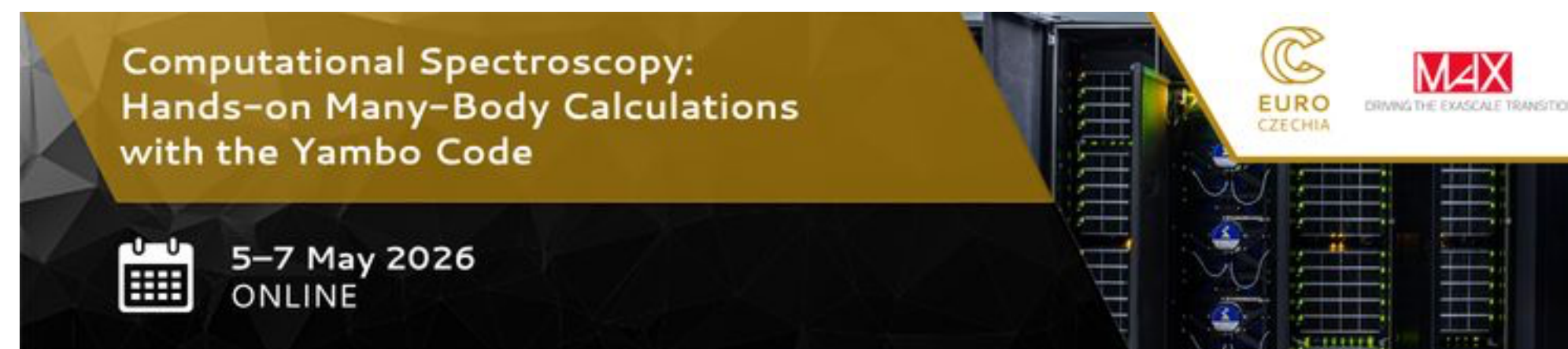


# Many-body perturbation theory calculations using the YAMBO code

Daniele Varsano

daniele.varsano@nano.cnr.it

 **CNRNANO** Modena, Italy  
ISTITUTO NANOSCIENZE CONSIGLIO NAZIONALE DELLE RICERCHE



 **MAX** DRIVING THE EXASCALE TRANSITION

Yambo. 

# Outline:

The MaX Centre of Excellence

Computational Materials Science: Historical Background

Basic concepts of Many Body Perturbation Theory

Overview of The Yambo code



### **Phase I (2015–2018):**

Focused on establishing the CoE foundation by porting flagship community codes to large-scale architectures and enhancing software interoperability.

### **Phase II (2018–2022):**

Targeted "pre-exascale" readiness by optimizing codes for heterogeneous hardware (GPUs) and transitioning toward high-throughput computing workflows

### **Phase III (2023–2026):**

Aims for full exascale performance on EuroHPC systems while integrating exascale workflows and prioritizing energy-efficient materials simulation.

# Motivation: HPC at the exascale

## the exascale challenge in high performance computing

- $10^{18}$  Flops/s
- $10^{18}$  Bytes
- abrupt technology changes
- **action is needed** for full exploitation
- **heterogeneous** machines (multiple HW and SW stacks)

### US DOE



**Frontier (@ORNL):** HDE+AMD  
=> 1194 PFlops



**Jupiter:** > 1 ExaFlops



**Leonardo:** Atos + NVIDIA A100  
(CUDA backend) => 239 PFlops



**EuroHPC**  
Joint Undertaking



**MareNostrum V:** Atos + NVIDIA  
H100 => 208 PFlops (estimated)



**LUMI:** CRAY + AMD cards  
(ROCm, HIP) => 309 PFlops

**quantum mechanics** based  
atomistic modelling of materials  
+  
interfacing with **multiscale** approaches

## Electronic Structure Methods

- highly accurate (predictive)
- computationally demanding
- **a case for HPC**

the **exascale** opportunity:

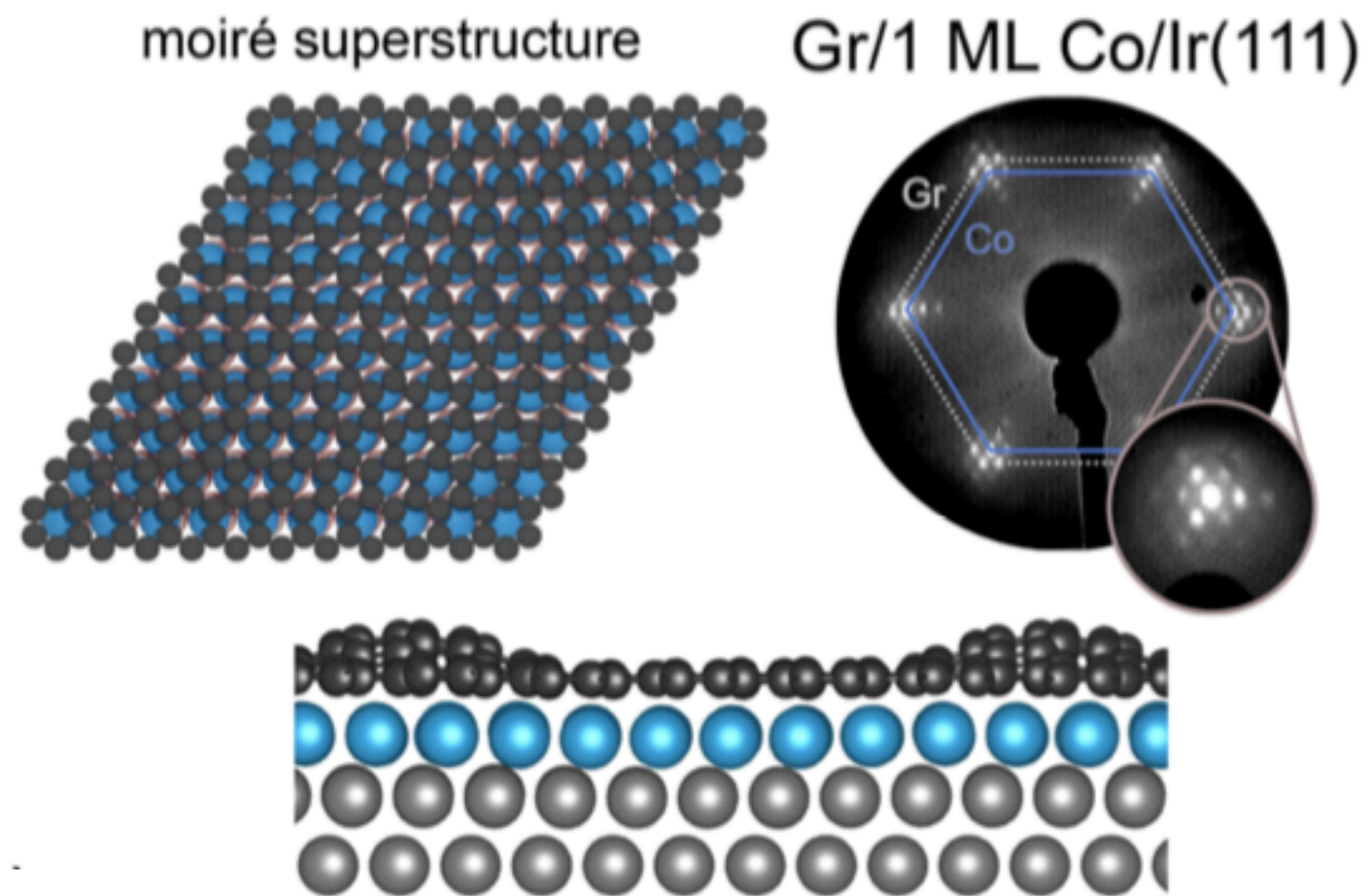


**Higher accuracy**

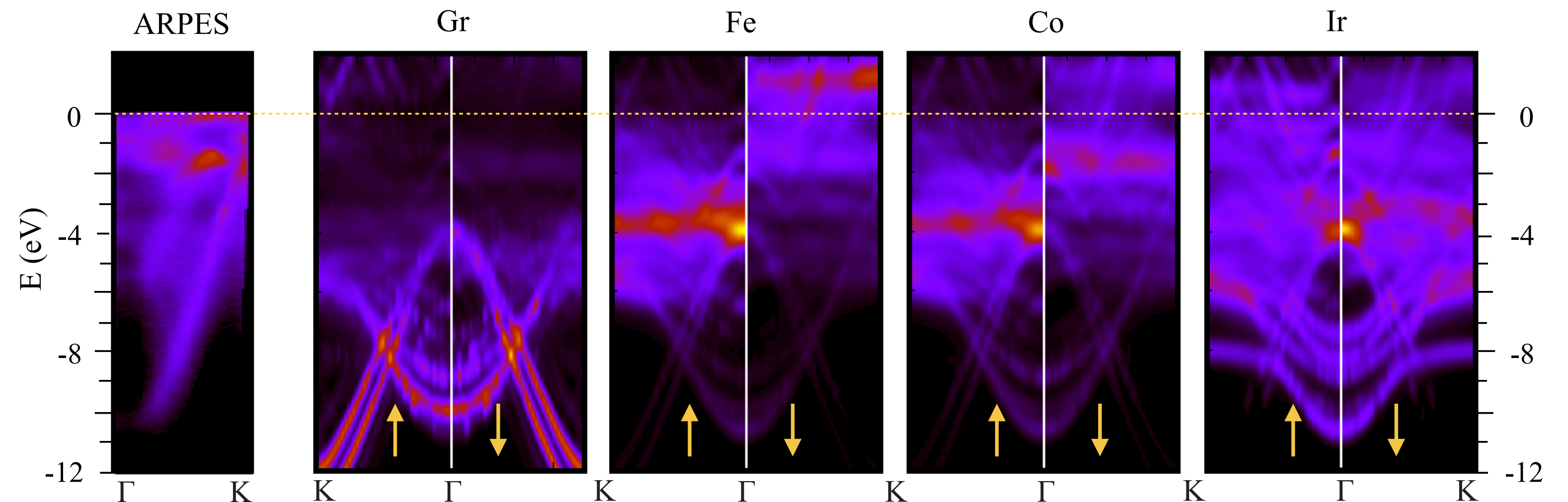
**High throughput  
screening**

**Improved modelling  
(complexity)**

# exascale opportunity: complexity

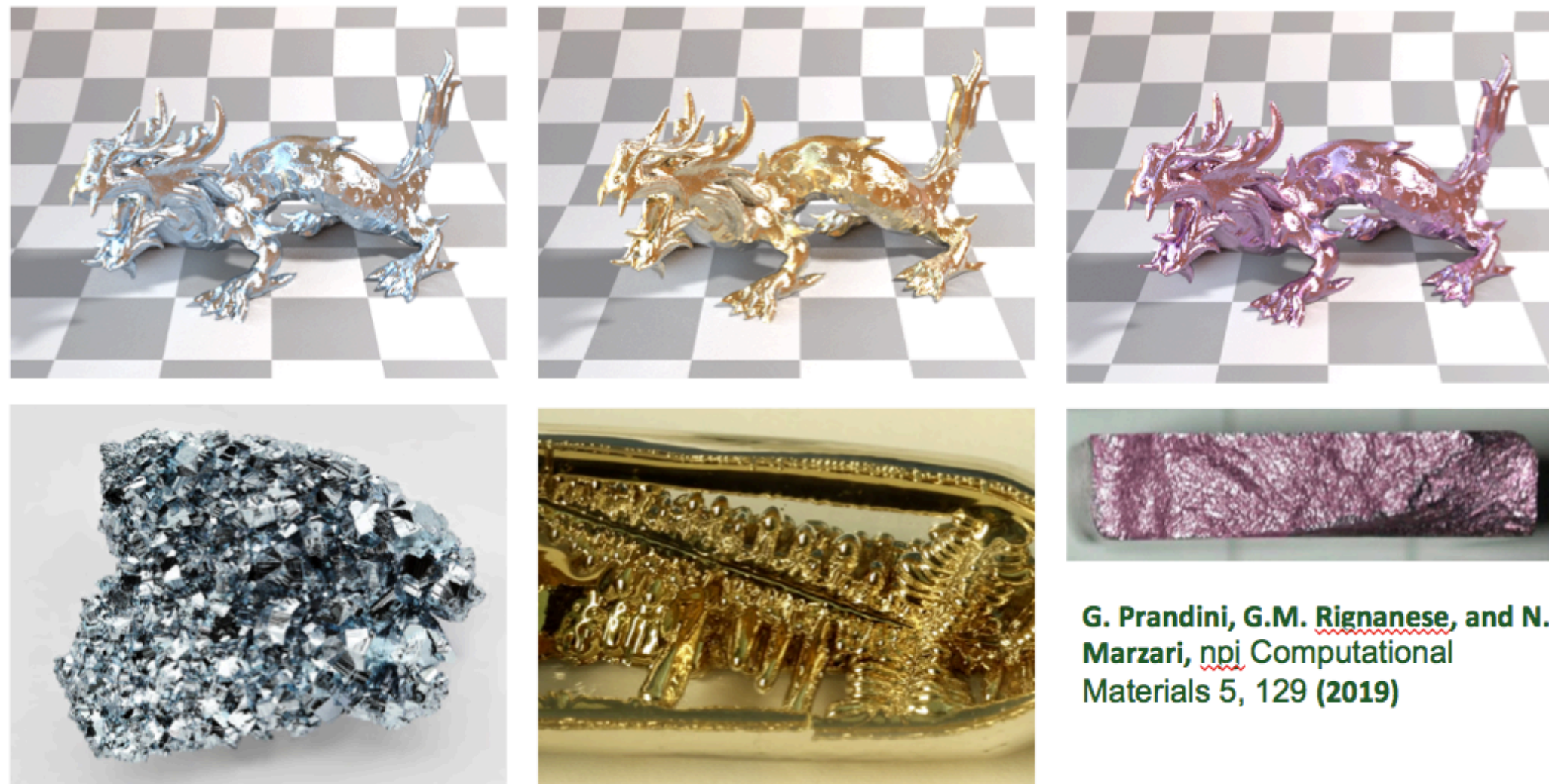
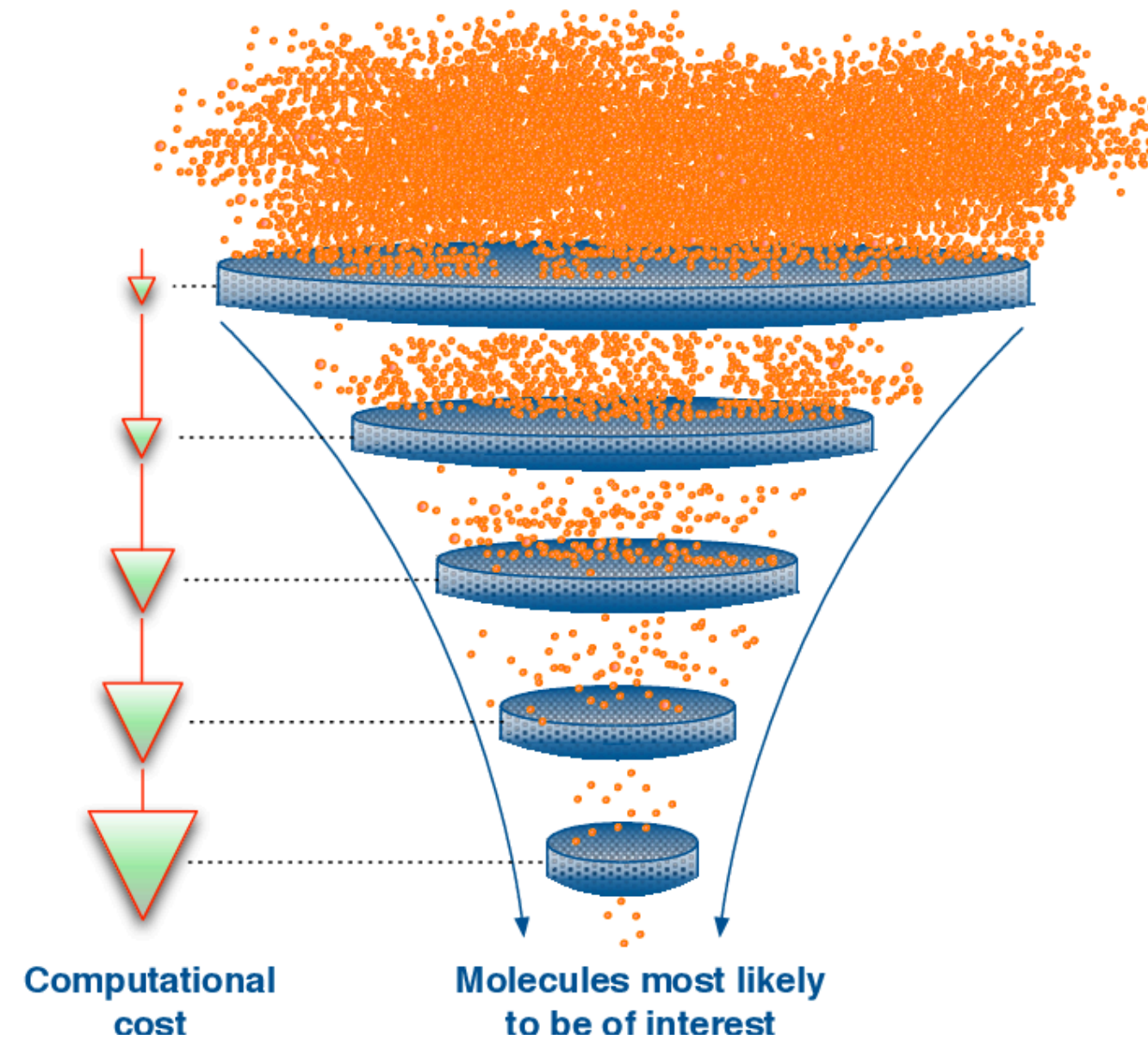


- Graphene / Transition Metal / Ir (111)
- **clear experimental evidence** for moiré' pattern (**lattice mismatch**) and **Gr corrugation**
- 10x10 Graphene, 9x9 Iridium => 605 atoms / unit cell
- **Precise treatment of the structure** is important for modelling

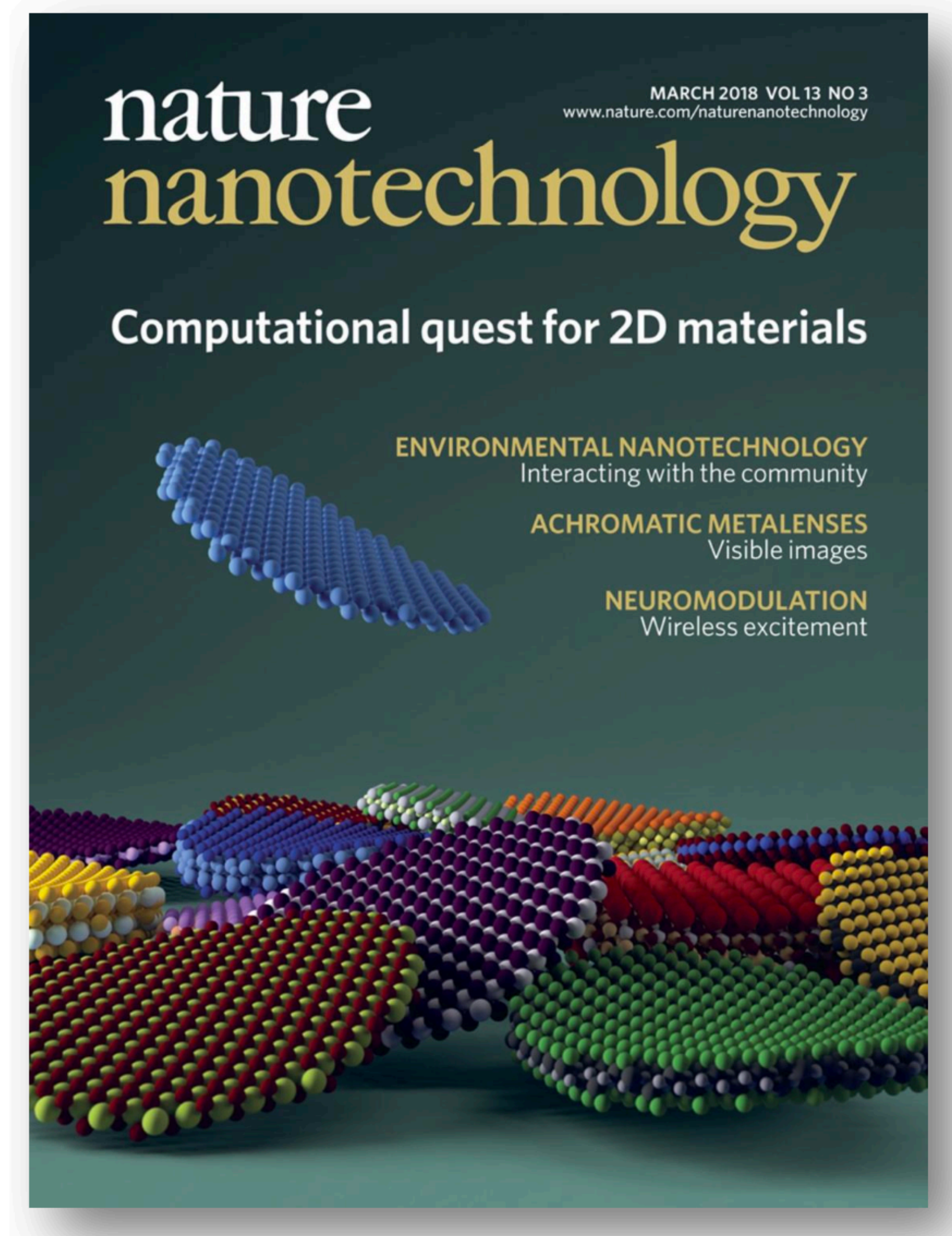
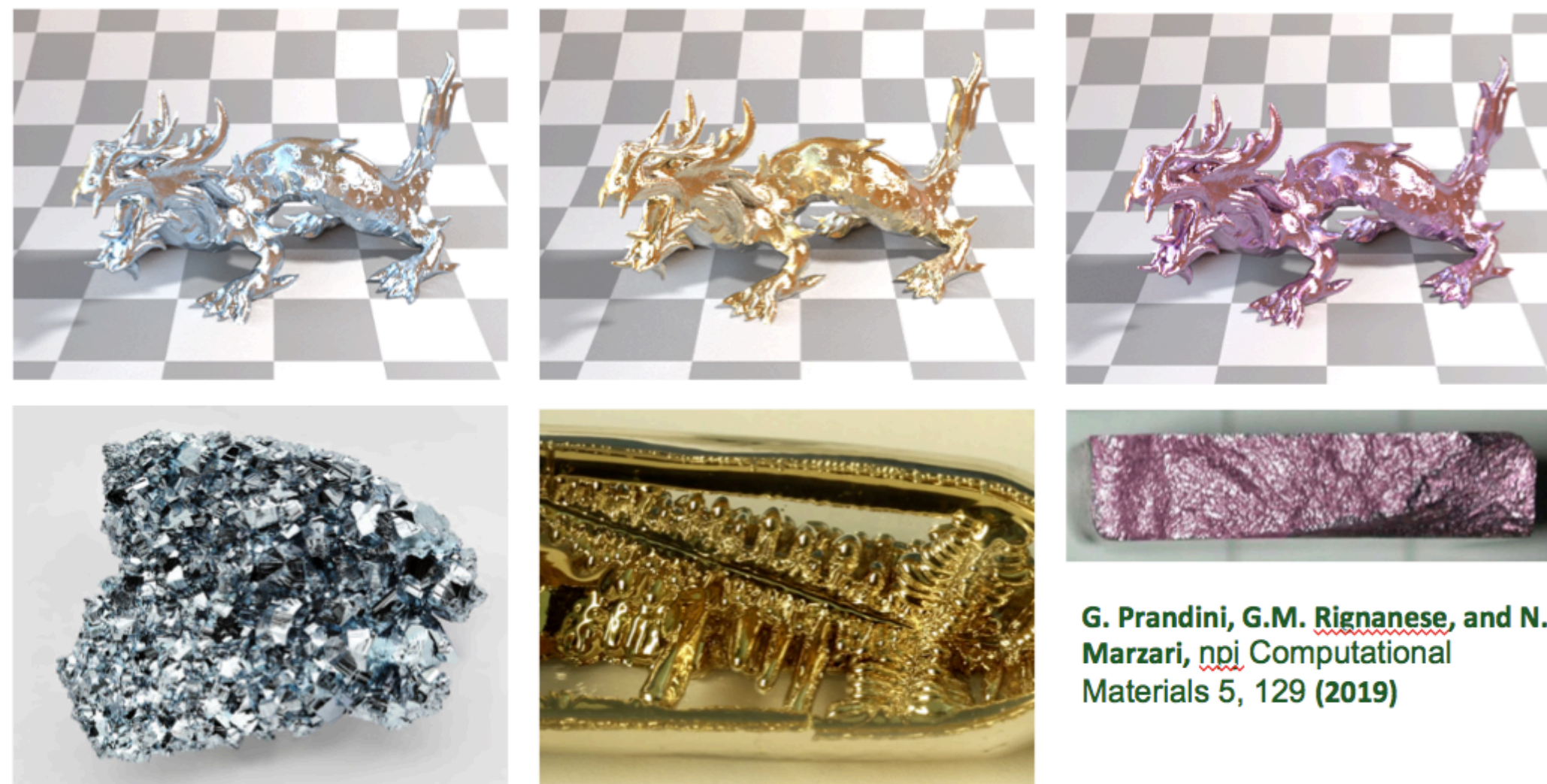
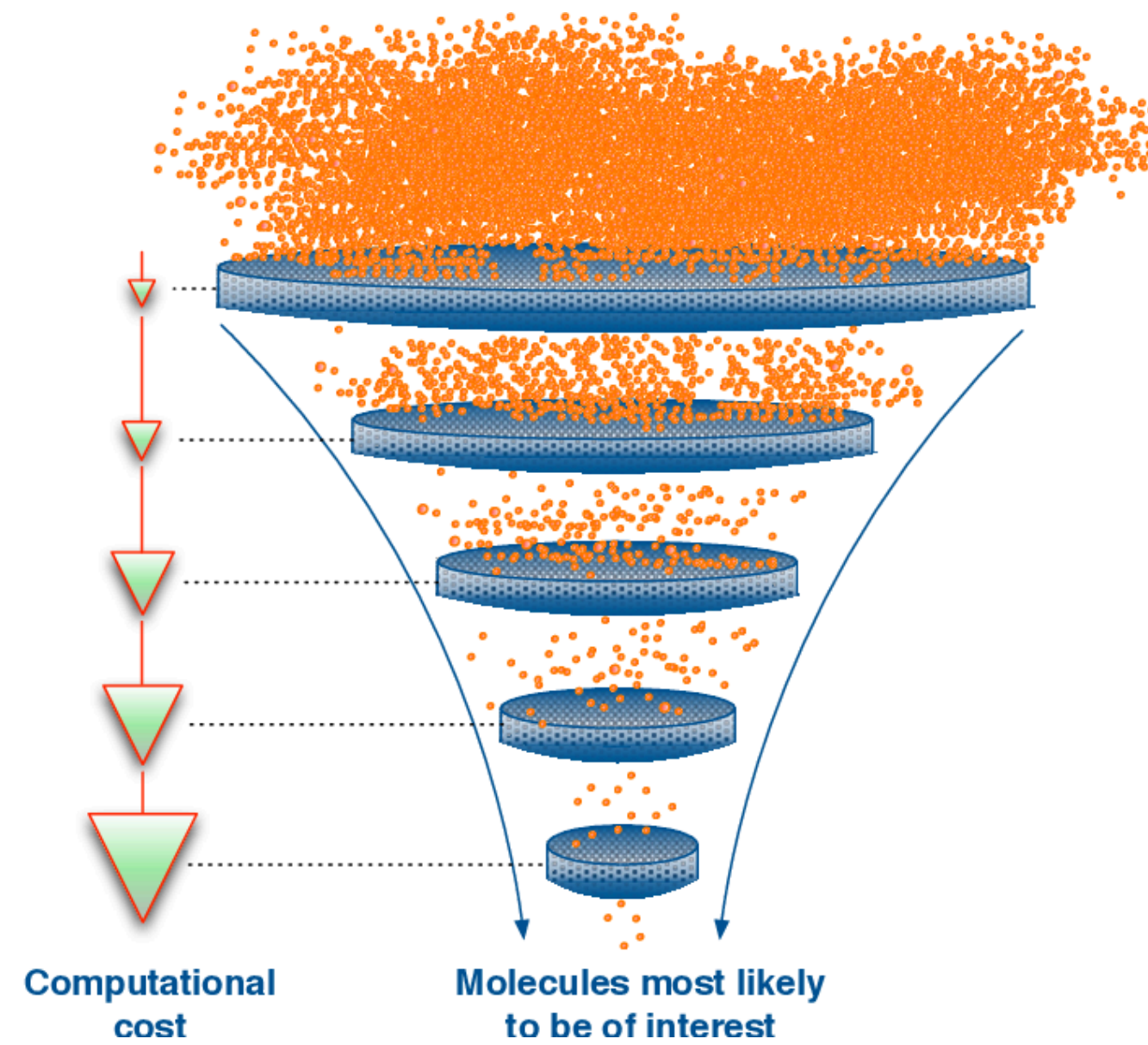


- Avvisati et al, J Phys. Chem. C **121**, 1639 (2017)
- Avvisati et al, Nano Lett. **18**, 2268 (2018)
- Calloni et al, J. Chem. Phys. **153**, 214703 (2020)
- Cardoso et al, Phys. Rev. Mat. **5**, 014405 (2021)
- Pacile' et al, Appl. Phys. Lett. **118**, 121602 (2021)

# exascale opportunity: high throughput screening



# exascale opportunity: high throughput screening



N. Mounet, ..., N. Marzari, *Nature Nanotechnology* 13, 246 (2018)  
D. Campi, N. Mounet, M. Gibertini, G. Pizzi, and N. Marzari, *ACS Nano* 17, 11268–11278 (2023)



## Materials Design at the Exascale

- European centre of Excellence in HPC applications
- funded for 3 phases (2015-2026)
- head-quartered at CNR-NANO, Modena
- focused on **electronic structure codes**



# A partnership with the required skills



LIGHTHOUSE  
CODES

DOMAIN EXPERTS  
& CODE DEVELOPERS

HPC EXPERTS  
& DATA CENTRES

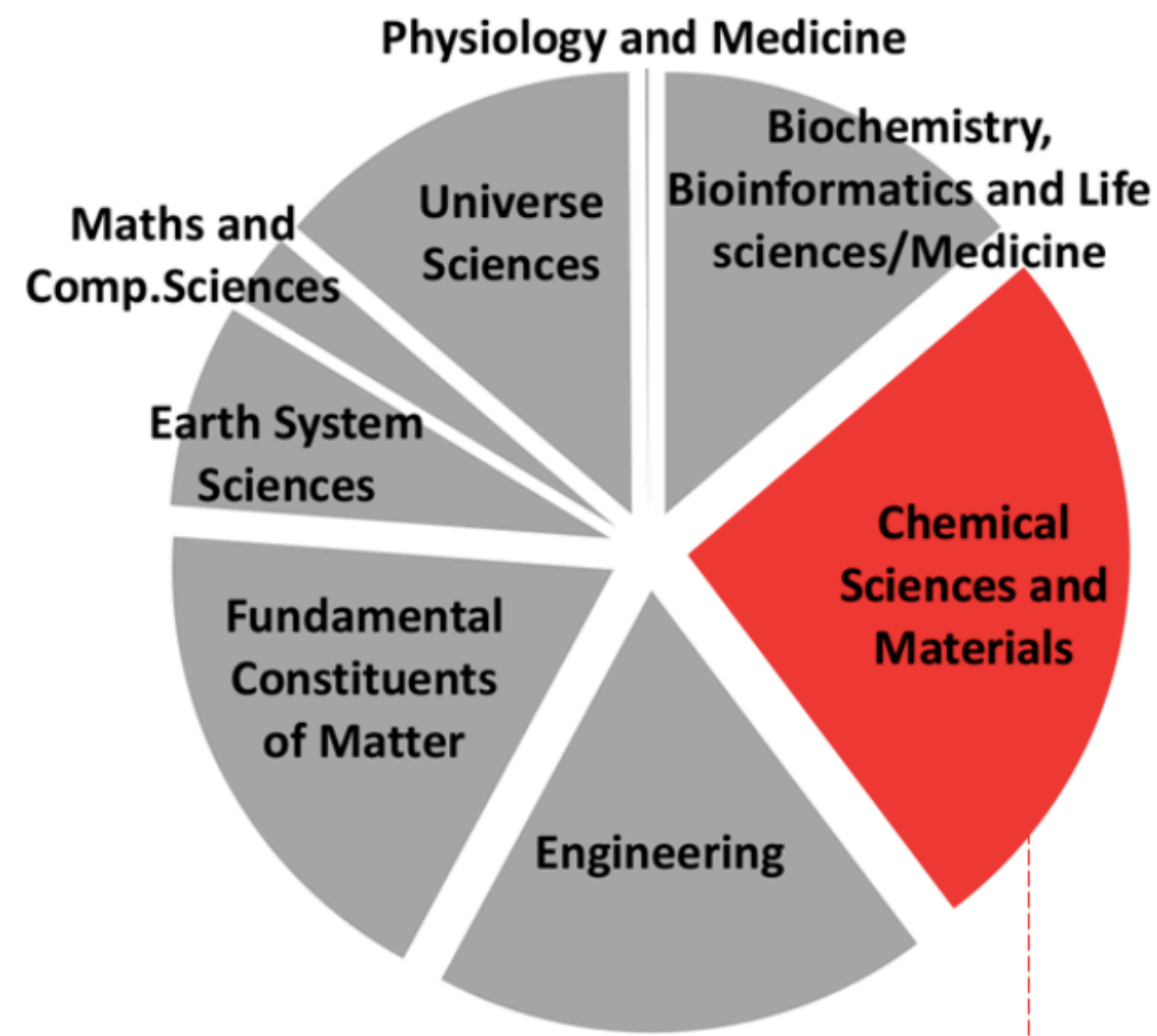
TECHNOLOGY &  
CO-DESIGN PARTNERS

MAX coordination and management: Cnr – Modena, Italy



<http://www.max-centre.eu/>

- widely used **open source, community codes** in electronic structure



## SELECTED ACTIVITIES

- parallel optimization and performance portability** are key to keep exploiting HPC resources
- All MaX flagship codes released for **production with GPU support**

- Design, of **exascale workflows** for selected scientific grand challenges

- hardware-software **codesign vehicles**
- energy-efficiency** of codes

- large effort on **education and training:** hands-on schools and hackathons

# Lhumos Platform: Learning Hub for Modeling and Simulation

Lhumos Spaces

### CECAM

Fostering computational science for societal progress

### MARVEL

MARVEL targets the accelerated design and discovery of novel materials, via a materials' informatics platform of database-driven high-throughput quantum simulations.

### MAX

MaX (MATERIALS design at the eXascale) is a European Centre of Excellence which enables materials modelling, simulations, discovery and design at the frontiers of the current and future High Performance Computing (HPC), High Throughput Computing (HTC) and data analytics technologies.

### MultiXscale

MultiXscale is a EuroHPC JU Centre of Excellence in multiscale modelling. It is a collaborative 4-year project between the CECAM network and EESSI that will allow domain scientists to take advantage of the computational resources that will be offered by EuroHPC.

### DOME

DOME 4.0 intends to offer an intelligent semantic industrial data ecosystem for knowledge creation across the entire materials to manufacturing value chains.

### E-CAM

Shared space for E-CAM related material

### Lhumos

this is a public space to showcase new features about the Lhumos training portal

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## MAX Webinars

6



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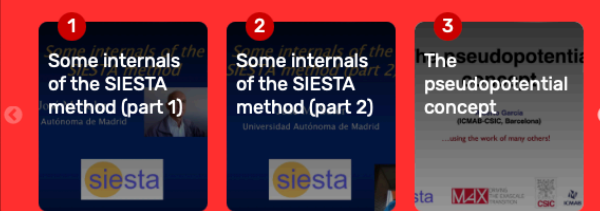
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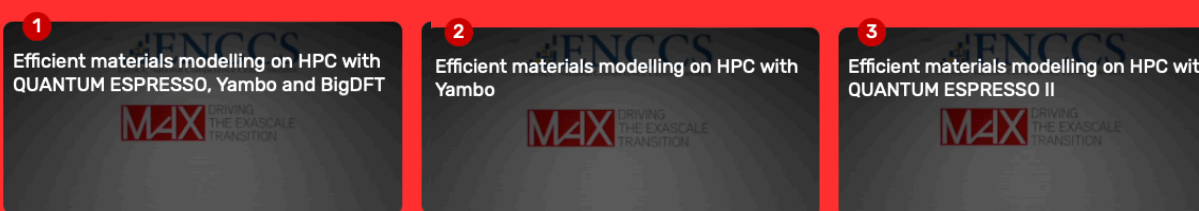
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# Lhumos Platform

Lhumos

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MAX DRIVING THE EXASCALE TRANSITION

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MAX DRIVING THE EXASCALE TRANSITION

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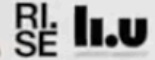




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Spaces → MAX → **Efficient materials modelling on HPC with QUANTUM ESPRESSO, Yambo and BigDFT**



EuroCC National Competence Centre Sweden



**DRIVING THE EXASCALE TRANSITION**

**Efficient materials modelling on HPC with QUANTUM ESPRESSO, Yambo and BigDFT**

14-17 November 2022

1 **ENCACS logo**

2 **Origin of the BigDFT project**

STREP European project: BigDFT (2005-2008)

In the beginning: Four partners, 35 people  
Now: around 10 active developers, Grenoble, Basel, Bristol, Catania, Trieste, Kobe  
Used in production since twelve years.

Aim: To develop an ab-initio DFT code based on Daubechies Wavelets, to be integrated in ABINIT.  
BigDFT 1.0 → January 2008

**Why have we done that?**

- Test the potential advantages of a new formalism
- A lot of outcomes and interesting results
- Future opportunities and ideas

3 **Daubechies wavelets**

**Wavelets**

A basis with optimal properties for expanding localized information

- Localized in real space
- Smooth (localized in Fourier space)
- Orthogonal basis
- Multi-resolution basis
- Adaptive
- Systematic

**From early 80's**

Applied in several domains interesting for DFT

4 **A brief description of wavelet theory**

**A Multi-Resolution real space basis**

All functions w/ compact support, centered on grid points. In the wavelet theory we have two kind of basis functions.

**Scaling Functions (SF)** **Wavelets (WF)**

The functions of low resolution level are a linear combination of high-resolution functions.

Contain the Dof needed to complete the information lacking due to the coarseness of the resolution.


**Increase the resolution without modifying grid space**

SF + WF = Degrees of Freedom of SF of higher resolution

BigDFT is an open source density functional theory code which uses a Daubechies wavelet basis set which facilitates optimal features of flexibility, performance and precision. In addition to the traditional cubic-scaling DFT approach, BigDFT also contains an approach which scales linearly with the number of atoms, enabling DFT calculations of large systems containing many thousands of atoms which were impractical to simulate even very recently. BigDFT consists of a package suite with a wide variety of features, from ground-state quantities to excited state quantities based on time-dependent DFT and constrained DFT, to potential energy surface exploration techniques. It uses dual space Gaussian type norm-conserving pseudopotentials including those with non-linear core corrections, which have proven to deliver all-electron precision. Its flexible Poisson solver can handle a number of different boundary conditions including free, wire, surface, and fully periodic, while it is also possible to simulate implicit solvents as well as external electric fields. Finally, BigDFT has been designed to exploit HPC from


1

Efficient materials modelling on HPC with QUANTUM ESPRESSO, Yambo and BigDFT




1

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2

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PDF

ENCACS-BigDFT-Driving Workshop

LG.pdf

pages: 32      BigDFT Session

7.906 MB

Flexibilities of wavelets as a

PDF

ENCACS-LSBIGDFT-LR.pdf

pages: 18

0.821 MB

Simulating Thousands of Atoms using Linear Scaling BigDFT

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Increase the resolution without modifying grid space

SF + WF = Degrees of Freedom of SF of higher resolution

BigDFT is an open source density functional theory code which uses a Daubechies wavelet basis set which facilitates optimal features of flexibility, performance and precision. In addition to the traditional cubic-scaling DFT approach, BigDFT also contains an approach which scales linearly with the number of atoms, enabling DFT calculations of large systems containing many thousands of atoms which were impractical to simulate even very recently. BigDFT consists of a package suite with a wide variety of features, from ground-state quantities to excited state quantities based on time-dependent DFT and constrained DFT, to potential energy surface exploration techniques. It uses dual space Gaussian type norm-conserving pseudopotentials including those with non-linear core corrections, which have proven to deliver all-electron precision. Its flexible Poisson solver can handle a number of different boundary conditions including free, wire, surface, and fully periodic, while it is also possible to simulate implicit solvents as well as external electric fields. Finally, BigDFT has been designed to exploit HPC from

**ENCACS-BigDFT-Driving Workshop**

PDF **LG.pdf** BigDFT Session

pages: 32  
7.906 MB

Flexibilities of wavelets as a

PDF **ENCACS-LSBIGDFT-LR.pdf**

pages: 18  
0.821 MB

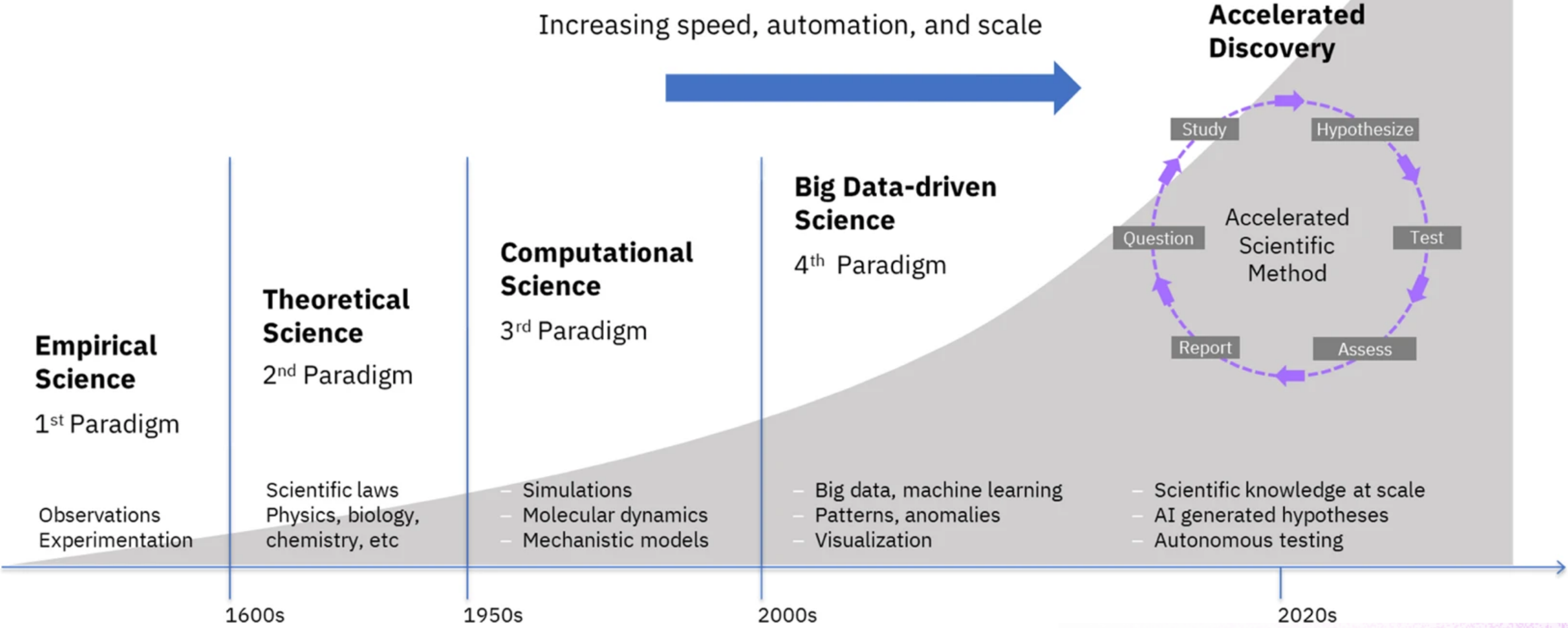
Calculating Thousands of Atoms using Linear Scaling BigDFT

[www.alpha.lhumos.org](http://www.alpha.lhumos.org)

# Computational Materials Science

Many Body Perturbation Theory:  
motivation and basic concepts

# Realization of the “fourth paradigm” of science in materials science



E. O. Pyzer-Knapp et al. *npj Computational Materials* 8, 84 (2022)  
 A. Agrawal, A. Choudhary *APL Mater.* 4, 053208 (2016)

# Computer meets theoretical physics



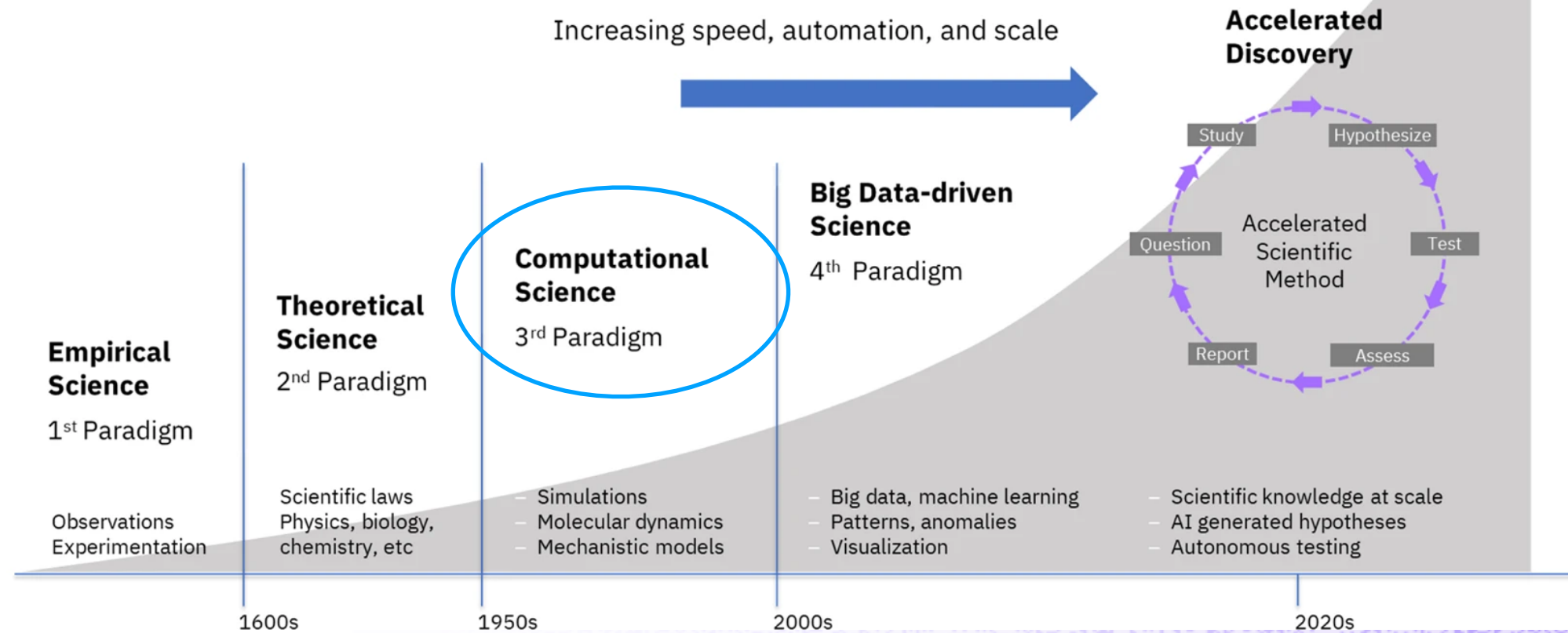
**Berni Julian Alder** (September 9, 1925 – September 7, 2020)



Boltzmann medal (2001)



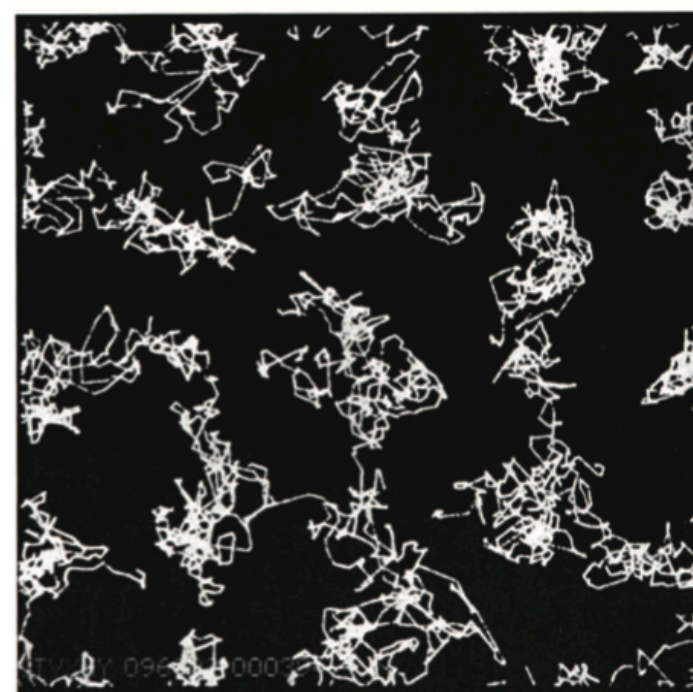
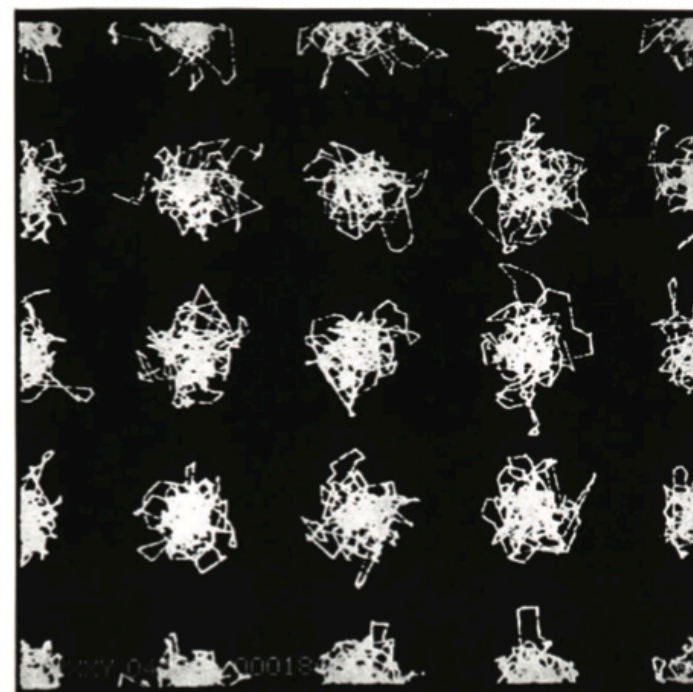
**Mary Ann Mansigh**  
(1932 – August 24, 2024)



1208 LETTERS TO THE EDITOR

relatively free diffusion, while in the low  $g(\sigma)$  states diffusion is much restricted.  
 The conjecture<sup>1</sup> that some high-order virial coefficients might be negative is not necessarily supported by the present results, since only to the left of the apparent transition do the latter give lower pressures than the five-term virial expression.  
 Some further investigation for both 32 molecule and larger systems will be made on the present calculators, but a satisfactory determination of the detailed behavior in the apparent transition region will require higher speed equipment. The possibility that a similar phenomenon for hard spheres in two dimensions may have been missed in the original Monte Carlo calculations<sup>2</sup> will also be investigated.  
 \* Work performed under the auspices of the U. S. Atomic Energy Commission.  
<sup>1</sup> M. N. Rosenbluth and A. W. Rosenbluth, *J. Chem. Phys.* **22**, 881 (1954).  
<sup>2</sup> Metropolis, Rosenbluth, Rosenbluth, Teller, and Teller, *J. Chem. Phys.* **21**, 1087 (1953).  
<sup>3</sup> B. J. Alder and T. Wainwright, *J. Chem. Phys.* **27**, 1208 (1957).  
<sup>4</sup> W. W. Wood and F. R. Parker, *J. Chem. Phys.* **27**, 720 (1957).  
 This paper discusses the Monte Carlo method in some detail, as well as giving computational results for Lennard-Jones molecules.  
<sup>5</sup> Kirkwood, Maun, and Alder, *J. Chem. Phys.* **18**, 1040 (1950).

A 32-particle system in a cube and initially in a face-centered cubic lattice proceeded at about 300 collisions an hour on the UNIVAC. For comparison a 96-particle system in a rectangular box and initially in a hexagonal arrangement has been calculated, however only at high densities so far. No differences in the pressures can be detected. It became apparent that some long runs were necessary at intermediate densities, accordingly the IBM-704 was utilized where, for 32 particles, an hour is required for 7000 collisions. Larger systems of 108, 256, and 500 particles can also conveniently be handled; in an hour 2000, 1000, and 500 collisions, respectively, can be calculated. The results for 256 and 500 particles are not now presented due to inadequate statistics.  
 The equation of state shown in Fig. 1 of the accompanying paper<sup>3</sup> for 32 and 108 particles is for the intermediate region of density, where disagreement was found with the previous Monte Carlo results. The volume,  $v$ , is given relative to the volume of close packing,  $v_0$ . Plotted also are the more extended Monte Carlo results; the agreement between these three systems is within the present accuracy of the pressure determination. This agreement provides an interesting confirmation of the postulates of statistical mechanics for this system.  
 Figure 1 of the accompanying paper shows two separate and overlapping branches. In the overlapping region the system can, at a given density, exist in two states with considerably different pressures. As the calculation proceeds the pressure is seen to jump suddenly from one level to the other. A study of the positions of the particles reveals that as long as the system stays on the lower branch of the curve the particles are all confined to the narrow region in space determined by their neighbors, while on the upper branch of the curve the particles have acquired enough freedom to exchange with the surrounding particles. Since the spheres are originally in ordered positions, the system starts out on the lower branch; the first jump to the upper branch can require very many collisions. The trend, as expected, is that at higher densities more collisions are necessary for the first transition, however, there are large deviations. At  $v/v_0=1.60$ , 5000 collisions were required; at 1.55, 25 000; while at 1.54 only 400; at 1.535, 7000; at 1.53, 75 000; and at 1.525, 95 000. Runs in excess of 200 000 collisions at  $v/v_0$  of 1.55 and 1.53 have not shown any return to the lower branch, while at 1.525 the system has returned several times, however only for relatively few collisions. The lowest density at which the system did not jump to the upper curve is at 1.50, however the run extends only to 50 000 collisions and at that density it might take very many collisions before the appropriate fluctuation occurs for a molecule to escape from its neighborhood. For comparison, the first jump for 108 particles occurred for  $v/v_0=1.55$  and 1.60 at about 2000 collisions. This is fewer collisions per particle than for the smaller system and is indicative of larger possible density fluctuations in larger systems. Apparently, the



*“The method consists of solving exactly the simultaneous classical equation of motion of several hundreds particles by means of fast electronic computers”*

Simulations of 32/108 hard spheres  
7000 collisions per hour

**computer simulation as a legitimate scientific method**



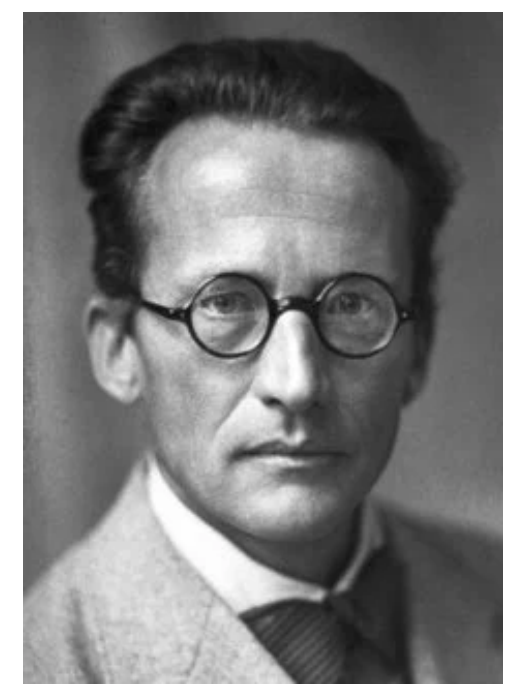
IBM-704 Los Alamos 1957  
~5000 Flops

~10<sup>8</sup>–10<sup>9</sup>× slower than a modern mobile phone

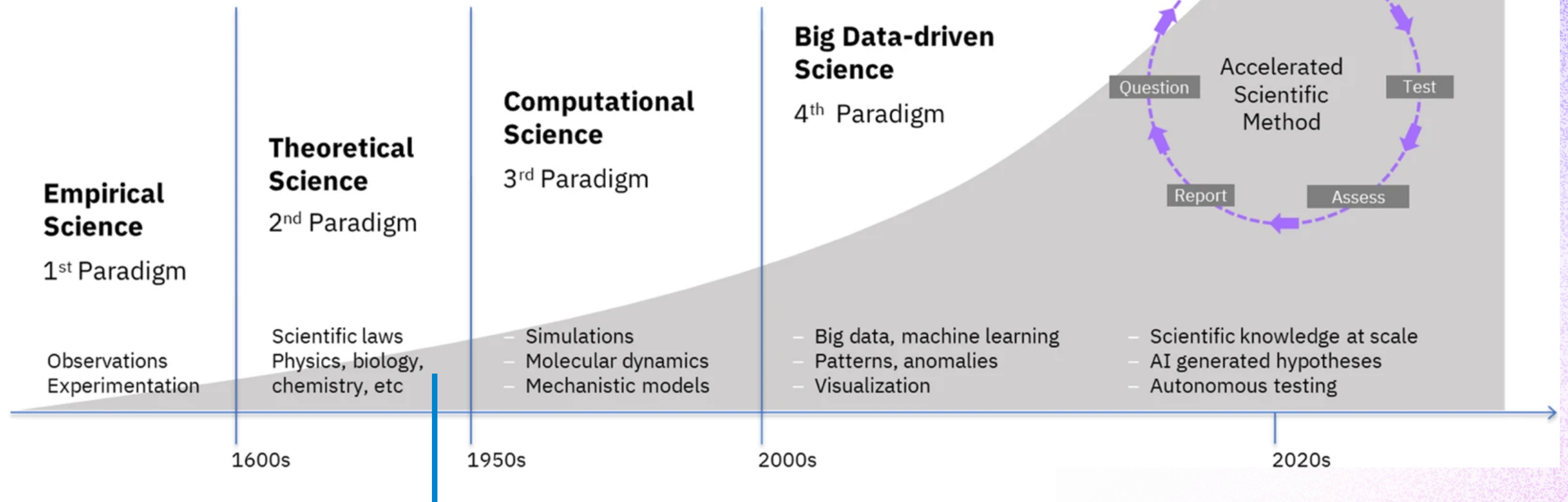
Alder, B. J.; Wainwright, . "Phase Transition for a Hard Sphere System". *J. Chem. Phys.* **27**, 1208–1209 (1957)

Online Computational Spectroscopy: Hands-on Many Body Calculation with the Yambo code. 5-7 May 2026

# The many body problem in Quantum Mechanics



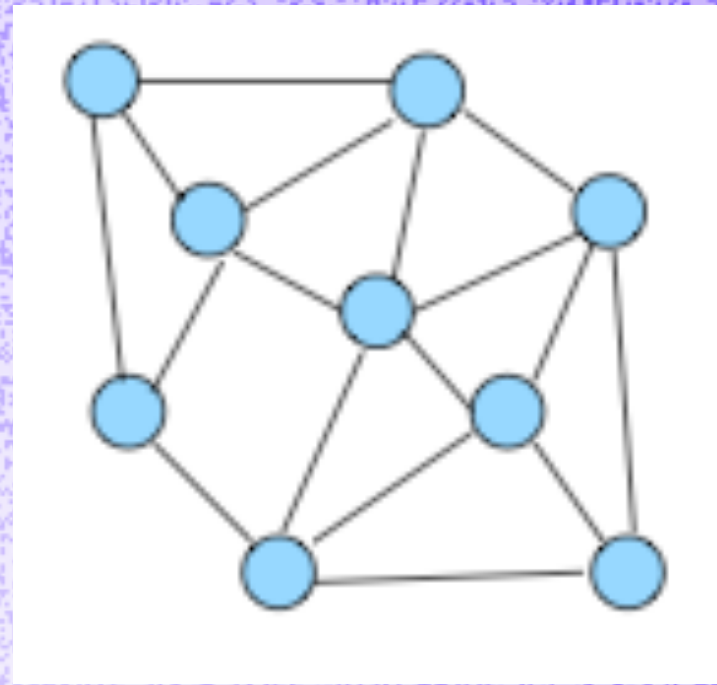
Nobel Prize in Physics 1933



Quantisierung als Eigenwertproblem (Quantization as an Eigenvalue Problem) E. Schrodinger Annalen der Physik 1926

# The many body problem in Quantum Mechanics

$$H\Psi(r_1, r_2, \dots, r_N) = E\Psi(r_1, r_2, \dots, r_N)$$

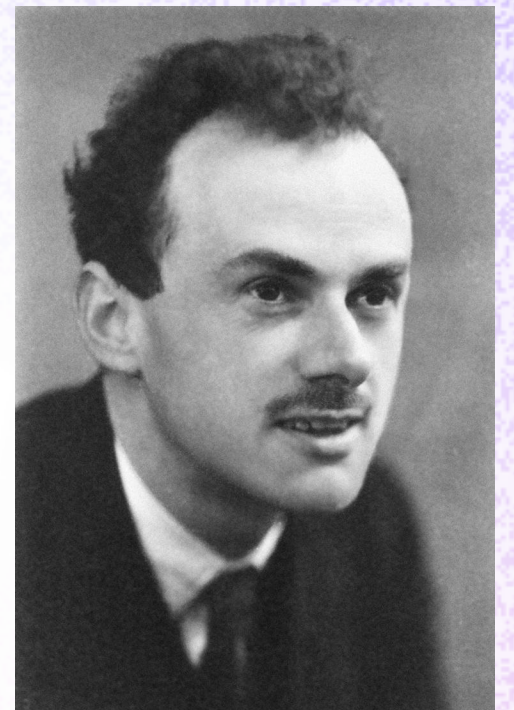


$$\hat{H} = -\frac{\hbar^2}{2m_e} \sum_{i=1}^N \nabla_i^2 + \frac{1}{4\pi\epsilon_0} \frac{1}{2} \sum_{i,j=1;i \neq j}^N \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} - \frac{1}{4\pi\epsilon_0} \sum_n^M \sum_i^N \frac{Z_n e^2}{|\mathbf{r}_i - \mathbf{R}_n|}$$

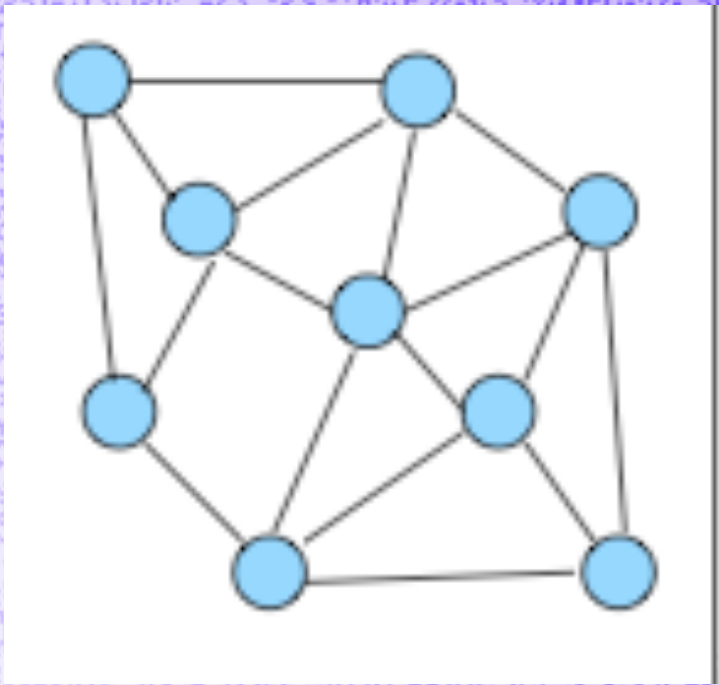
Hamiltonian of a System of N interacting electrons

Exact solutions of the many-electron Schrödinger equation scale exponentially with the number of electrons due to the growth of the Hilbert space (“exponential wall”).

*“The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble.”*  
— P. A. M. Dirac, *Proceedings of the Royal Society A* **123**, 714 (1929)



# The many body problem in Quantum Mechanics

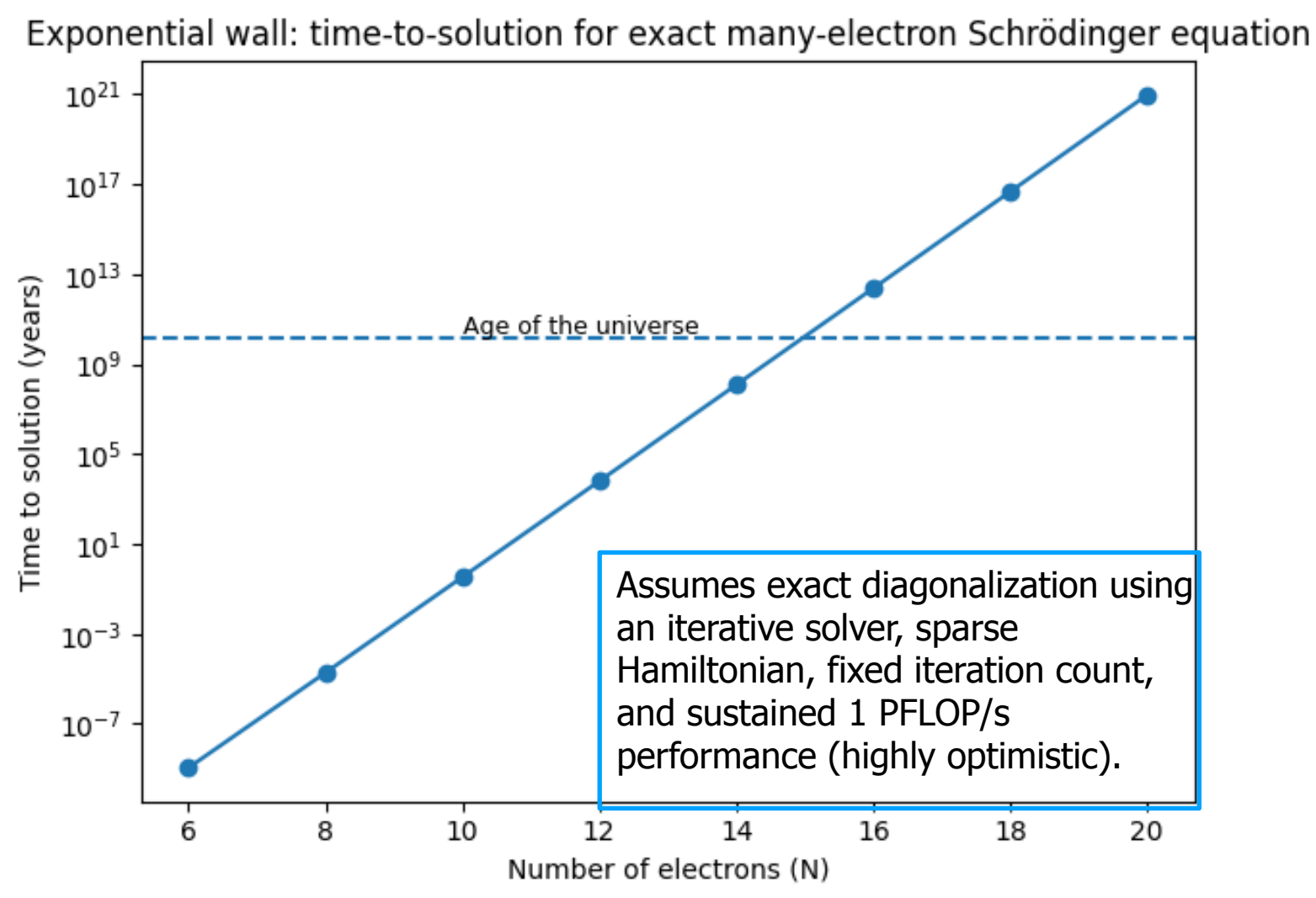
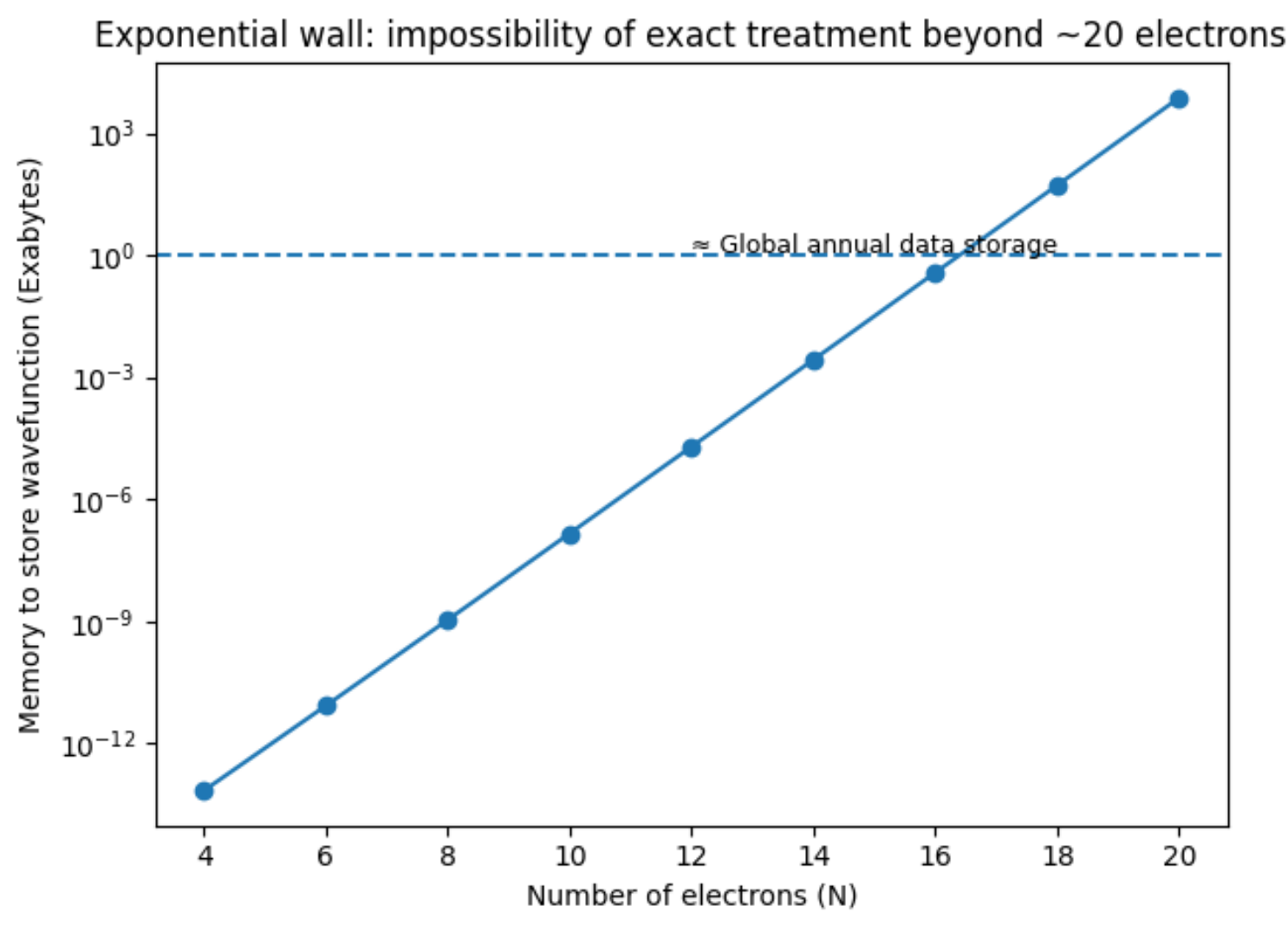


$$H\Psi(r_1, r_2, \dots, r_N) = E\Psi(r_1, r_2, \dots, r_N)$$

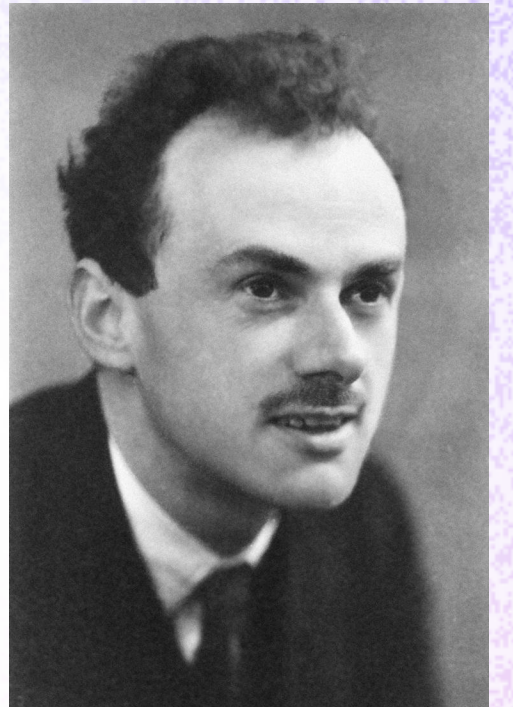
$$\hat{H} = -\frac{\hbar^2}{2m_e} \sum_{i=1}^N \nabla_i^2 + \frac{1}{4\pi\epsilon_0} \frac{1}{2} \sum_{i,j=1; i \neq j}^N \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} - \frac{1}{4\pi\epsilon_0} \sum_n^M \sum_i^N \frac{Z_n e^2}{|\mathbf{r}_i - \mathbf{R}_n|}$$

Hamiltonian of a System of N interacting electrons

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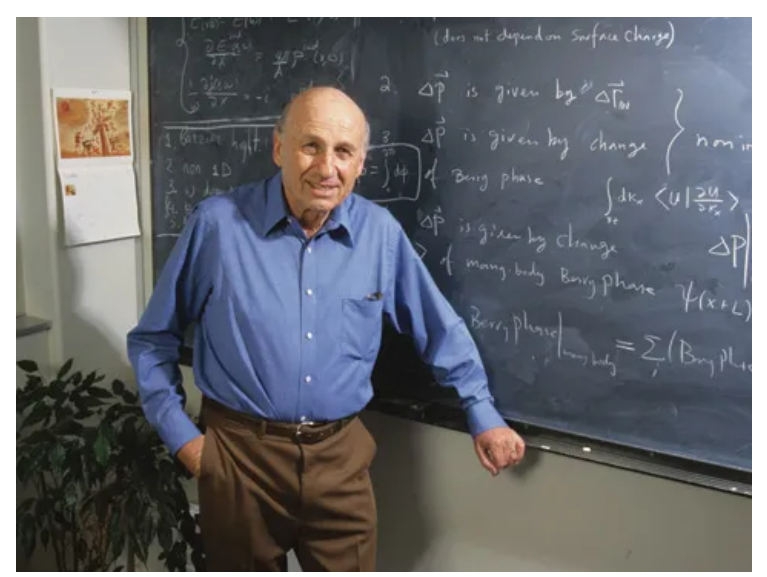


*“The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble.”*  
 — P. A. M. Dirac, *Proceedings of the Royal Society A* **123**, 714 (1929)

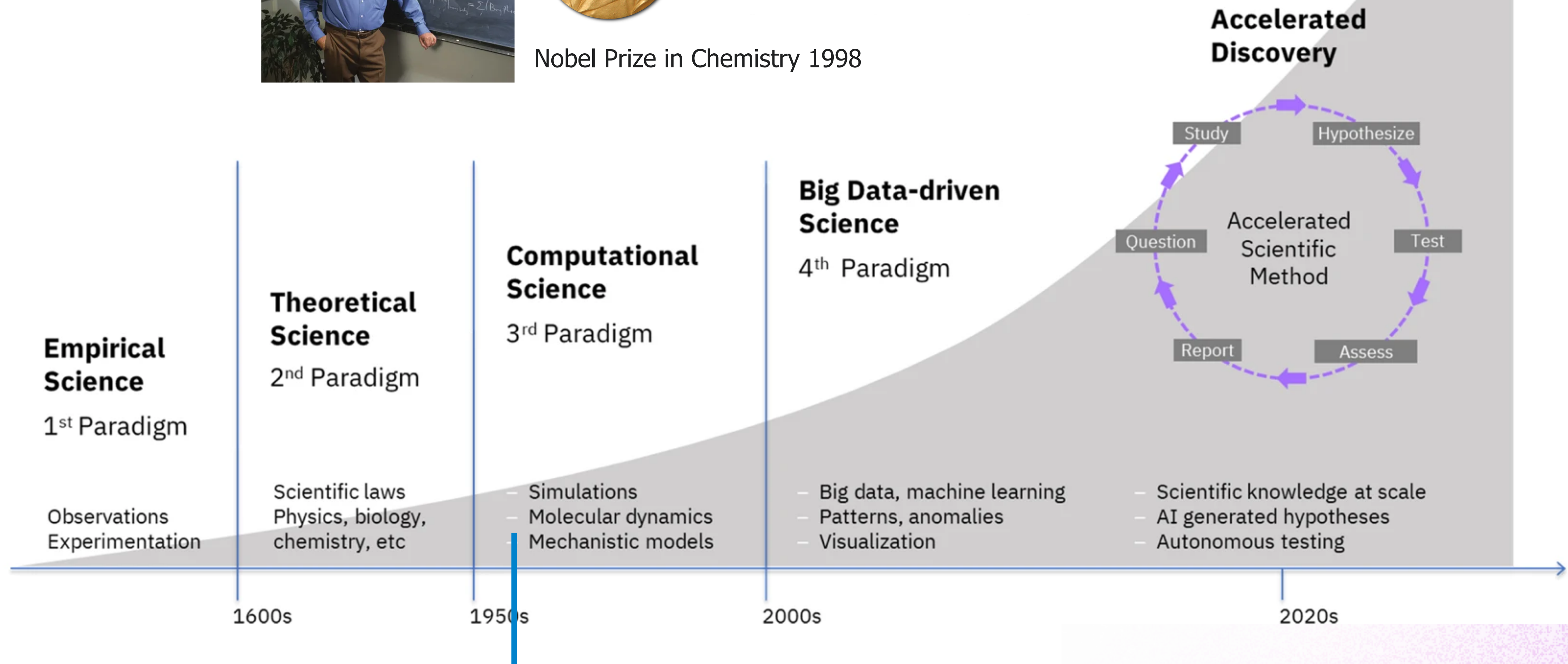


Exact solutions of the many-electron Schrödinger equation are prohibited by exponential scaling in both memory and time. It is not a merely technological issue.

# The many body problem in Quantum Mechanics



Nobel Prize in Chemistry 1998



- P. Hohenberg, and W. Kohn, "Inhomogeneous Electron Gas," *Physical Review*, **136**, B864–B871 (1964)
- W. Kohn, and L. J. Sham, "Self-Consistent Equations Including Exchange and Correlation Effects," *Physical Review*, **140**, A1133 (1965)

# Breaking the exponential wall: The density functional theory

$$H\Psi(r_1, r_2, \dots, r_N) = E\Psi(r_1, r_2, \dots, r_N)$$

$$n(r) = N \int |\Psi(r_1, \dots, r_N)|^2 dr_2 \dots dr_N$$

## Hohenberg-Kohn Theorems:

The ground-state density  $n(r)$ , a function of only **3 variables**, fully determines all ground-state properties.

$$n_{gs}(r) \leftrightarrow V_{ext}$$

ground state density determines the external potential in which the electrons move and thus the Hamiltonian and all physical properties of the system.

Exists an universal functional  $F_{HK}(n)$  such that:

$$E_{V_0}[n] = F_{HK}[n] + \int d^3r v_0(r)n(r)$$

$$E_0 = E_{v_0}[n_0] < E_{v_0}[n] \quad \text{Variational principle}$$

**Useless:**  $F_{HK}(n)$  is unknown: The theorems do not provide a way to calculate anything!

# Breaking the exponential wall: Kohn-Sham construction, making DFT practical

## Kohn-Sham DFT: An Effective One-Particle Picture

Map the interacting many-electron system onto a fictitious non-interacting system with the same ground-state density.

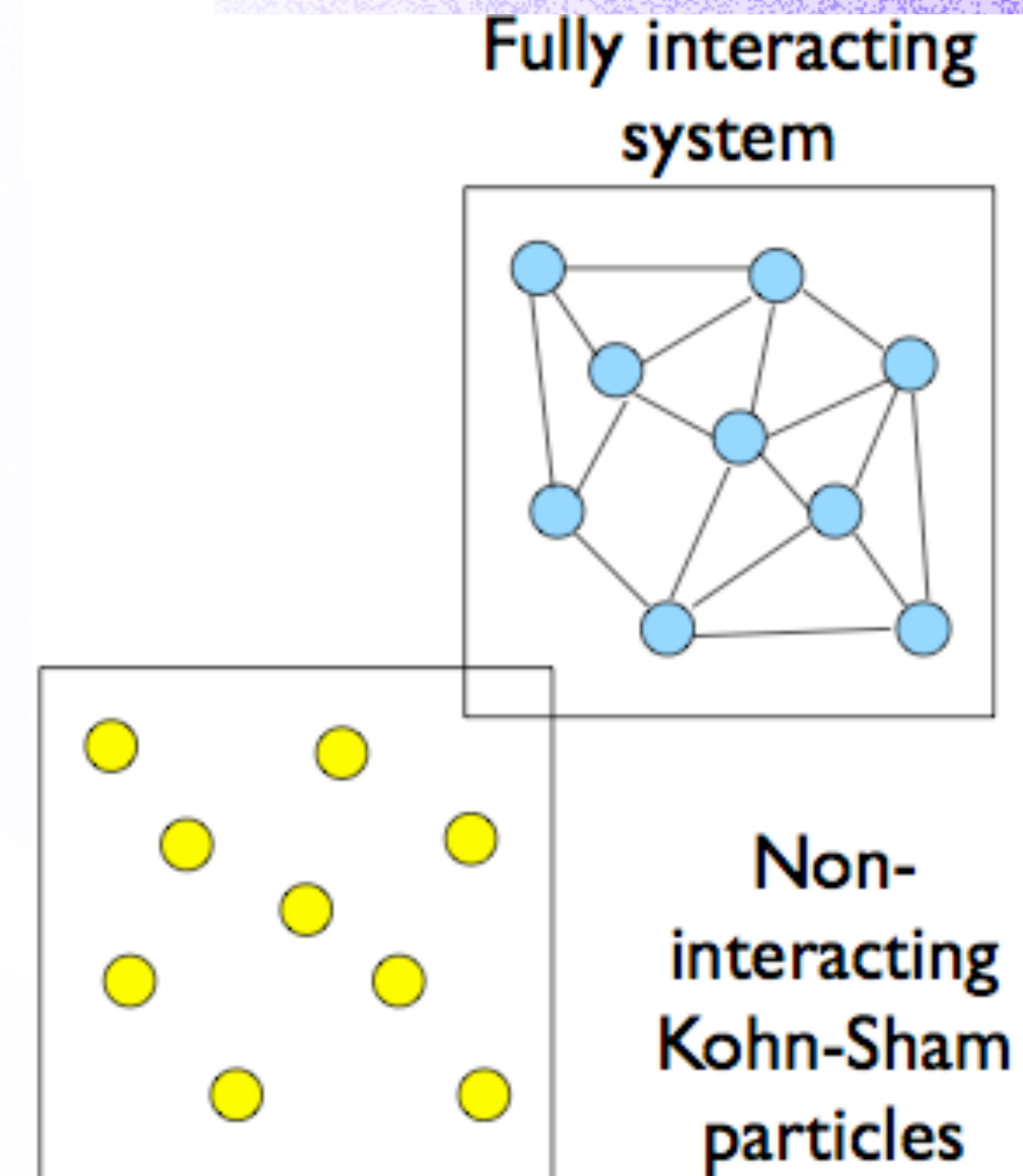
- Kohn-Sham functional - rewriting the Hohenberg-Kohn functional
- Auxiliary system of independent particles

$$n_0(r) = \sum_{i=1} |\psi_i(r)|^2$$

$$E_{KS} = \underbrace{T_{ip}[n]}_{\text{Equation for independent particle soluble}} + \int dr V_{ext}(r)n(r) + \underbrace{E_{Hartree}[n]}_{\text{Exchange-Correlation Functional - Exact formulation but unknown functional!}} + E_{xc}[n]$$

Equation for independent particle soluble

Exchange-Correlation Functional – Exact formulation but **unknown** functional!



DFT replaces an exponentially complex wavefunction with a tractable density, at the price of an approximate exchange–correlation functional.

Polynomial scaling  $\sim N^3$

Treats  $10^2$  -  $10^4$  electrons

# Breaking the exponential wall: Kohn-Sham construction, making DFT practical

$$E_{KS} = T_{ip}[n] + \int dr V_{ext}(r)n(r) + E_{Hartree}[n] + E_{xc}[n]$$

Equation for independent particle soluble

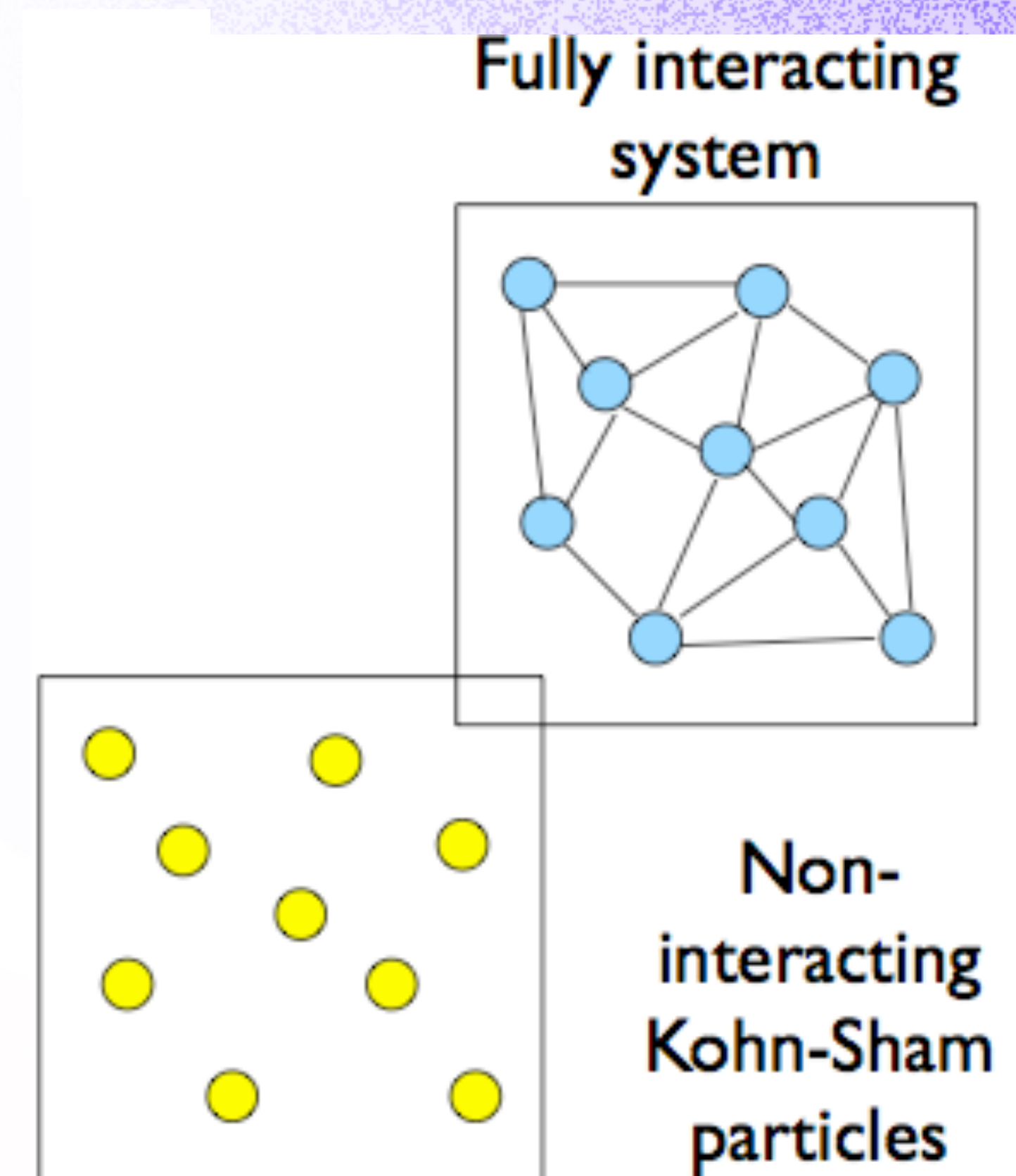
Exchange-Correlation Functional – Exact formulation but **unknown** functional!

In principle is exact

In practice it makes possible useful approximation

Finding a good approximation for  $E_{xc}[n]$  requires information about the interacting many-body problem

A new field of research – find **useful, approximate**  $E_{xc}[n]$  functionals



# Exchange-Correlation Potential

How to find a [approximate] functional  $E_{xc}[n]$  ?

Use a model where the exchange correlation energy can be calculated

Local Density Approximation (LDA):

At each point in space, the exchange–correlation energy is approximated by that of a **uniform electron gas** with the same local density.

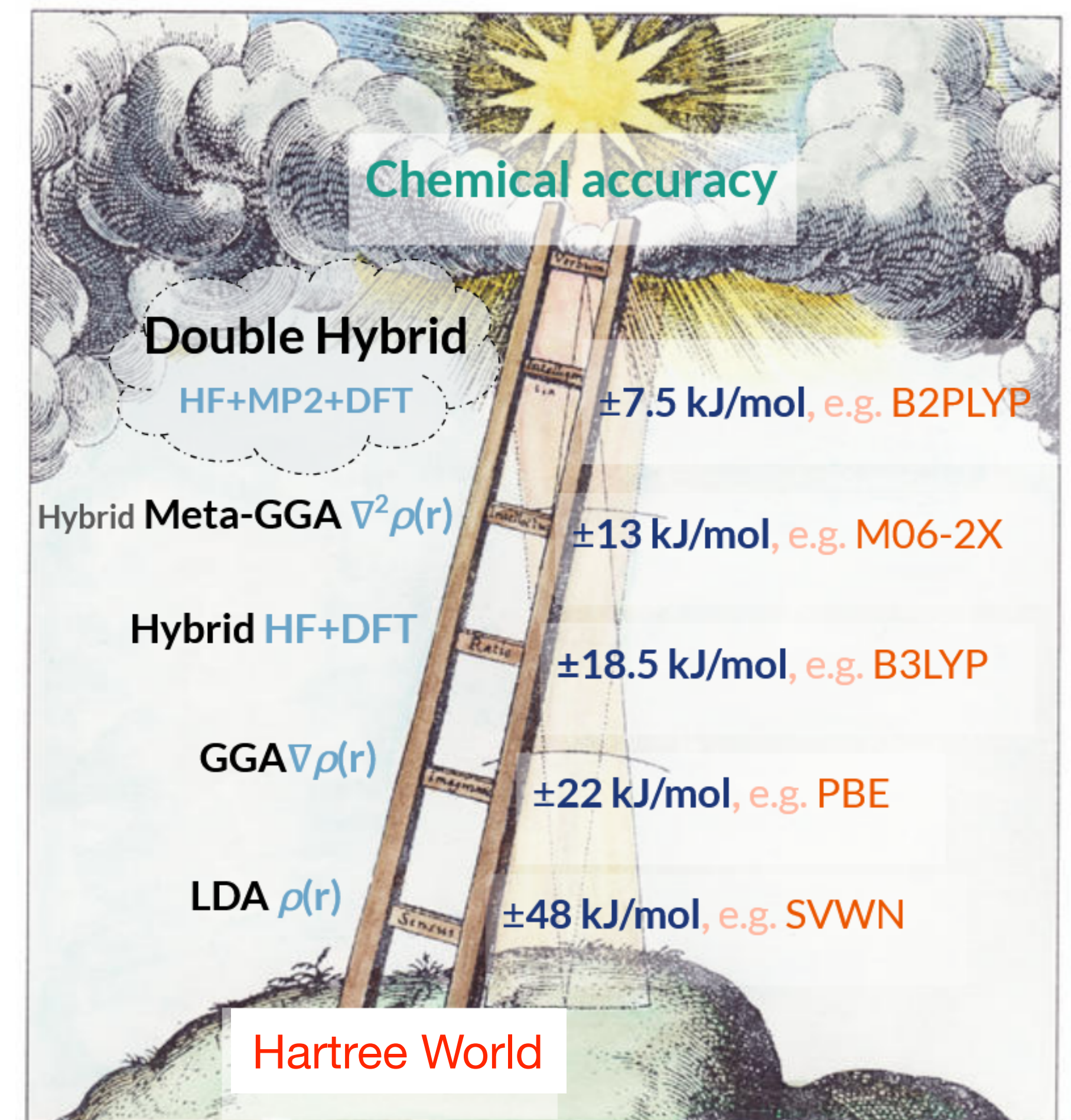
$$E_{xc}^{LDA}[n] = \int n(r) \epsilon_{xc}^{UEG}(n(r)) dr$$

$\epsilon_{xc}^{UEG}(n(r))$  exchange–correlation energy per particle of the **uniform electron gas**

$\epsilon_{xc}^{UEG}(n)$  was been calculated as a function of density using quantum Monte Carlo methods.

D. Ceperley and B. Alder Phys. Rev. Lett. 45, 566 (1980)

J. P. Perdew, A. Zunger Phys. Rev. B **23**, 5048 (1981)



Picture adapted from K. Rowell PhD thesis

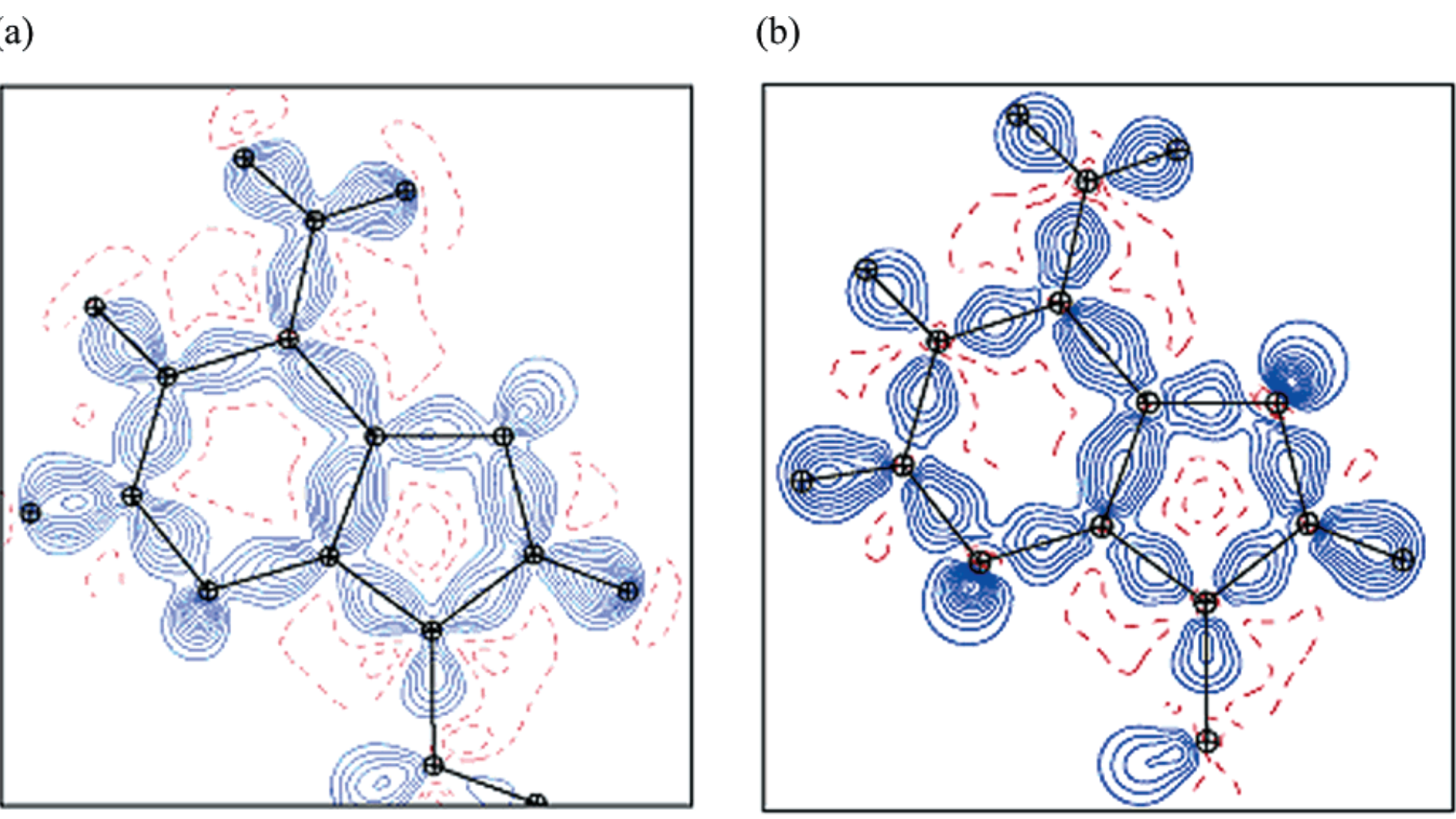
See. J. Perdew and K. Schmidt AIP Conf. Proc. 577, 1 (2001)

**modern deep learning-based XC functional**

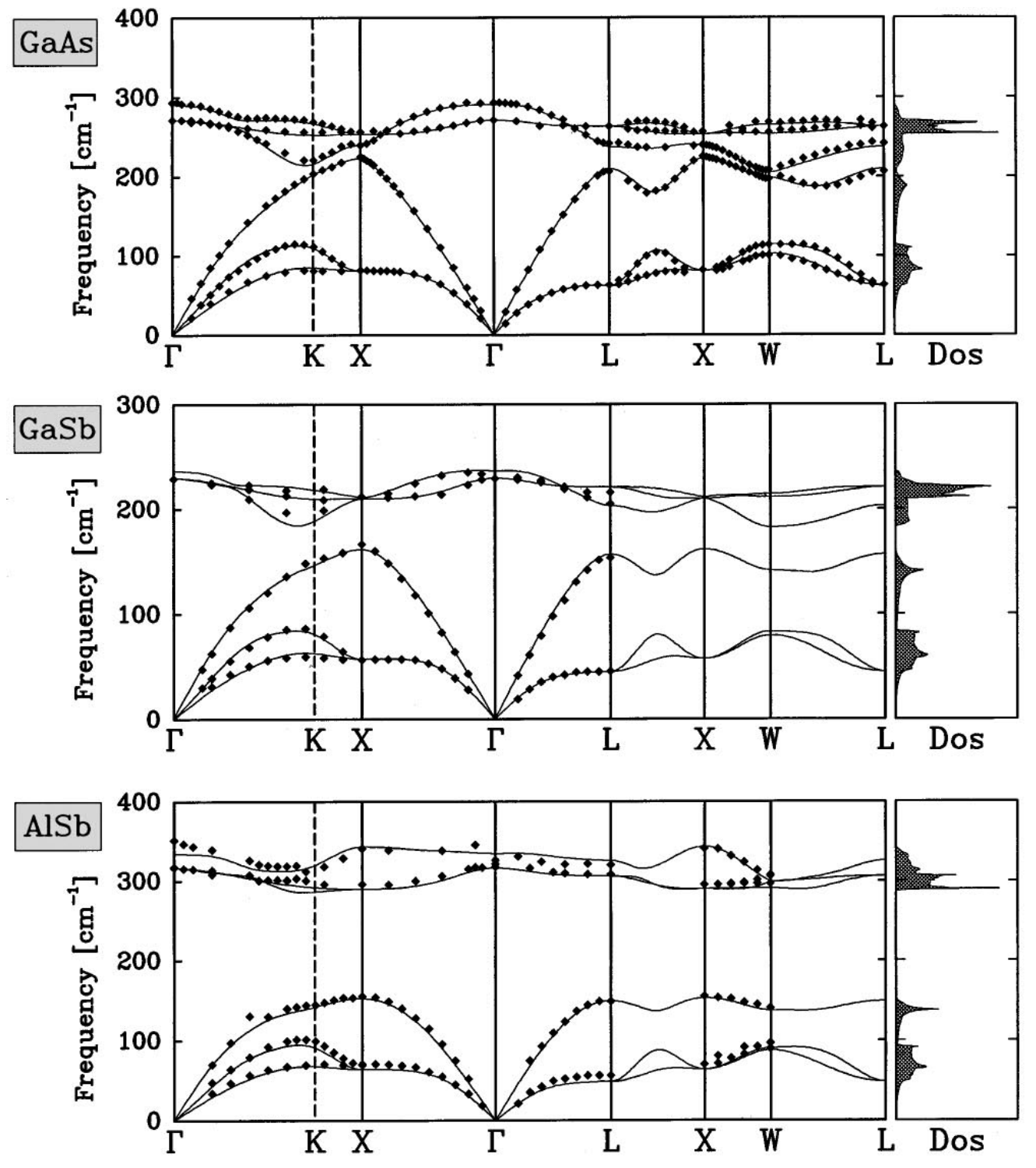
arXiv preprint arXiv:2506.14665

# Success of Density Functional Theory

from X ray experiment      DFT calculation (PBE)

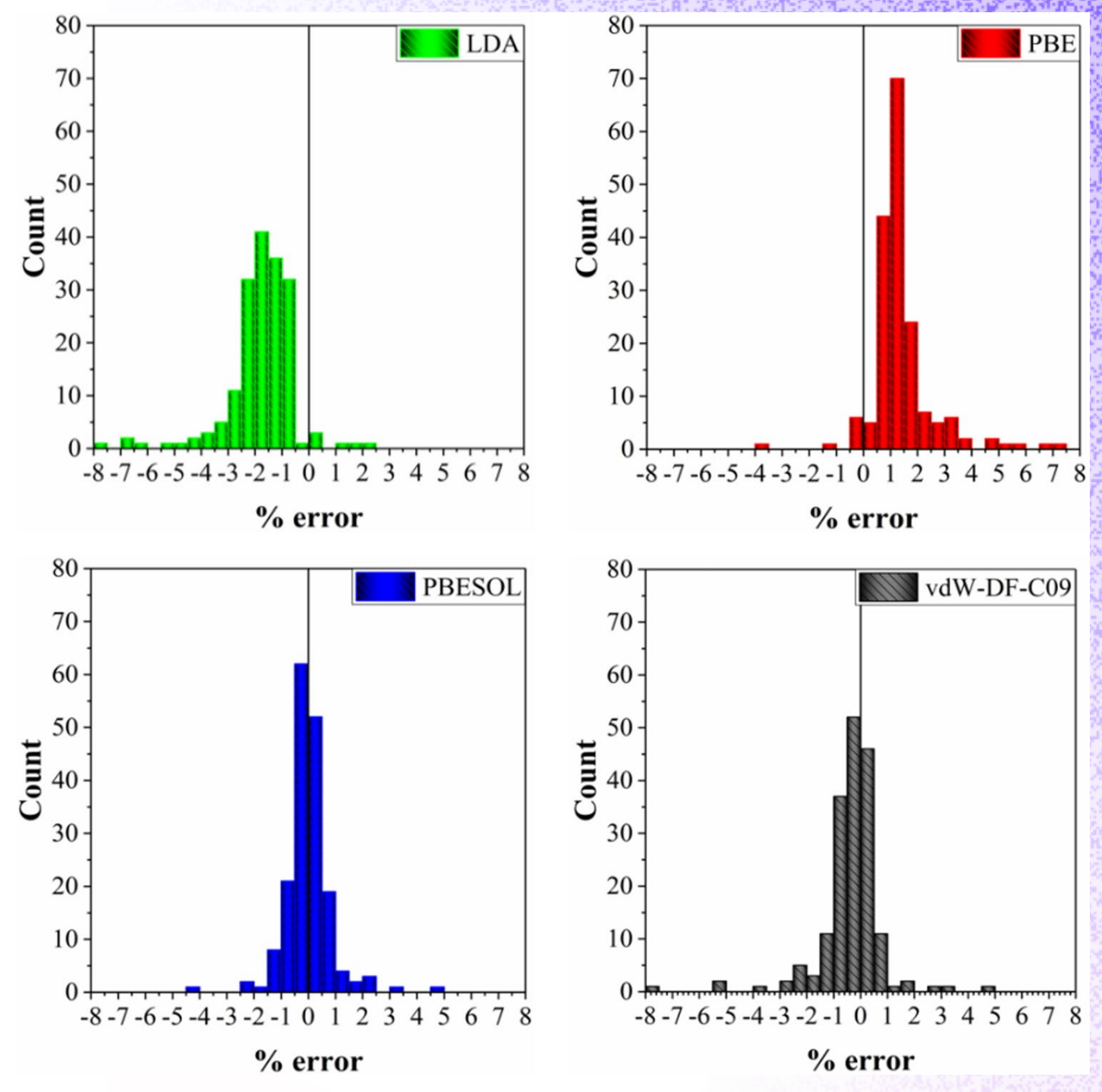


B. Guillot et al. J. Phys. Chem. B 107, 9109 ( 2003)



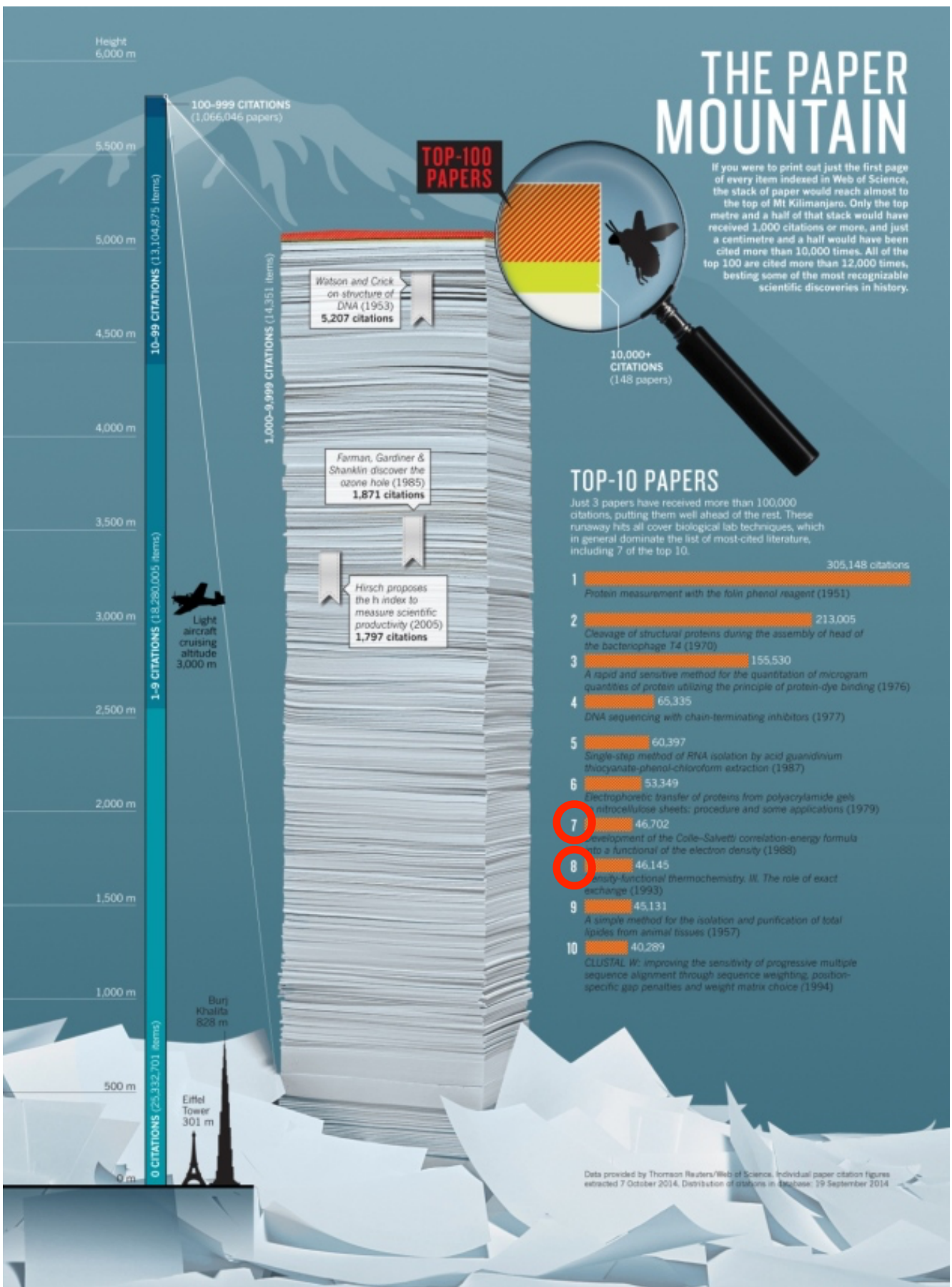
Giannozzi, P., S. de Gironcoli, P. Pavone, and S. Baroni, Phys. Rev. B 43, 7231 (1991)

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)

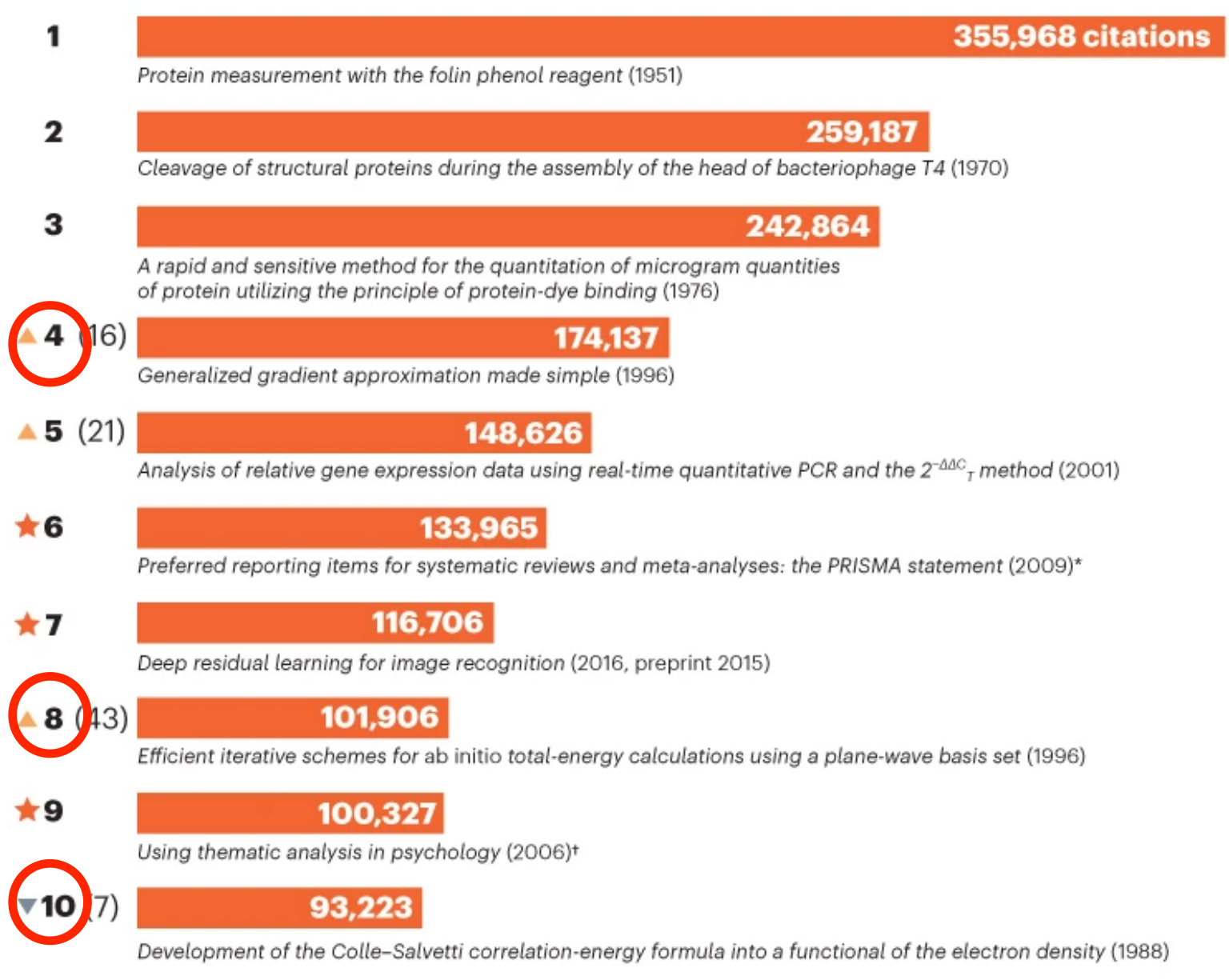
# Impact of Density Functional Theory



Nature News 514, 550 (2014)

**TOP TEN CITED PAPERS**

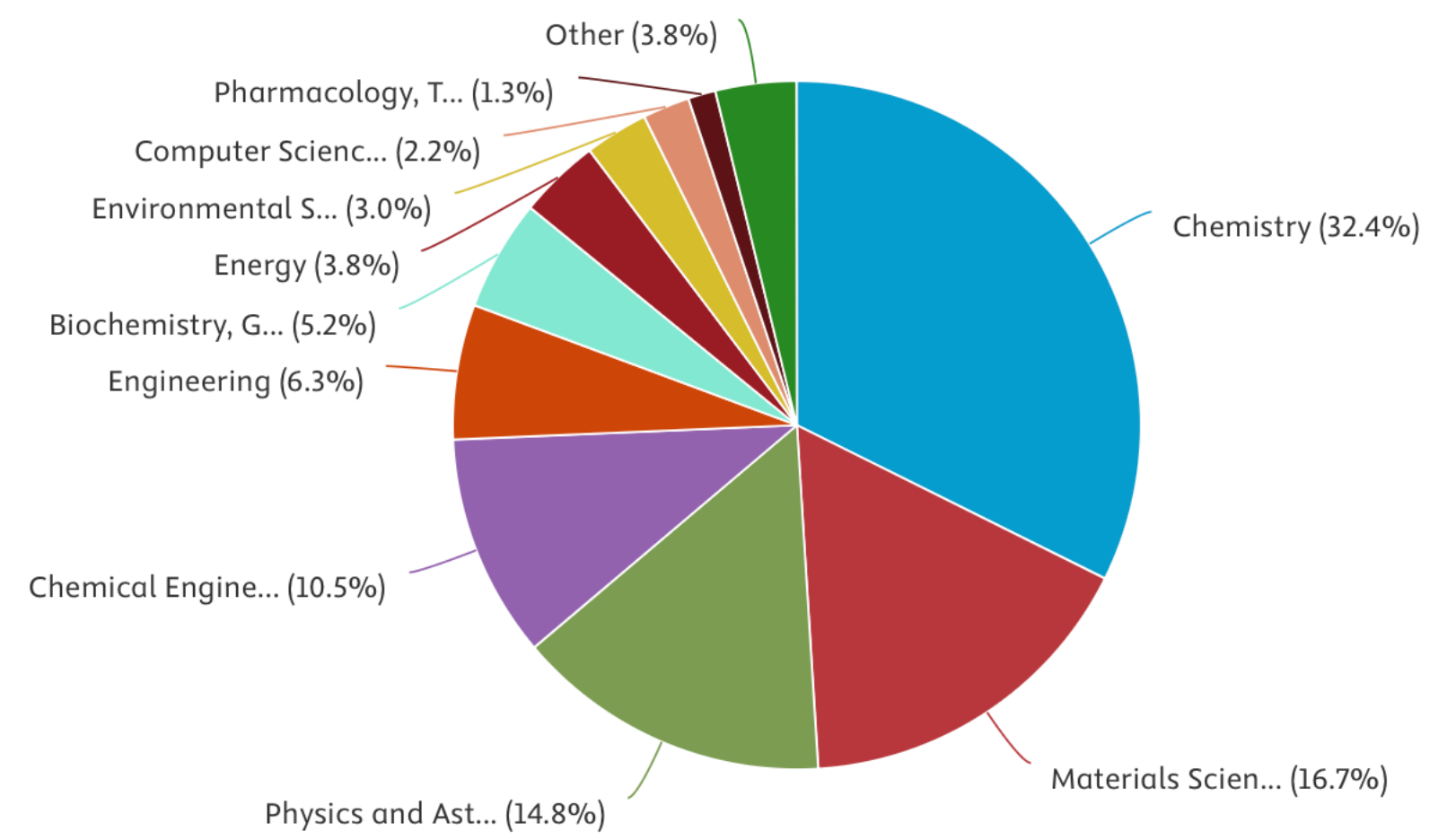
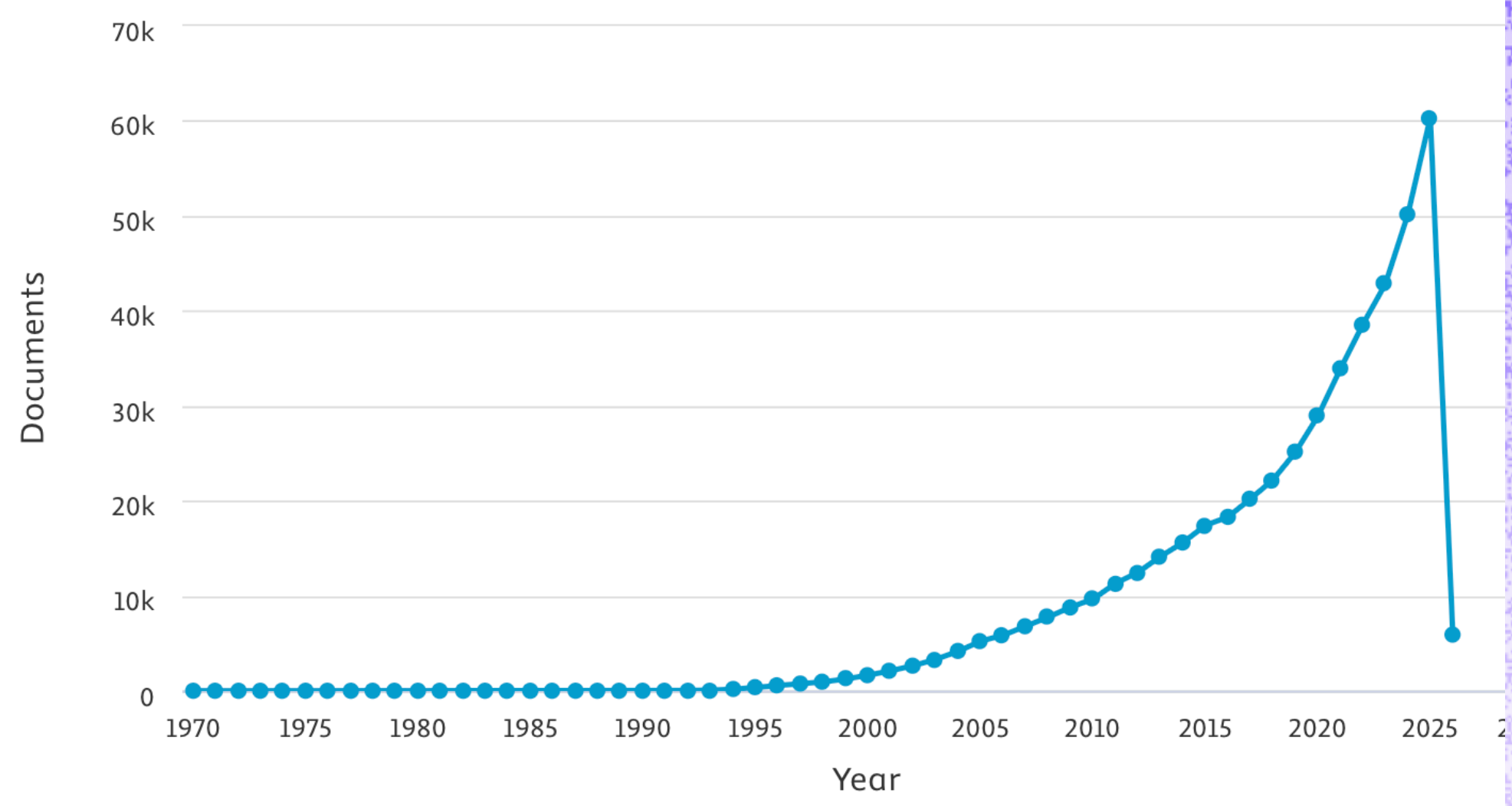
Just 3 papers have more than 200,000 citations each, according to the Web of Science database. All three cover biological laboratory techniques. This update to a 2014 list of most-cited articles shows that the top three papers remain unchanged. But there have been shifts in the positions of others (triangles), 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](http://go.nature.com/425g9dn)).



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.

Nature 640, 591 (2025)

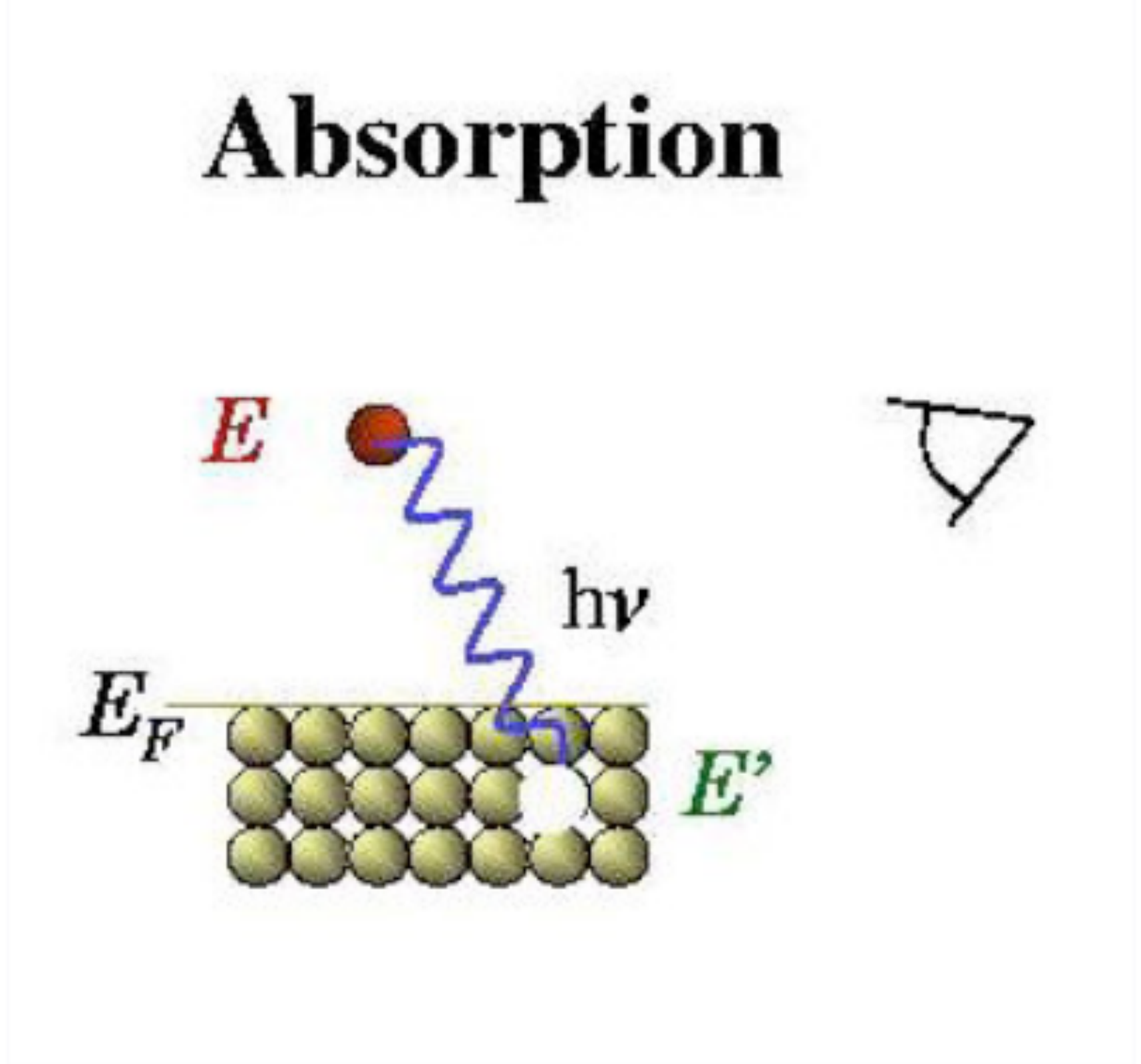
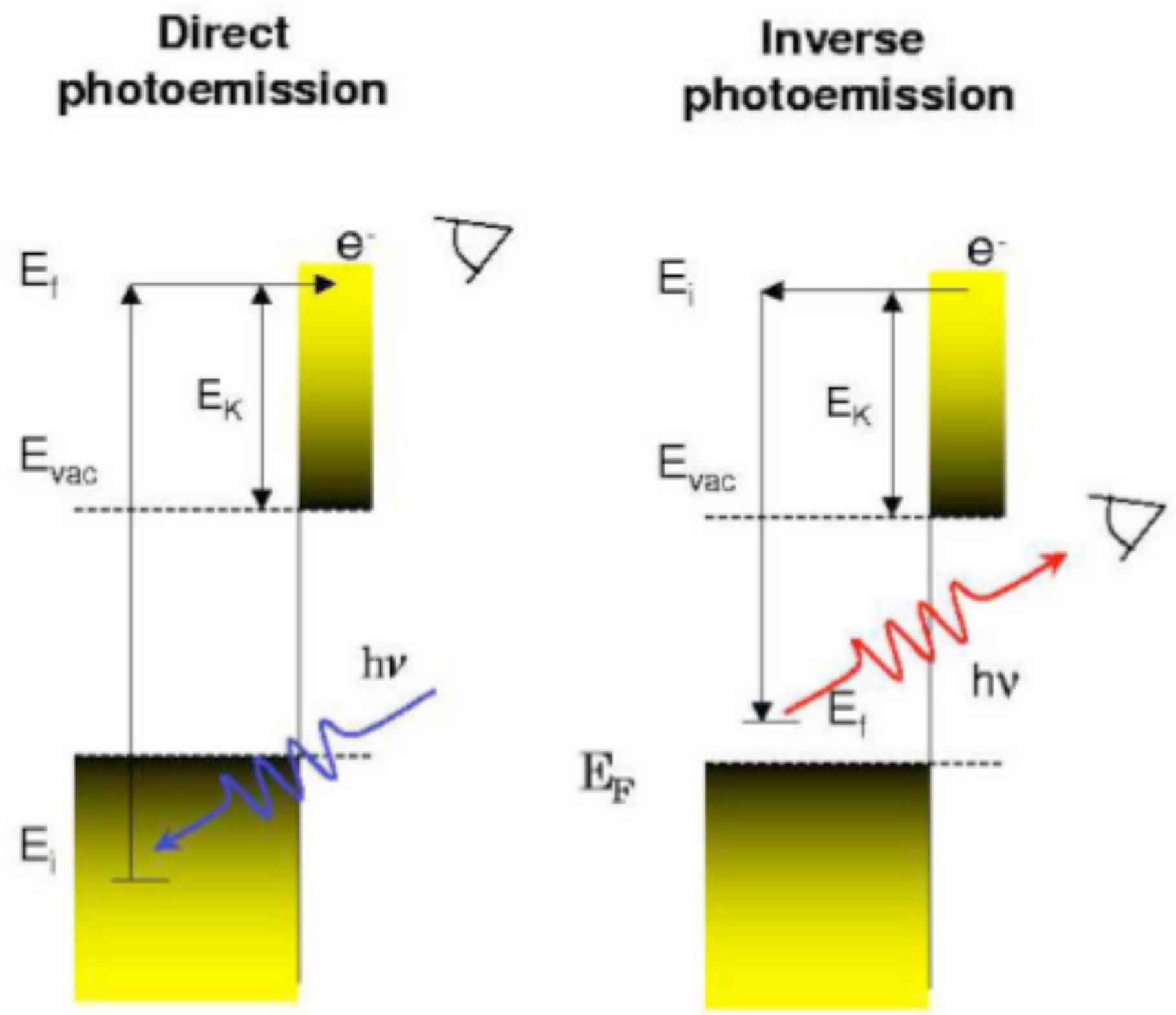
## Documents by year



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

Online Computational Spectroscopy: Hands-on Many Body Calculation with the Yambo code. 5-7 May 2026

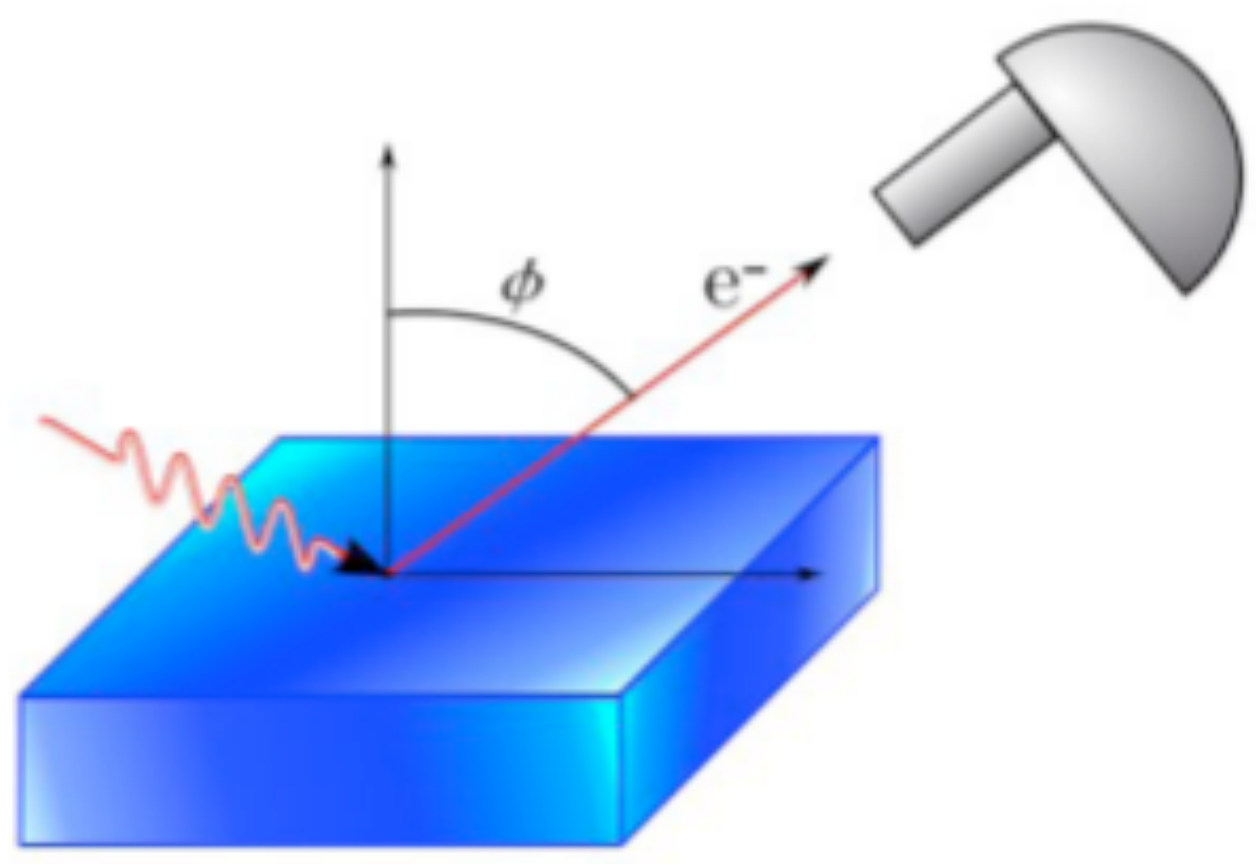
# Excited states of Materials: Spectroscopy



**Charged excitations:** photoemission and inverse photoemission

**Neutral excitations:** absorption

# Excited states of Materials: Direct Photoemission

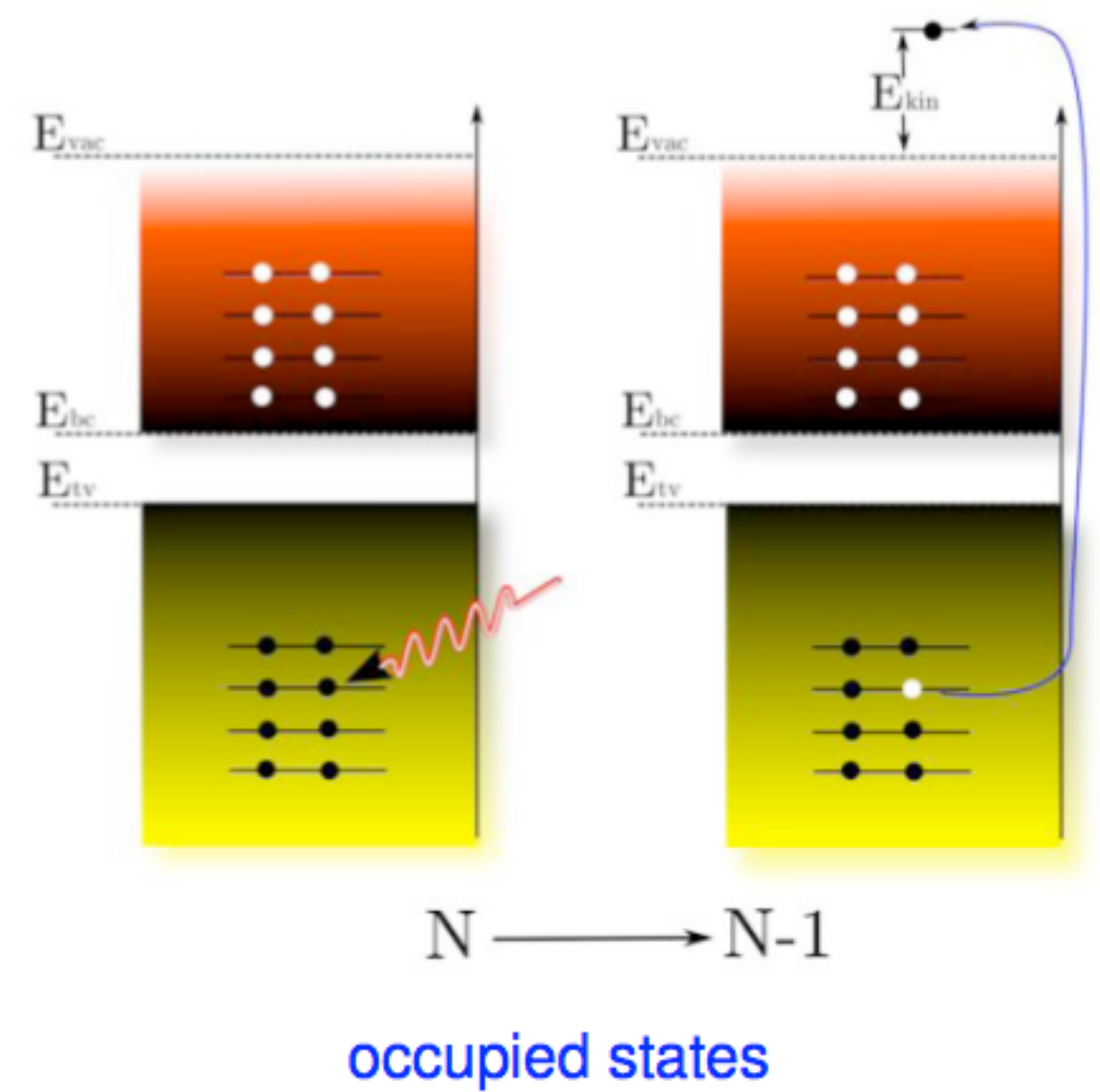


$$E(N) + h\nu = E(N-1) + [\Phi_W + E_{kin}]$$

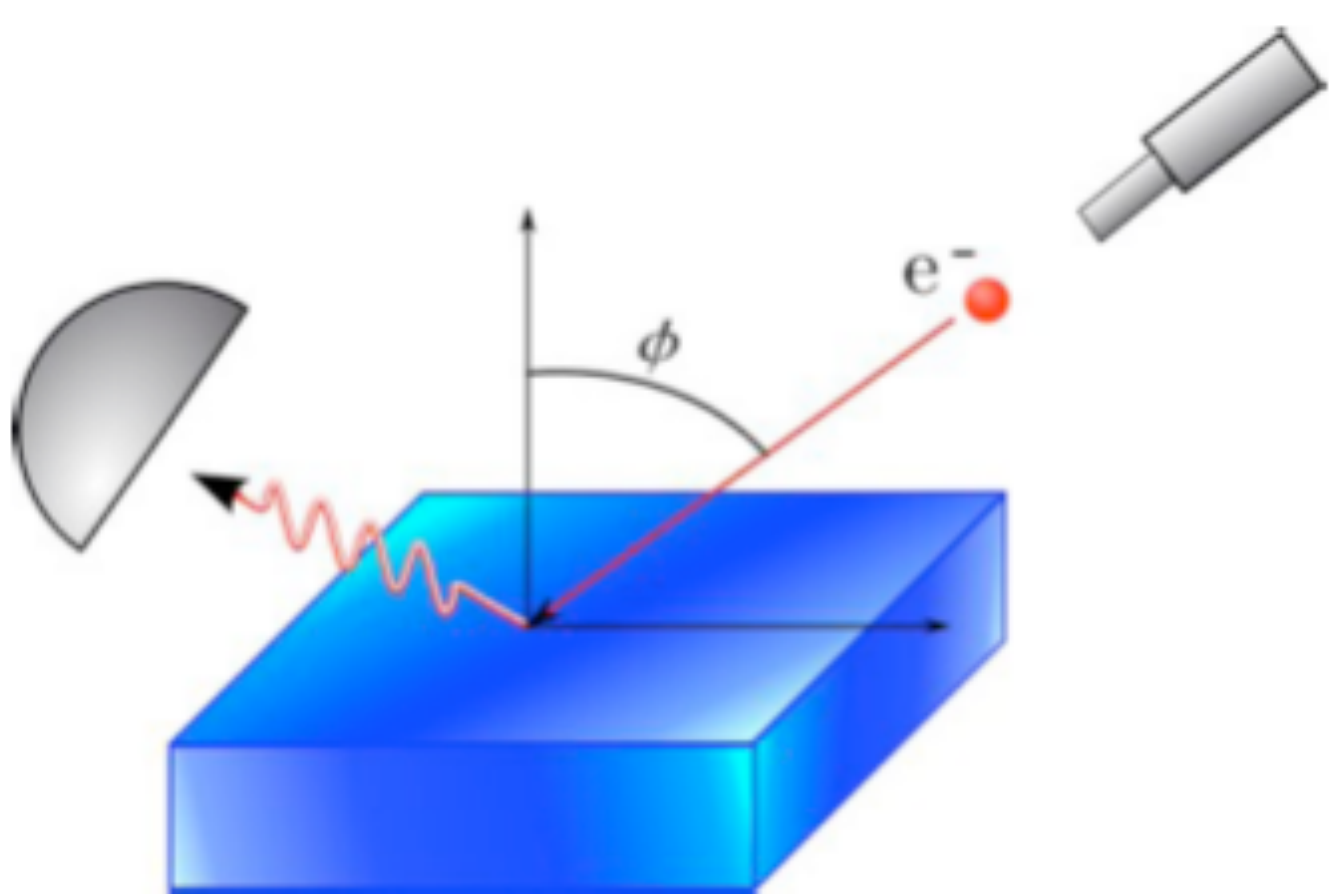
$$E(N) - E(N-1) = [\Phi_W + E_{kin}] - h\nu$$

...plus momentum conservation  $\Rightarrow$  ARPES

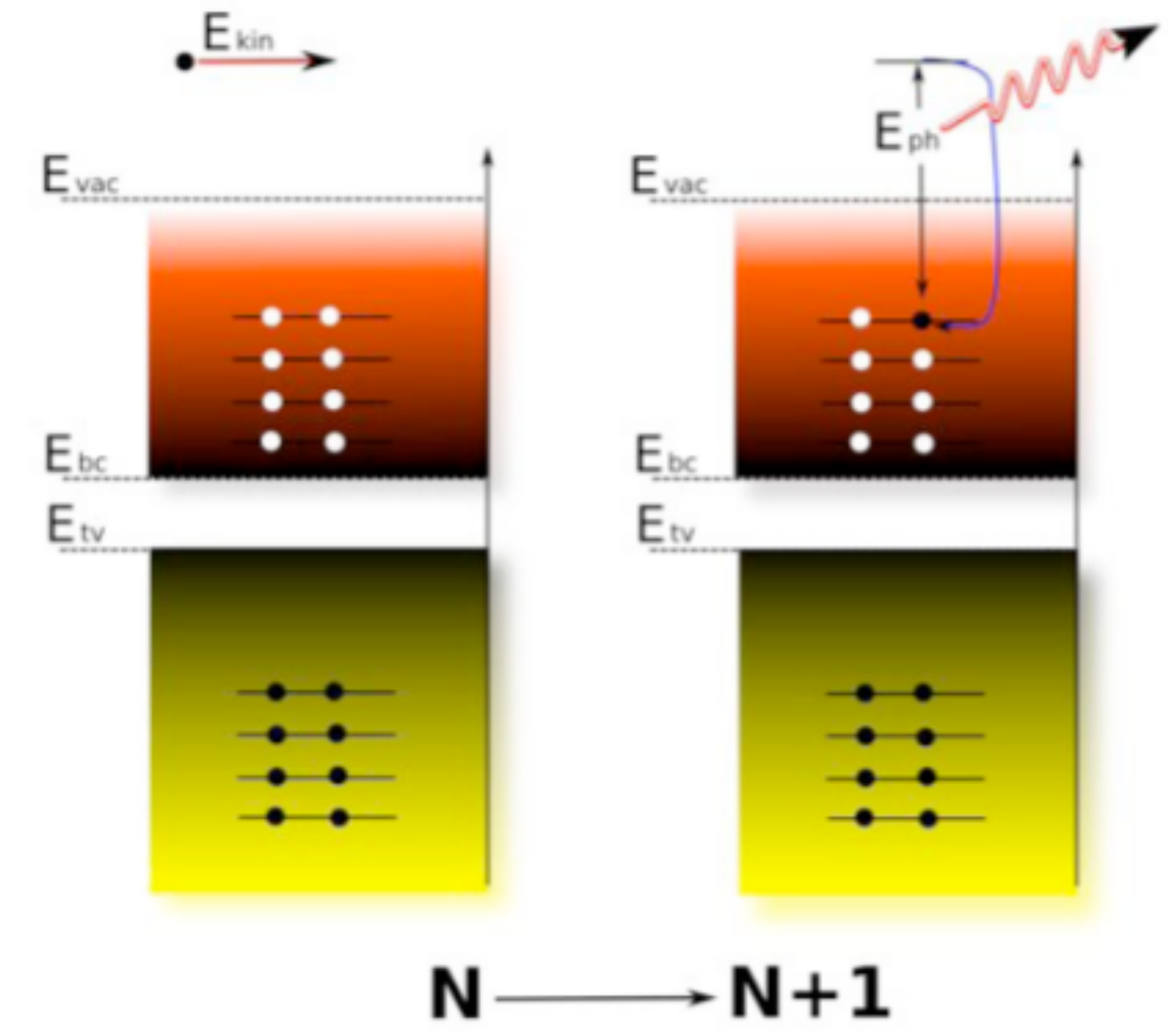
Measure the density of occupied states



# Excited states of Materials: Inverse Photoemission



electron in - photon out

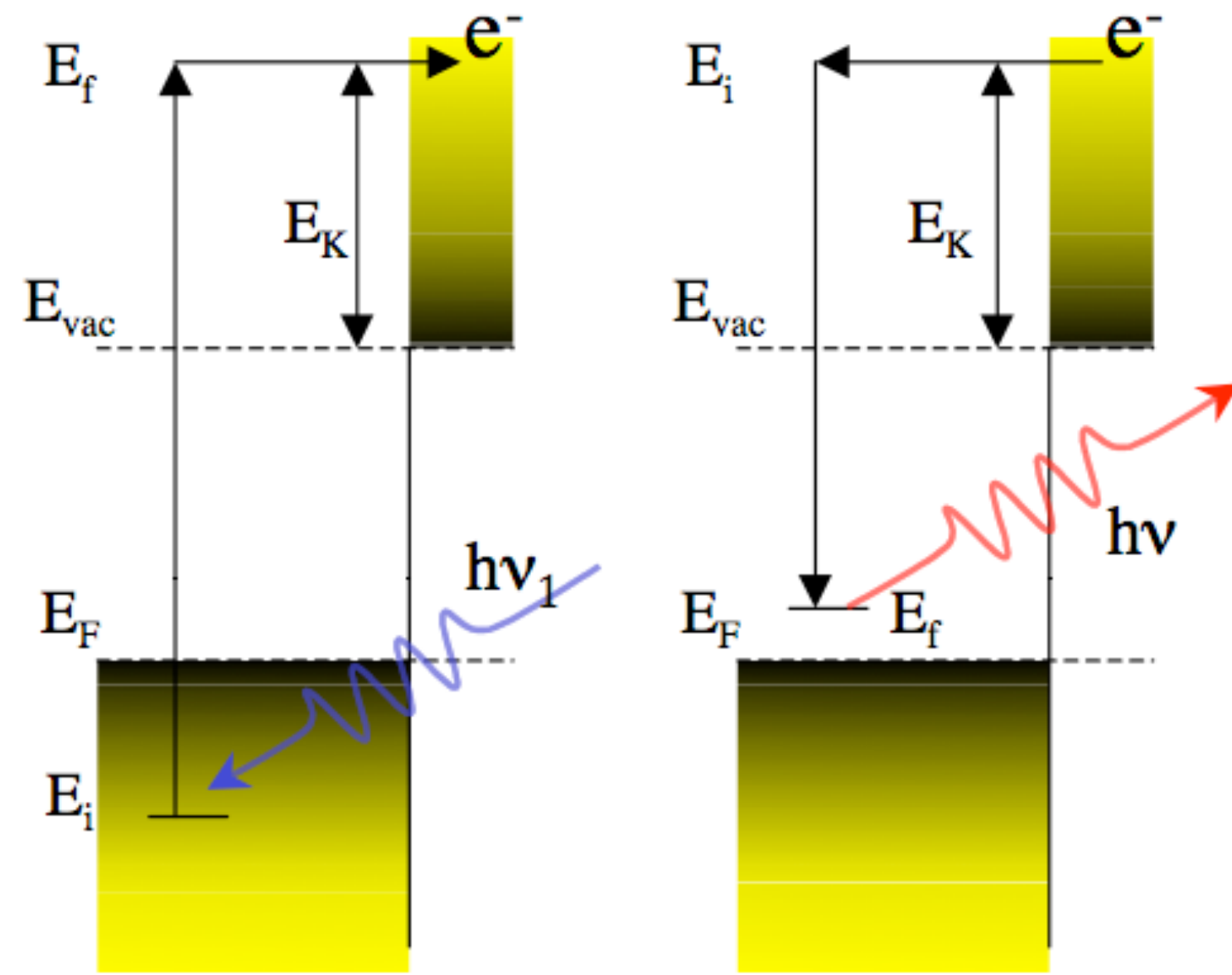


empty states

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

Measure the density of unoccupied 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

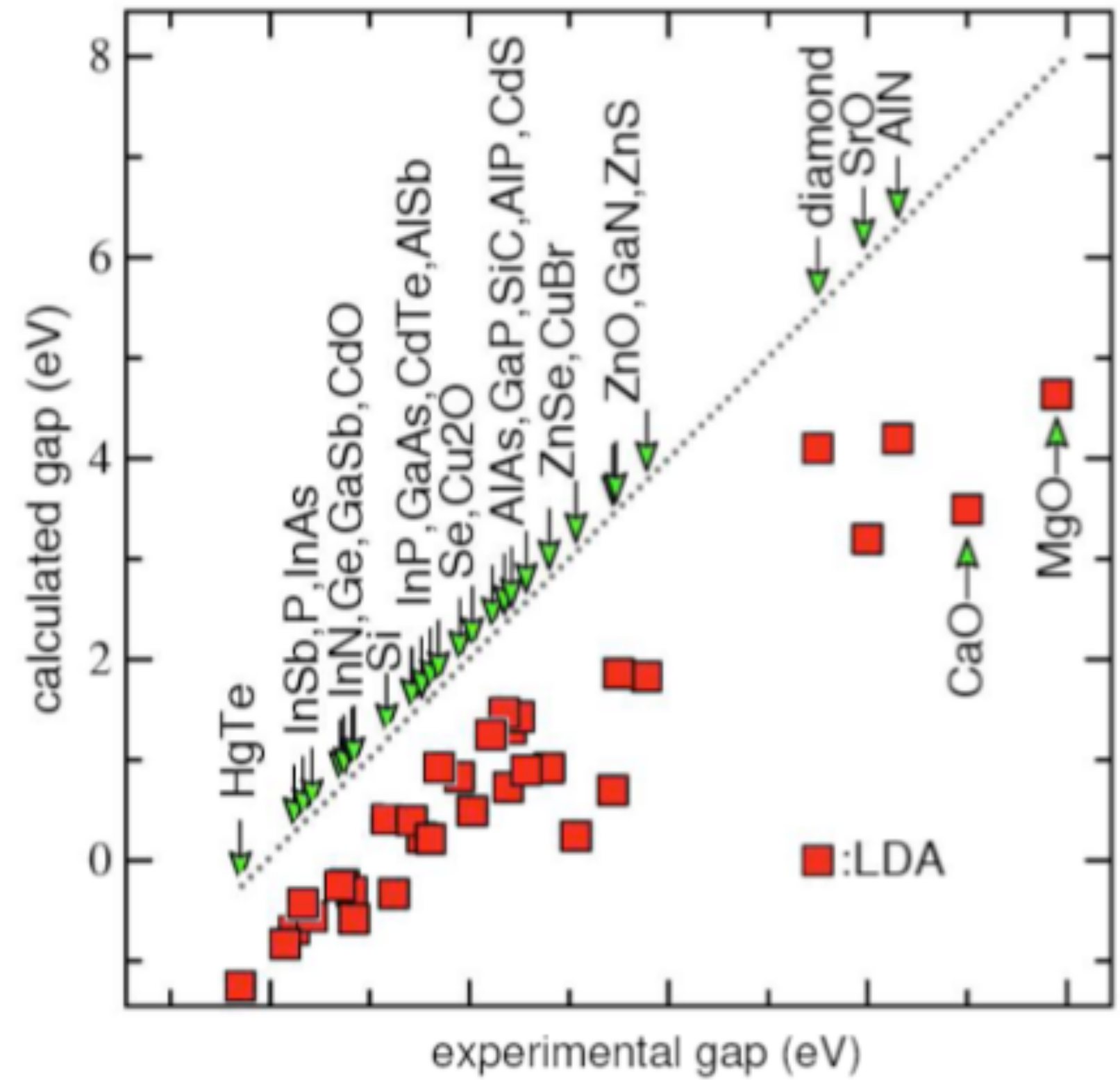
## Inverse photoemission

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

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

$$E_{gap} = \underbrace{(E_{N+1} - E_N)}_{\text{electron affinity}} - \underbrace{(E_N - E_{N-1})}_{\text{ionization potential}}$$

# Excited states of Materials: The Band Gap Problem



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

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

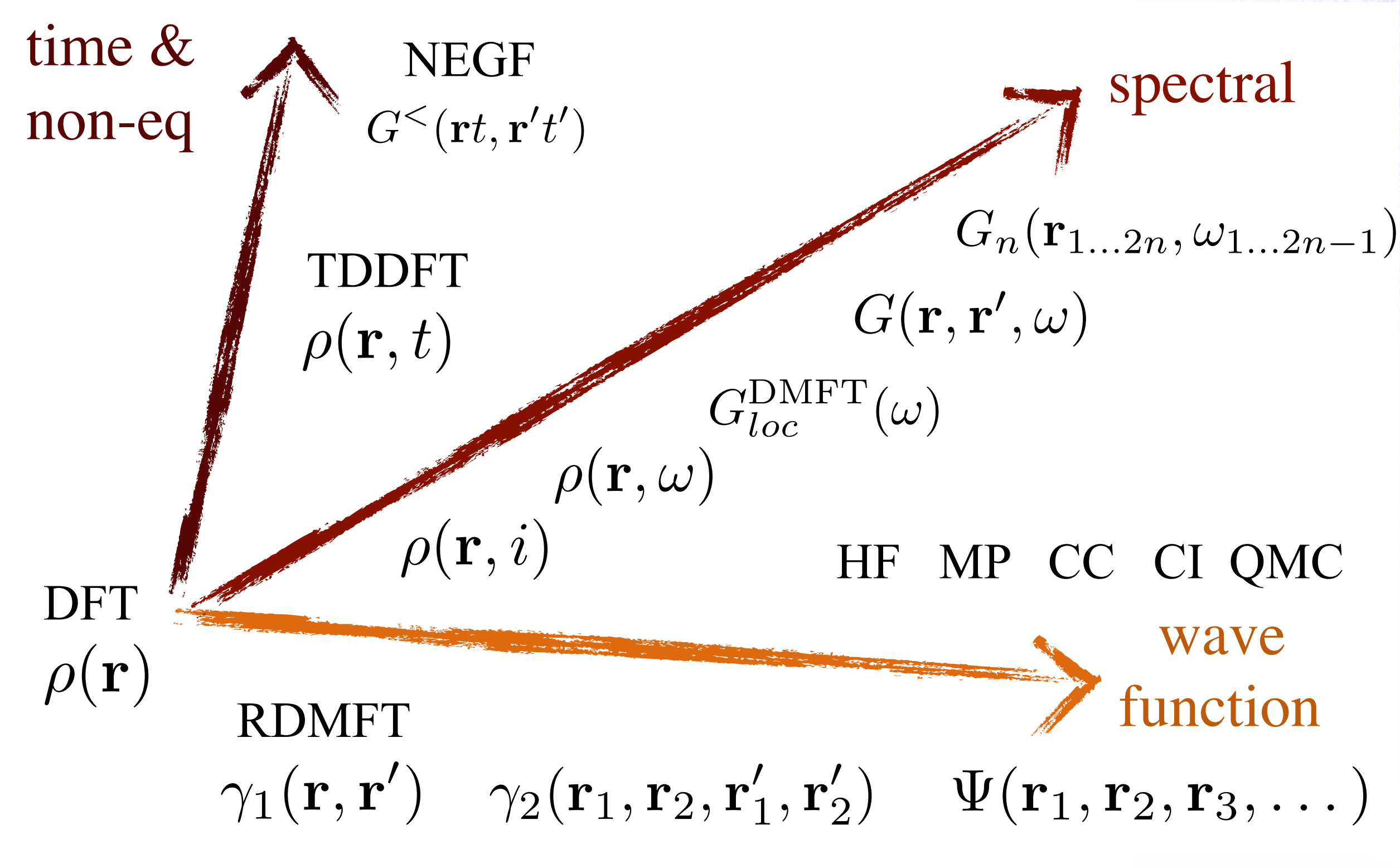
Adapted from M. van Schilfgaarde *et al.* PRL **96** (2006)

## Huge discrepancy not due to the LDA

# Excited states of Materials: Theoretical spectroscopy

The zoo of computational methods.

Accuracy and computational cost

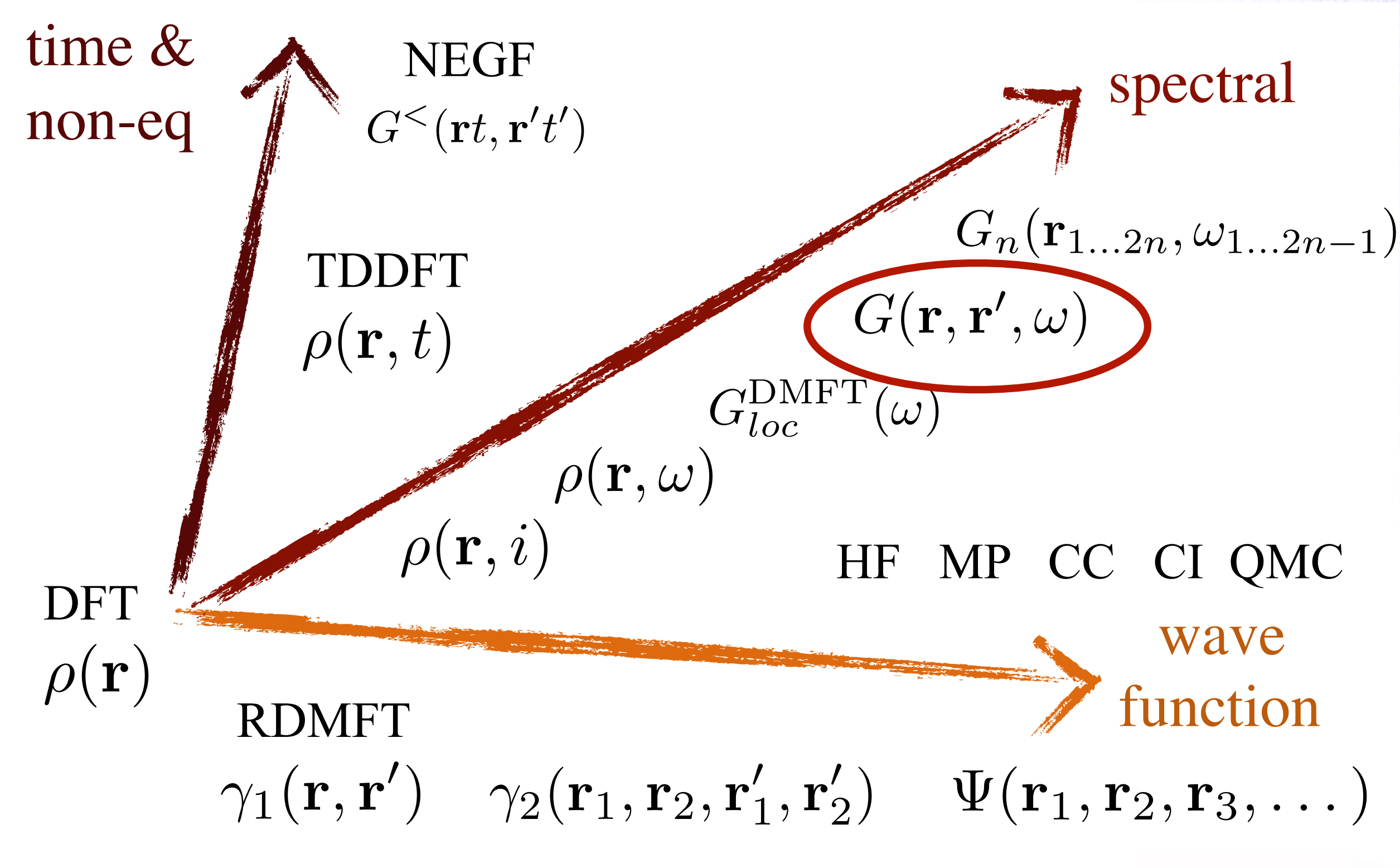


N. Marzari, A. Ferretti and C. Wolverton Nature Materials, 20, 736 (2021)

# Excited states of Materials: Theoretical spectroscopy

The zoo of computational methods.

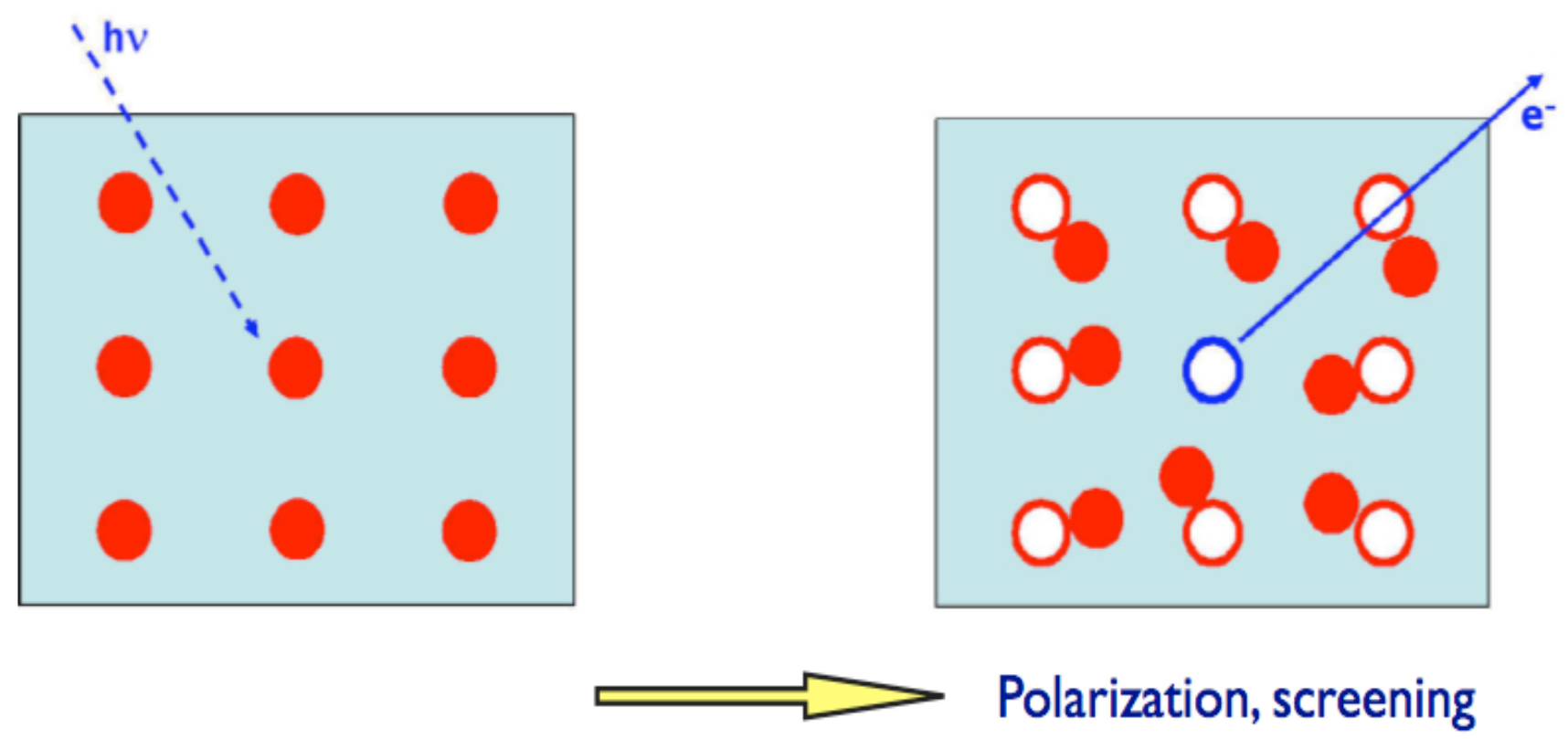
Accuracy and computational cost



N. Marzari, A. Ferretti and C. Wolverton Nature Materials, 20, 736 (2021)

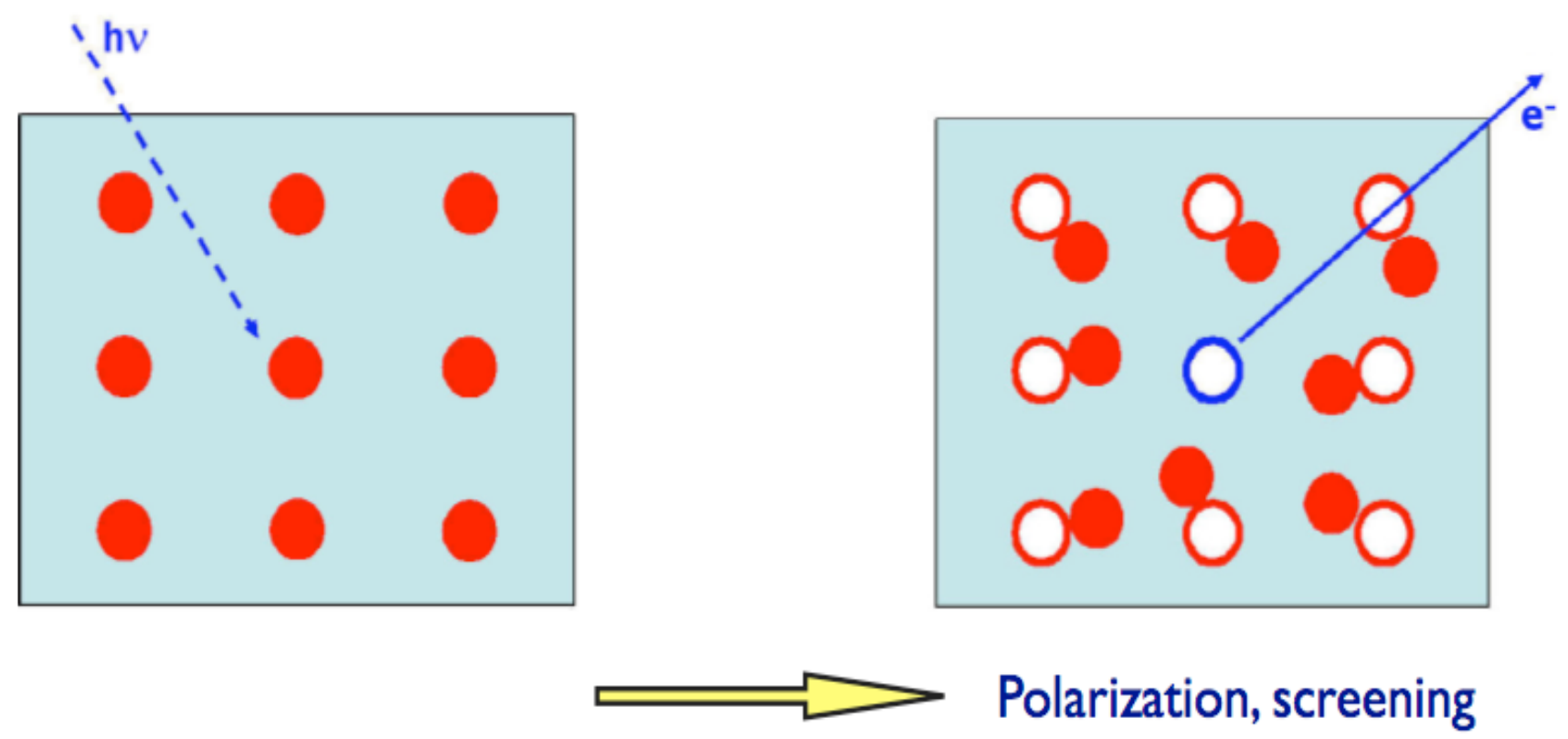
# Excited states of Materials: The Quasiparticle

$$E_{gap} = \underbrace{(E_{N+1} - E_N)}_{\text{electron affinity}} - \underbrace{(E_N - E_{N-1})}_{\text{ionization potential}}$$



# Excited states of Materials: The Quasiparticle

$$E_{gap} = \underbrace{(E_{N+1} - E_N)}_{\text{electron affinity}} - \underbrace{(E_N - E_{N-1})}_{\text{ionization potential}}$$



**Electron injection**  
Repulsive Coulomb interaction creates a repulsive Coulomb hole around the the additional electrons

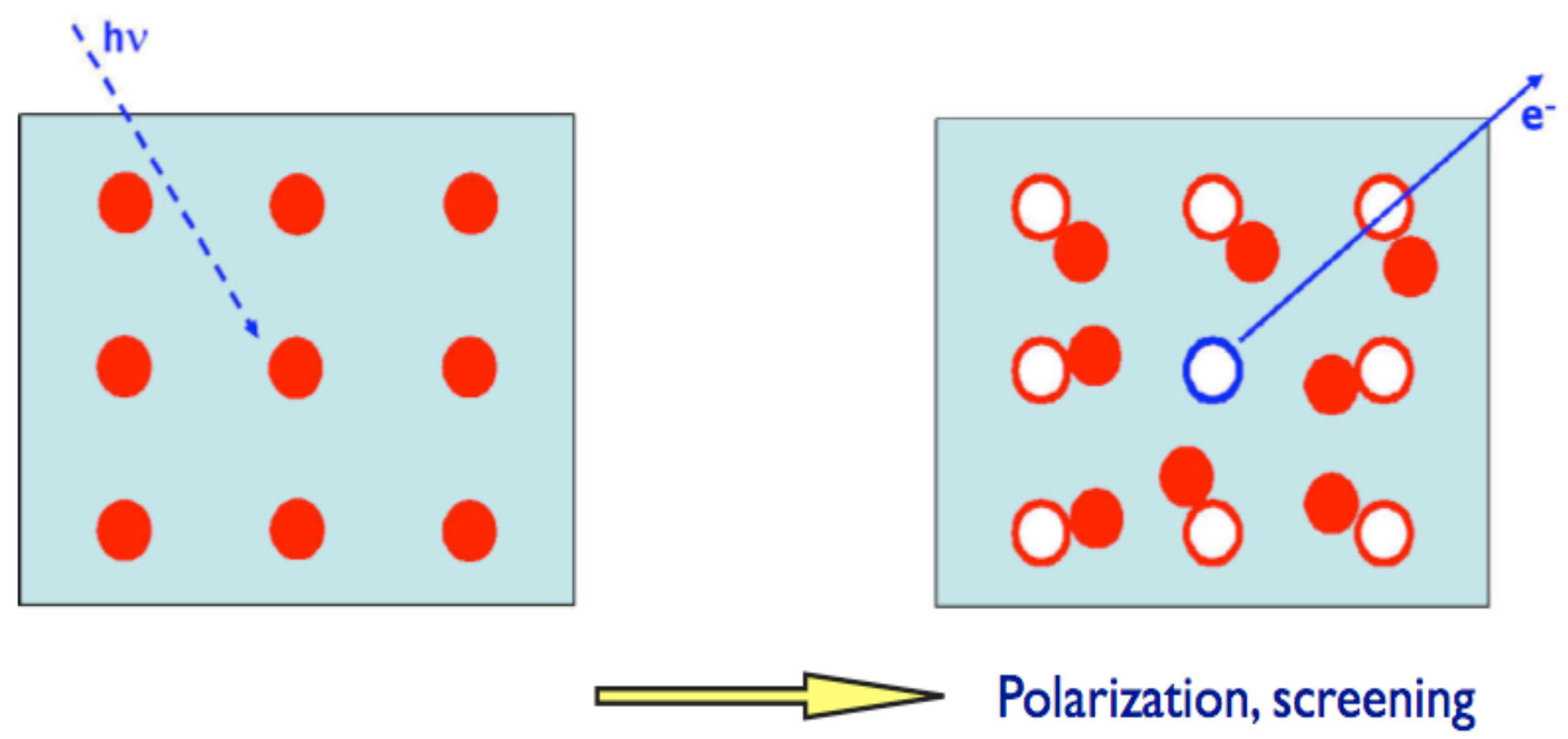
**Direct photemission**  
an electron leaves the system: also the Coulomb hole disappear

**Relaxation - Screening - Correlation**

# Excited states of Materials: The Quasiparticle

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

electron affinity
ionization potential

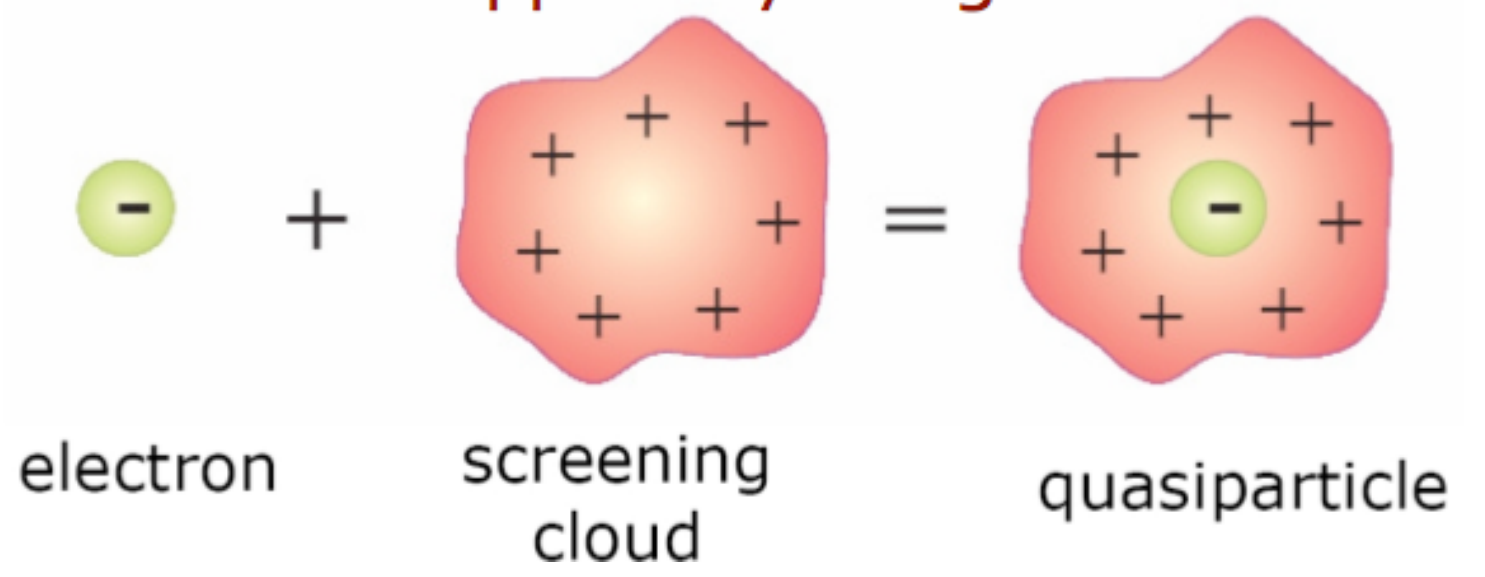


**Electron injection**  
 Repulsive Coulomb interaction creates a repulsive Coulomb hole around the the additional electrons

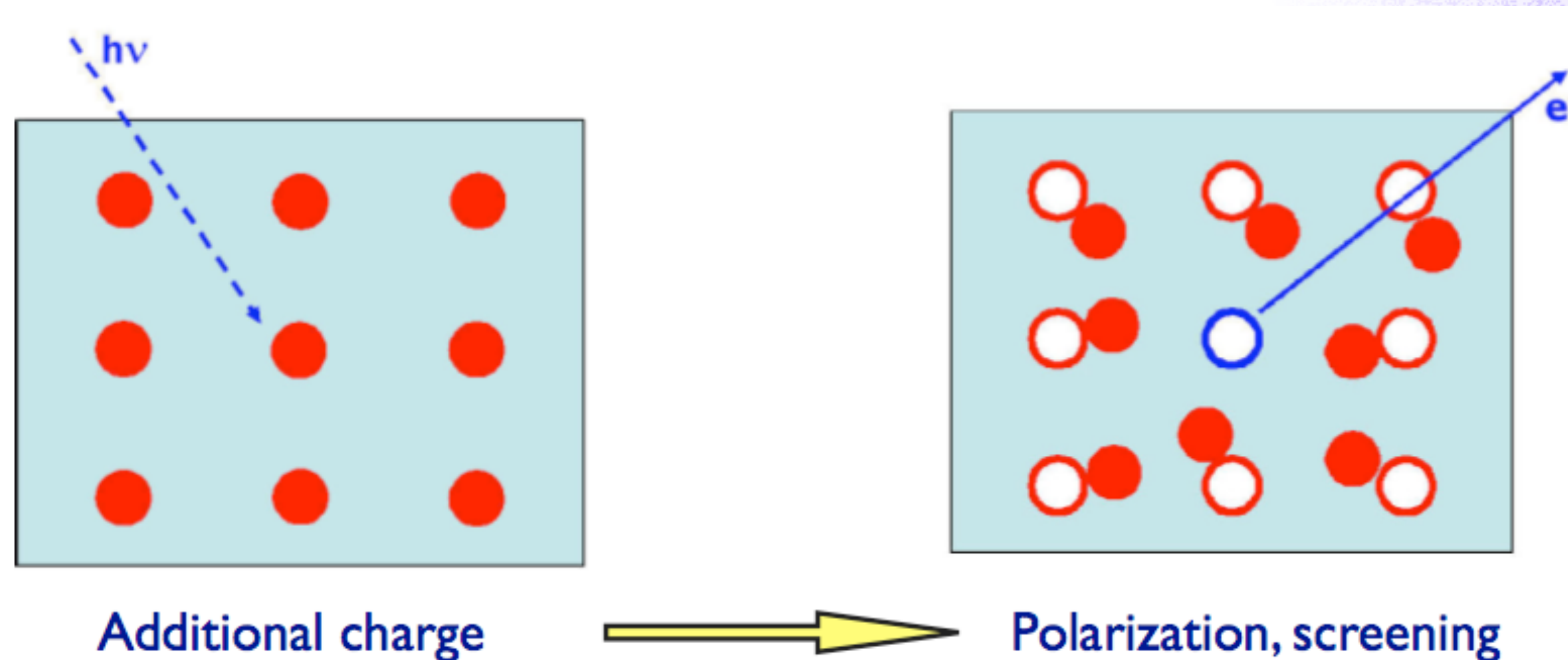
**Direct photemission**  
 an electron leaves the system: also the Coulomb hole disappear

**Relaxation - Screening - Correlation**

Relative to the ground- state N-electron system, the addition (removal) of an electron in indirect (direct) photoemission hence creates (annihilates) an ensemble consisting of the bare electron and its oppositely charges Coulomb hole.



# The Green Function



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

## Many Body Perturbation Theory

$$G(\mathbf{r}t, \mathbf{r}'t')$$

Green Function as a  
central variable

Contains the excitation energy  $\epsilon_i$   
excitation lifetime  
ground state density

expectation value one-particle operator, Total Energy etc.

# The Green Function

Definition and meaning of G

$$G^e(\mathbf{r}_1 t_1, \mathbf{r}_2 t_2)$$

**probability amplitude** for the propagation of an **additional electron** from  $(\mathbf{r}_2, t_2)$  to  $(\mathbf{r}_1, t_1)$   
in a many body electron system with interacting H

$$\hat{H} = \int d\mathbf{r} \hat{\psi}^\dagger(\mathbf{r}) \hat{T}(\mathbf{r}) \hat{\psi}(\mathbf{r}) + \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') V(\mathbf{r}, \mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r})$$

$$G^e(\mathbf{r}_1 t_1, \mathbf{r}_2 t_2) =$$

# The Green Function

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$$G^e(\mathbf{r}_1 t_1, \mathbf{r}_2 t_2) = \langle \Psi_0^N(t_2) |$$

# The Green Function

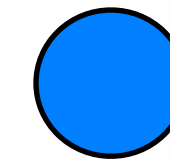
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$(\mathbf{r}_2, t_2)$



$$G^e(\mathbf{r}_1 t_1, \mathbf{r}_2 t_2) = \hat{\psi}^\dagger(\mathbf{r}_2) |\Psi_0^N(t_2)\rangle$$

# The Green Function

Definition and meaning of G

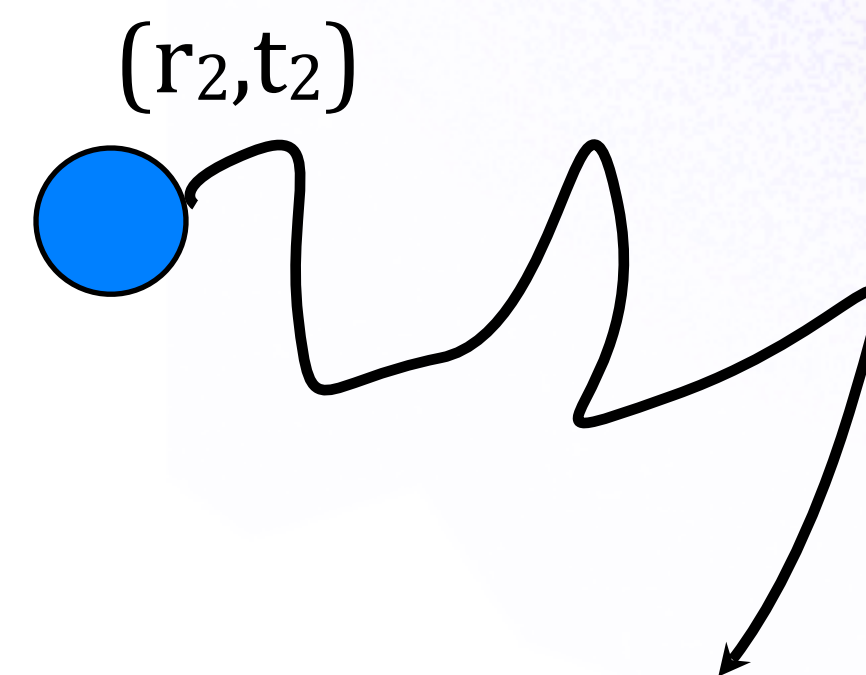
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$$G^e(\mathbf{r}_1 t_1, \mathbf{r}_2 t_2) = U(t_1, t_2) \hat{\psi}^\dagger(\mathbf{r}_2) |\Psi_0^N(t_2)\rangle$$

$$\hat{U}(t_1, t_2) = e^{\frac{-i}{\hbar} \hat{H}(t_1 - t_2)} \quad t_1 > t_2$$



# The Green Function

Definition and meaning of G

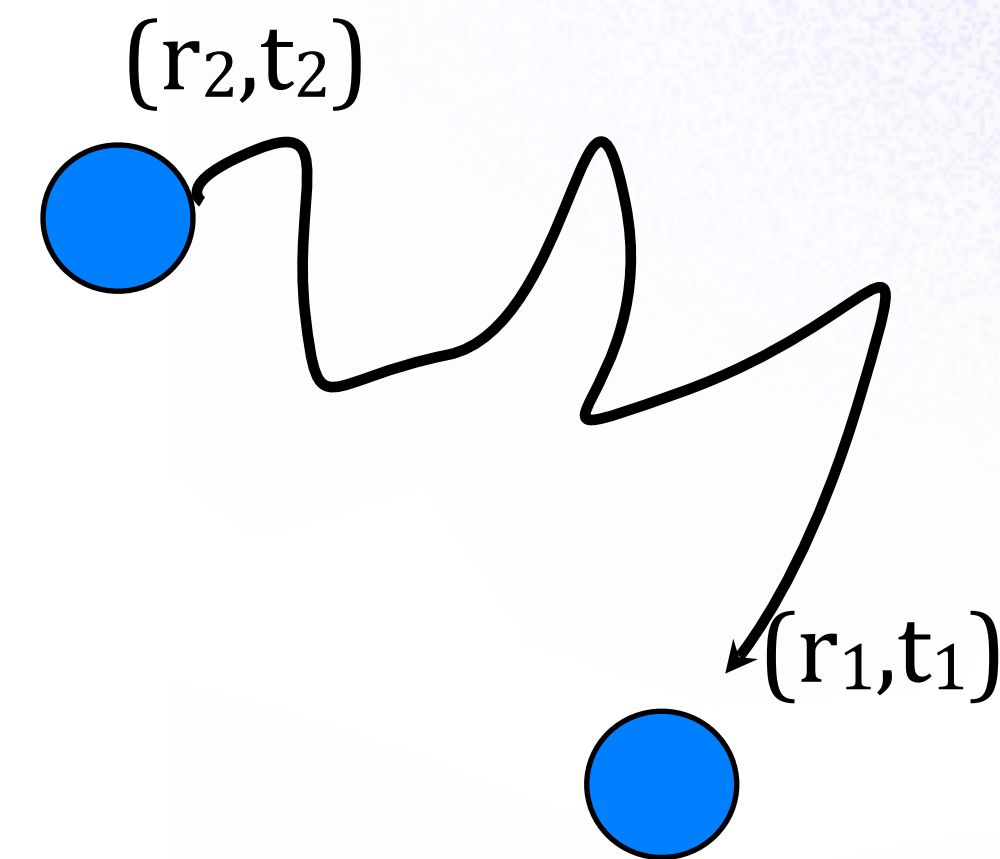
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# The Green Function

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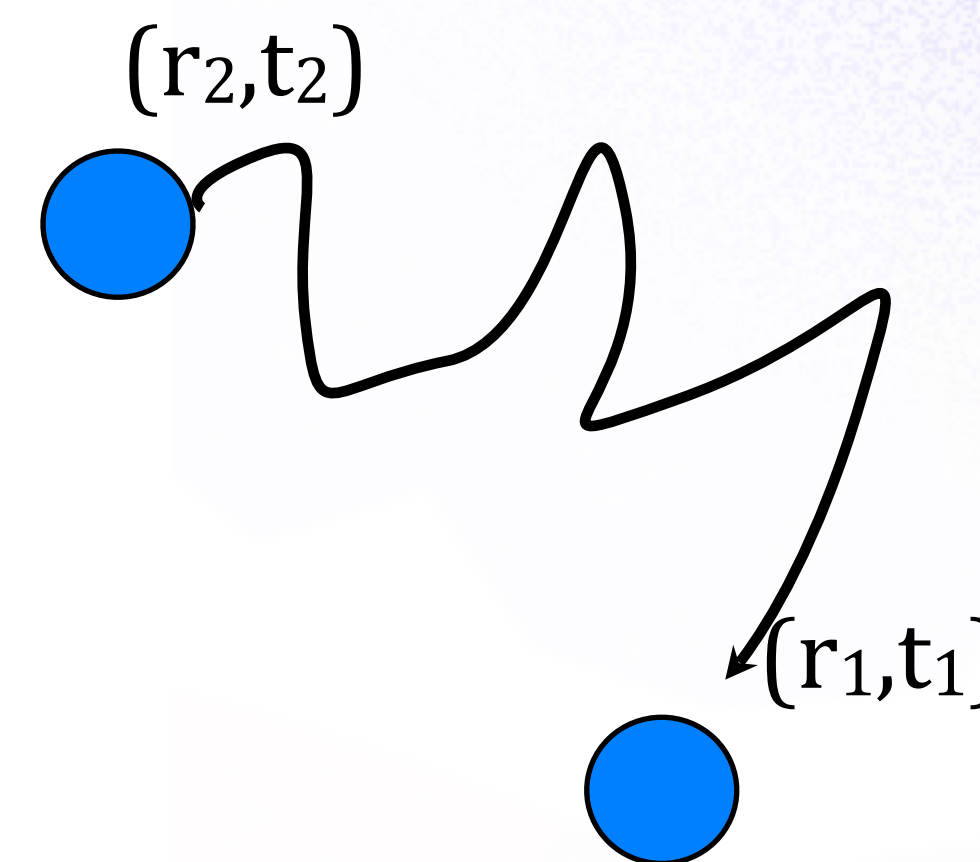
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$$G^e(\mathbf{r}_1 t_1, \mathbf{r}_2 t_2) = -\frac{i}{\hbar} \langle \Psi_0^N | \hat{\psi}(\mathbf{r}_1, t_1) \hat{\psi}^\dagger(\mathbf{r}_2, t_2) | \Psi_0^N \rangle \theta(t_1 - t_2)$$

# The Green Function

Similarly for an hole propagation

$$G^h(\mathbf{r}_2 t_2, \mathbf{r}_1 t_1) = -\frac{i}{\hbar} \langle \Psi_0^N | \hat{\psi}^\dagger(\mathbf{r}_2, t_2) \hat{\psi}(\mathbf{r}_1, t_1) | \Psi_0^N \rangle \theta(t_2 - t_1)$$

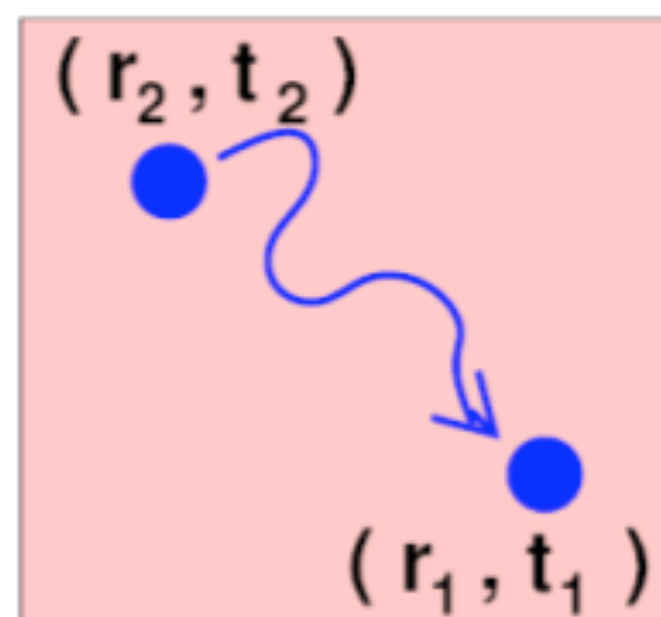
We define G as:

Time-ordered Green Function

$$G(\mathbf{r}_1 t_1, \mathbf{r}_2 t_2) = G^e(\mathbf{r}_1 t_1, \mathbf{r}_2 t_2) - G^h(\mathbf{r}_2 t_2, \mathbf{r}_1 t_1) = -\frac{i}{\hbar} \langle \Psi_0^N | \hat{T}[\hat{\psi}(\mathbf{r}_1, t_1) \hat{\psi}^\dagger(\mathbf{r}_2, t_2)] | \Psi_0^N \rangle$$

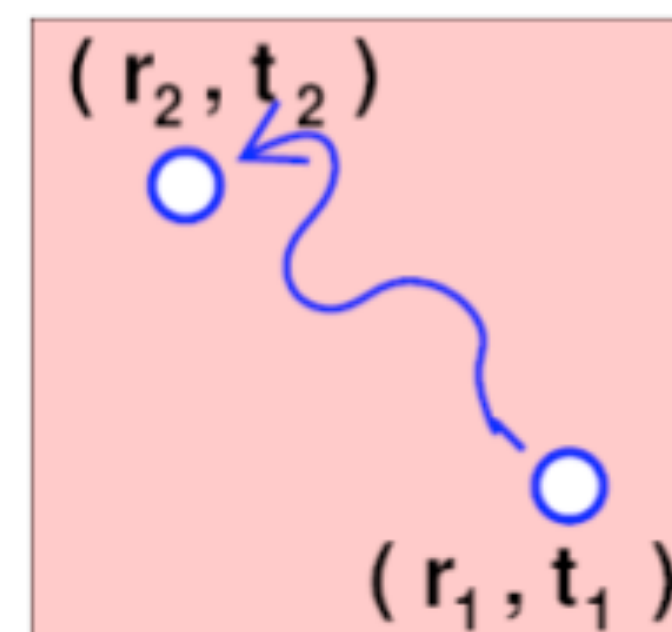
$$t_1 > t_2$$

$$\langle \Psi_0^N | \hat{\psi}(\mathbf{r}_1, t_1) \hat{\psi}^\dagger(\mathbf{r}_2, t_2) | \Psi_0^N \rangle$$



$$t_1 < t_2$$

$$-\langle \Psi_0^N | \hat{\psi}^\dagger(\mathbf{r}_2, t_2) \hat{\psi}(\mathbf{r}_1, t_1) | \Psi_0^N \rangle$$



# The Green Function

$$G(\mathbf{r}_1 t_1, \mathbf{r}_2 t_2) = -i \sum_i f_j(\mathbf{r}_1) f_j^*(\mathbf{r}_2) e^{-i\epsilon_j(t_1 - t_2)} \left[ \theta(t_1 - t_2) \theta(\epsilon_j - \mu) - \theta(t_2 - t_1) \theta(\mu - \epsilon_j) \right]$$

Fourier Transforming in frequency domain:

$$G(\mathbf{r}_1, \mathbf{r}_2, \omega) = \sum_j \frac{f_j(\mathbf{r}_1) f_j^*(\mathbf{r}_2)}{\omega - \epsilon_j + i\eta \operatorname{sgn}(\epsilon_j - \mu)}$$

$$\epsilon_j = \begin{cases} E(N+1, j) - E(N) & \epsilon_j > \mu \\ E(N) - E(N-1, j) & \epsilon_j < \mu \end{cases} \quad f_j(\mathbf{r}_1) = \begin{cases} \langle \Psi_0^N | \hat{\psi}(\mathbf{r}_1) | \Psi_j^{N+1} \rangle & \epsilon_j > \mu \\ \langle \Psi_j^{N-1} | \hat{\psi}(\mathbf{r}_1) | \Psi_0^N \rangle & \epsilon_j < \mu \end{cases}$$

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

How to obtain  $G$ ??

# The Green Function

How to obtain  $G$ ??

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

Let's say we know  $G_0(\omega)$  that corresponds to the Hamiltonian  $H_0$  (e.g. non interacting electrons)

$H = H_0 + H_1$ , where the interaction is put in  $H_1$

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Let's say we know  $G_0(\omega)$  that corresponds to the Hamiltonian  $H_0$  (e.g. non interacting electrons)

$H = H_0 + H_1$ , where the interaction is put in  $H_1$

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 mean field system defined by

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

Introducing the Lehmann representation for  $G$

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

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

QP equation: looks similar to KS equation but:

$\Sigma$  contains many body effects (as  $V_{xc}$ )

$\Sigma$  is not Hermitian, non-local, frequency dependent

$\Sigma$  potential felt by an added (removed) electron to (from) the system

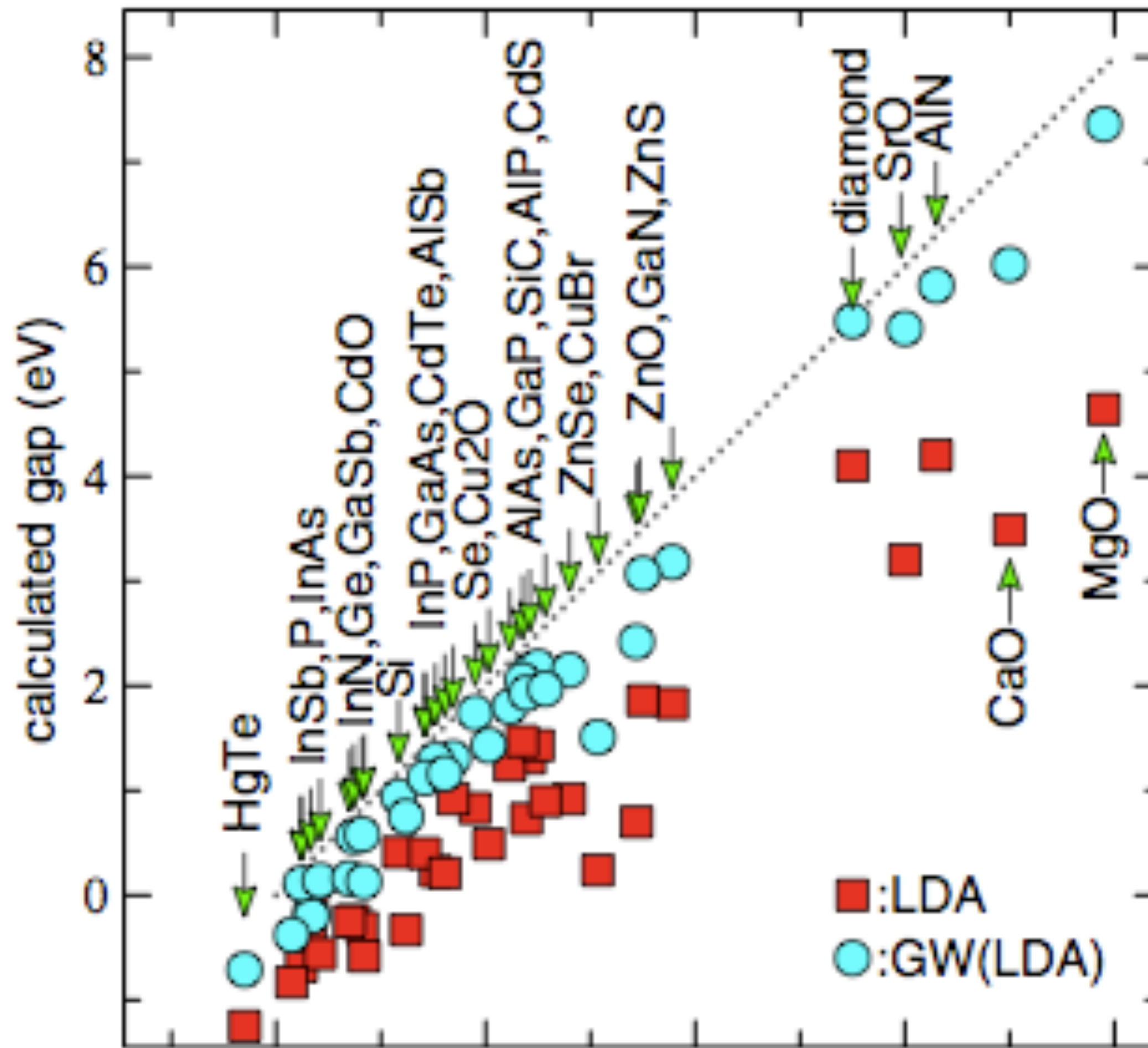
$f_s$  not orthonormal

$\epsilon_s$  are complex

$V_{xc}$  is local and not frequency dependent

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

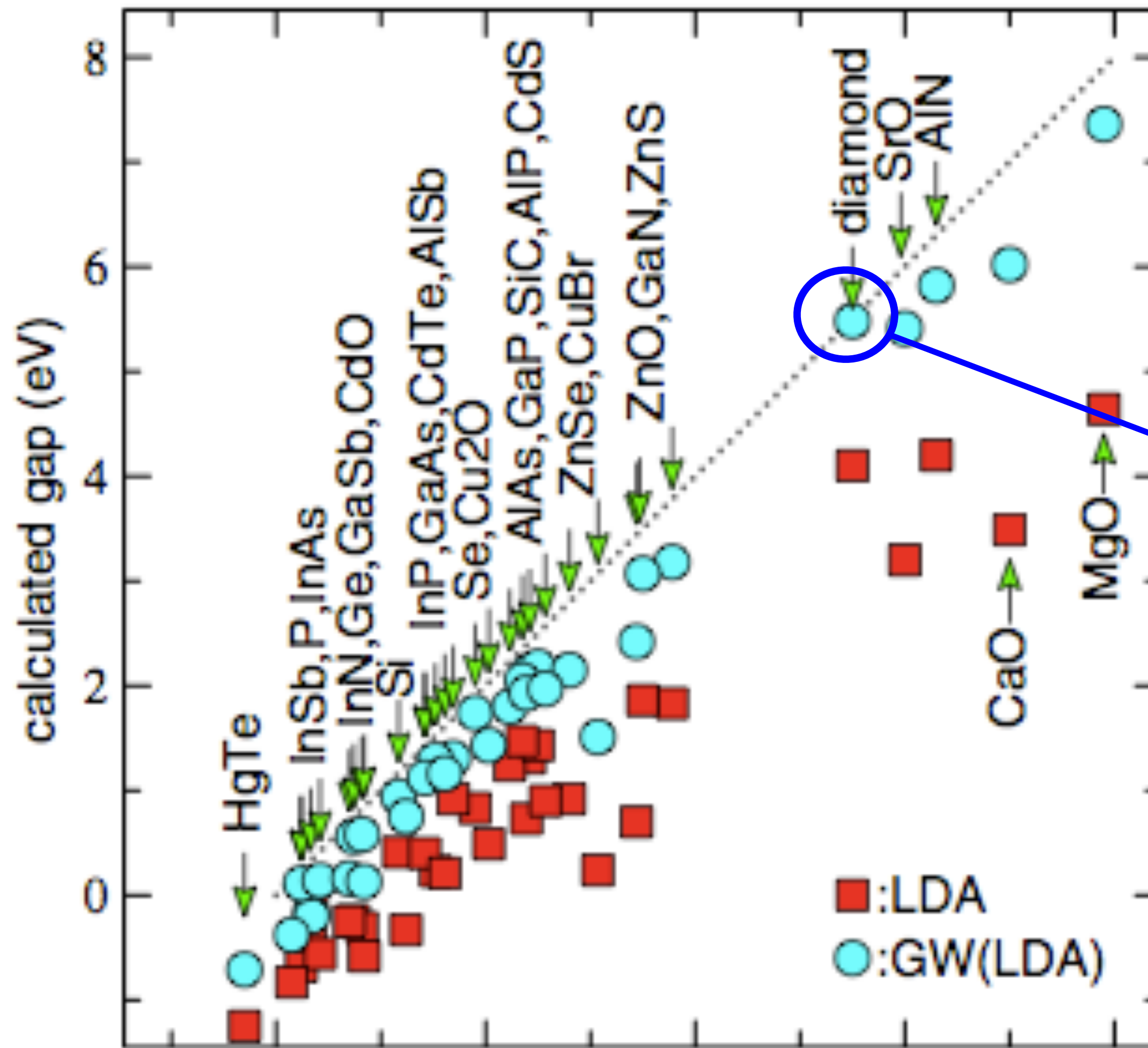
# Some GW results: semiconductor band gaps



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

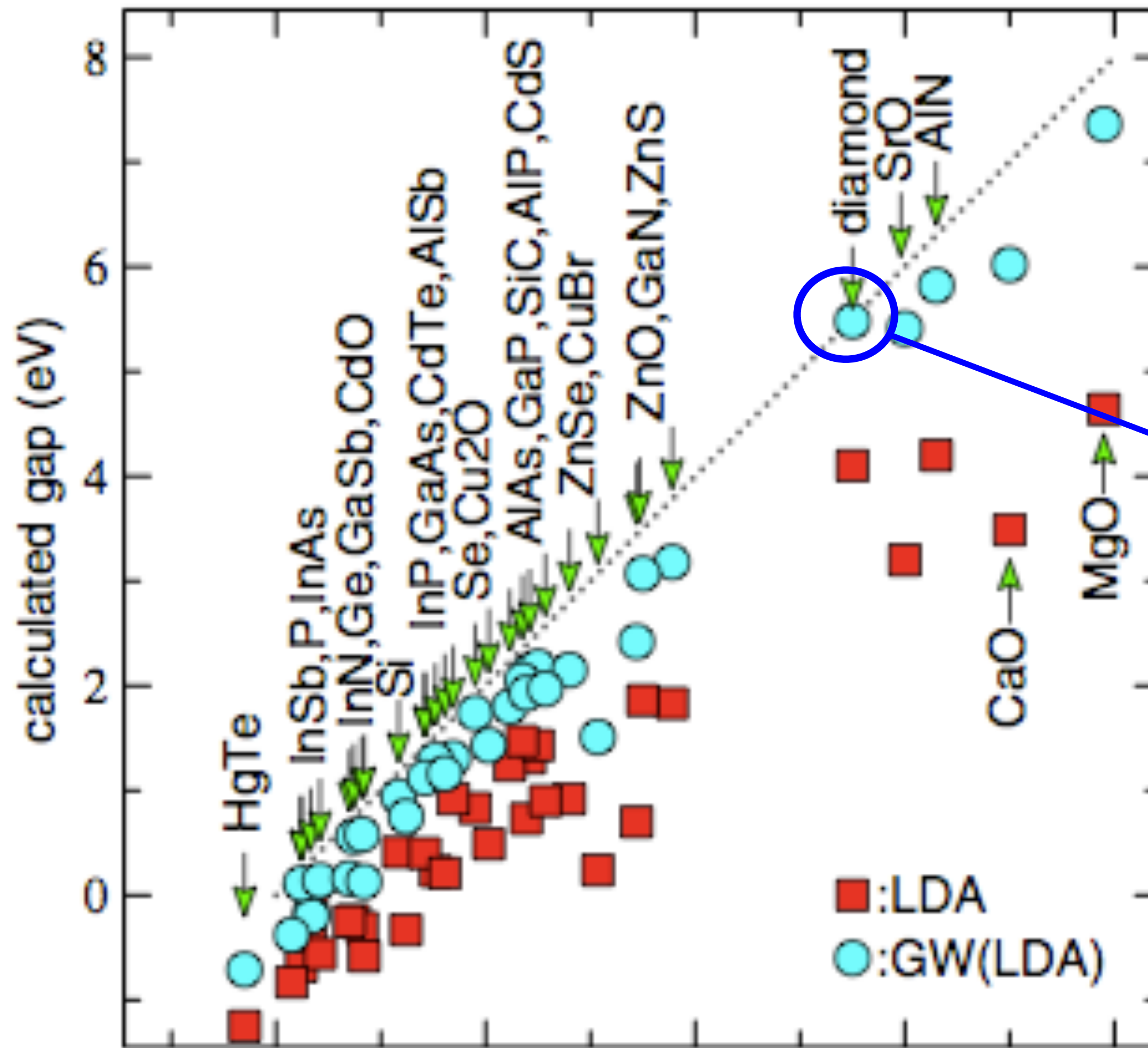


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# Some GW results: semiconductor band gaps



GW band gaps: huge improvement wrt the LDA

Very good agreement with the experiment!!

**But for a wrong reason!!!!**

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

# 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 unoccupied states, 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](https://arxiv.org/abs/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  $\sim 10^5$  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)

# The Yambo code

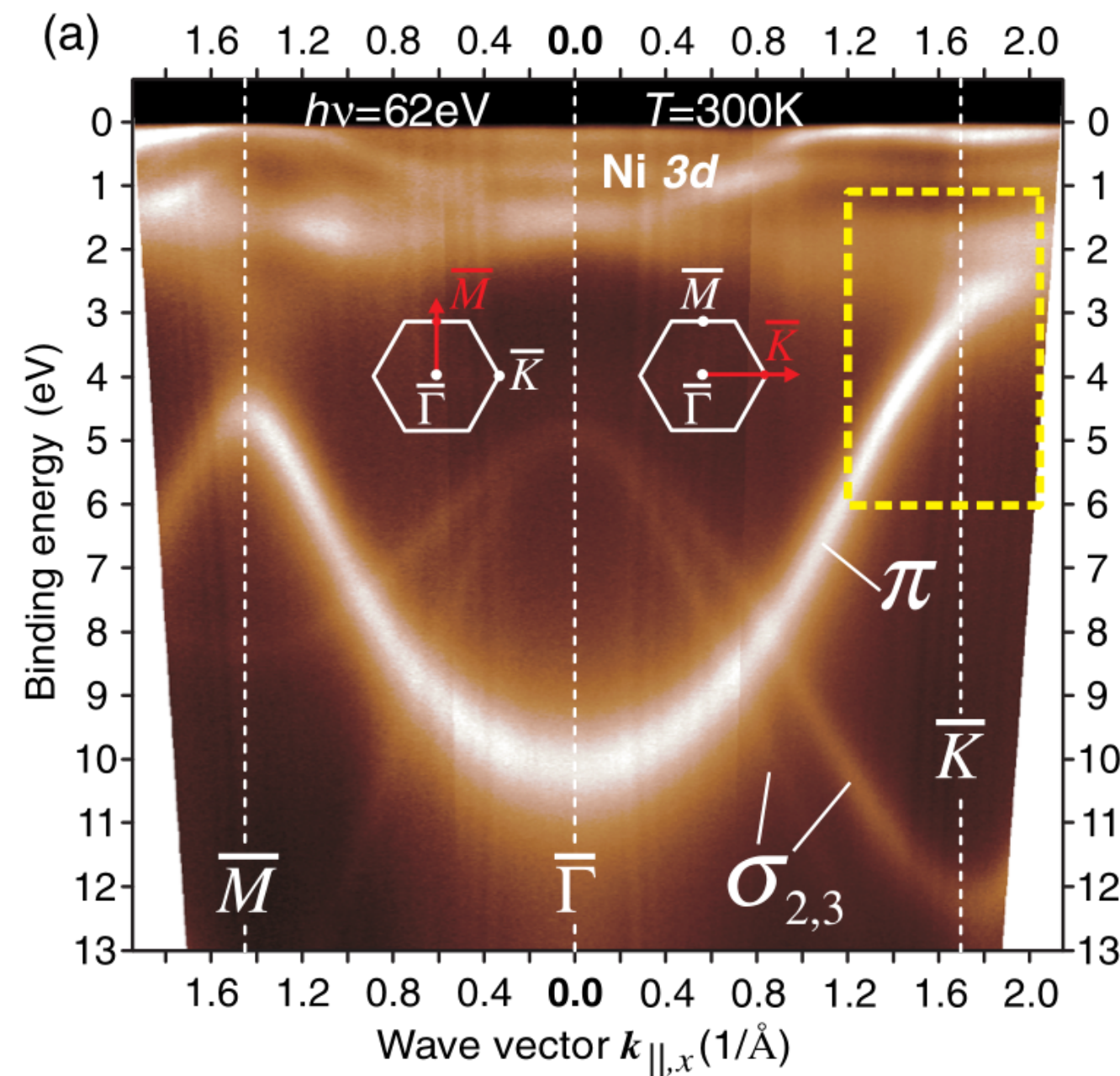


# The Yambo code



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)

<https://www.yambo-code.eu>



Varykhalov et al, PRX **2**, 041017 (2012)

- Implements **many-body methods** (post-DFT) for finite and extended systems
- eg: quasiparticle energies (GW), optical absorption (BSE), spectroscopies
- **plane wave basis set** and pseudopotentials
- Natively interfaced to Quantum ESPRESSO and Abinit

$$\Sigma_{\text{GW}} = \text{[Self-energy diagrams]} + \dots$$

$$\text{BSE} \quad \text{[Diagram with } \Xi \text{]} = \text{[Diagram with } v \text{]} + \text{[Diagram with } W \text{]}$$

# Ab initio many-body perturbation theory (MBPT)

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

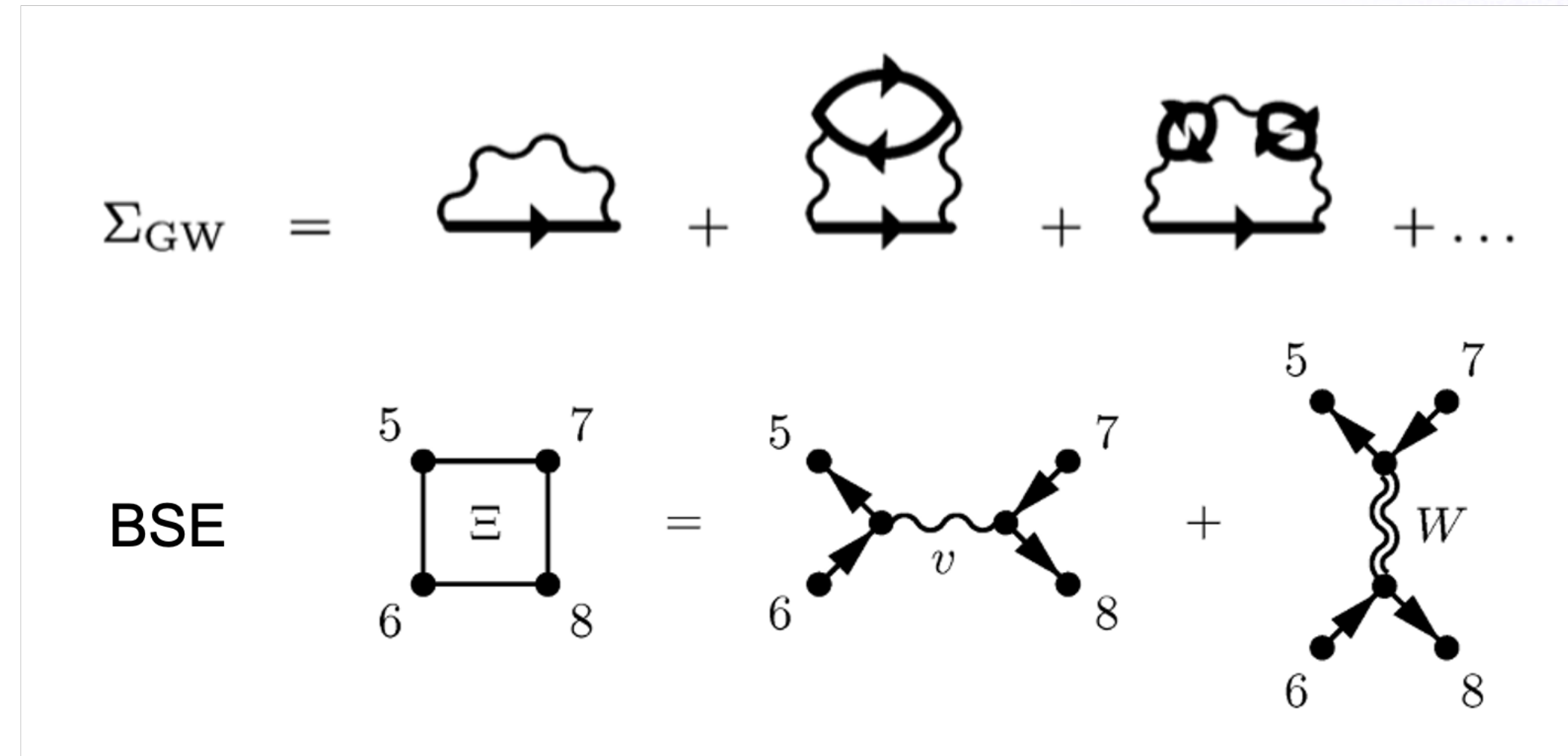
- **DFT simulation as input**
- interfaced to QE (MaX), Abinit

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

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

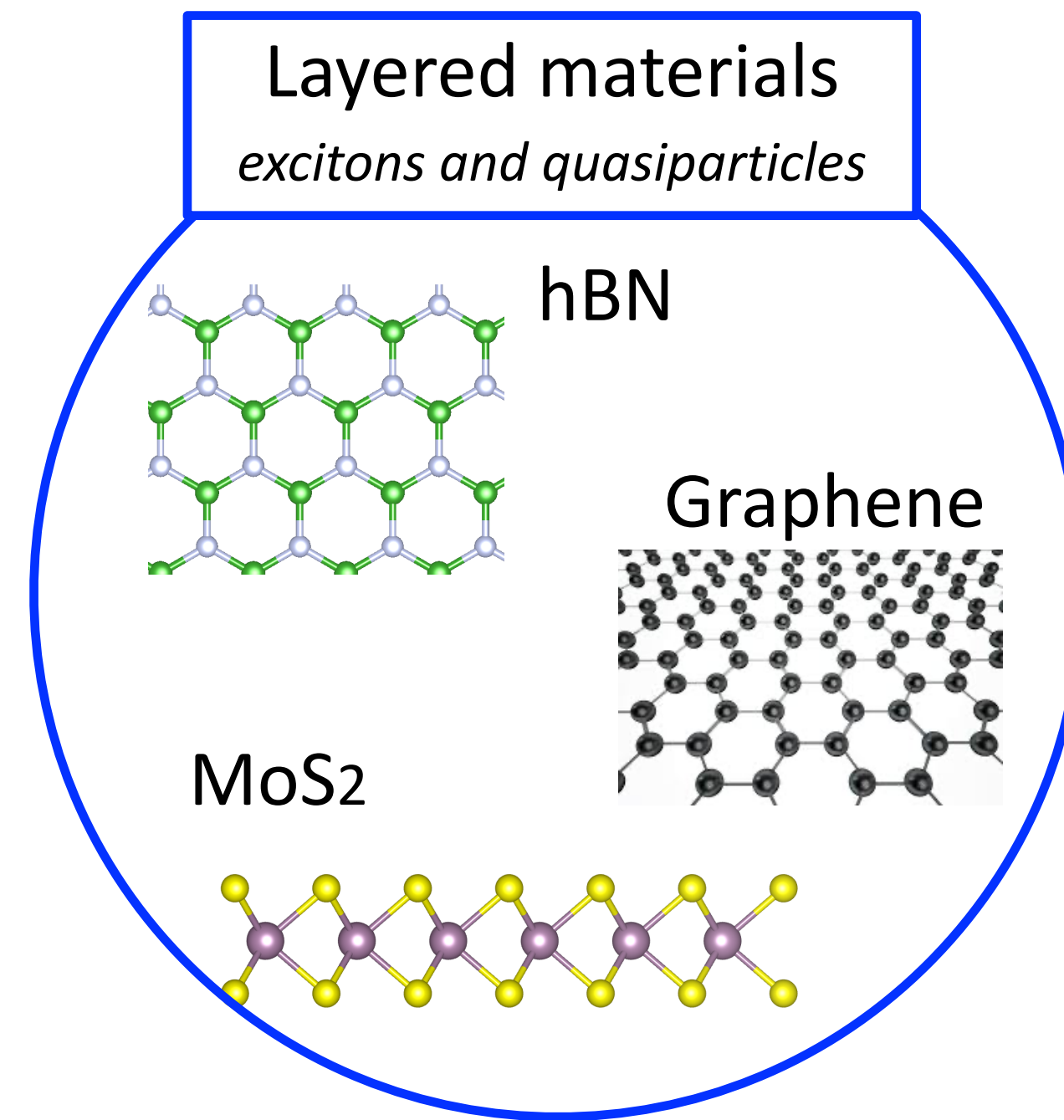
- microscopic screening

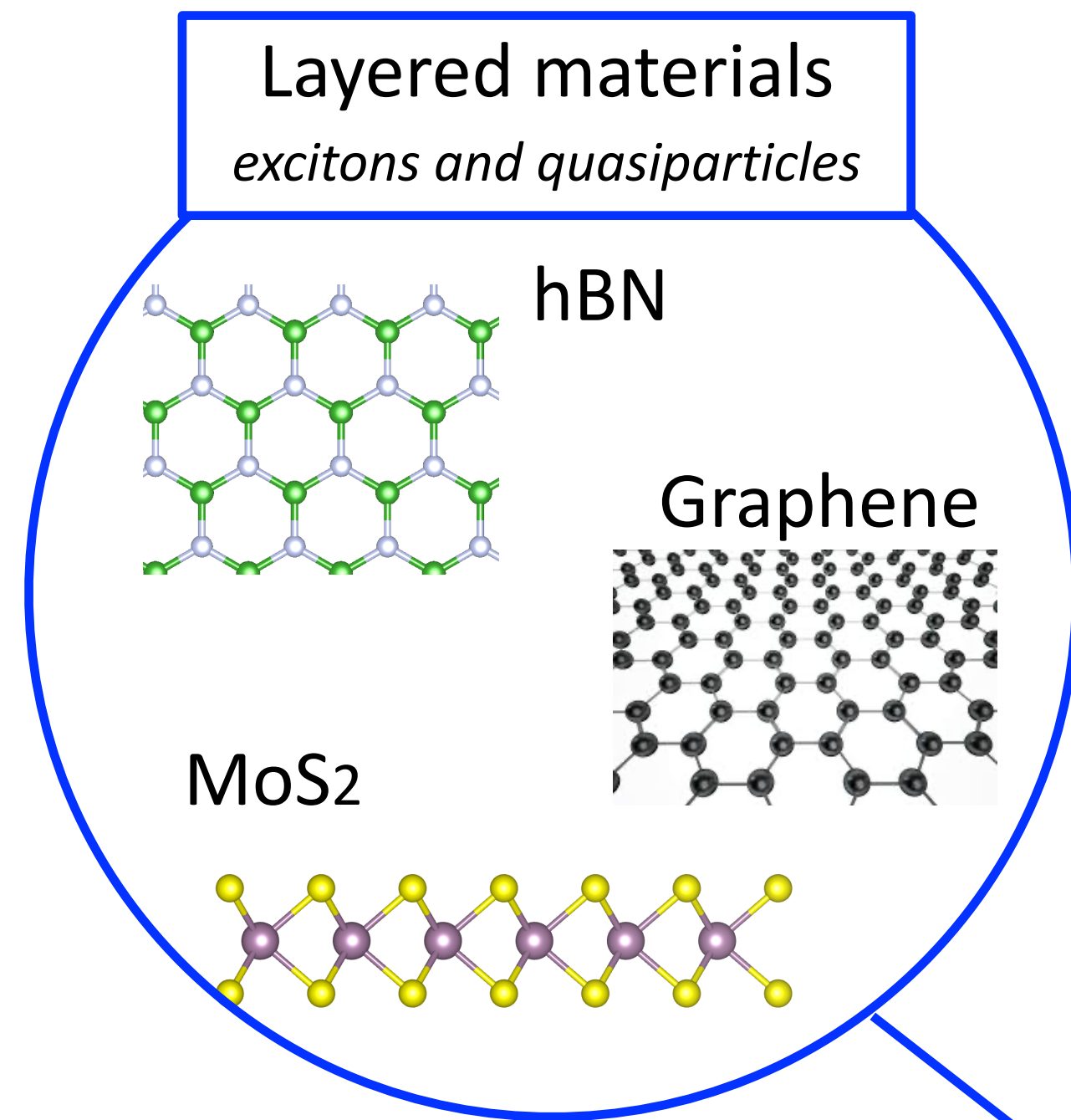
$$\chi_{\mathbf{q}}(\mathbf{G}, \mathbf{G}', \omega)$$



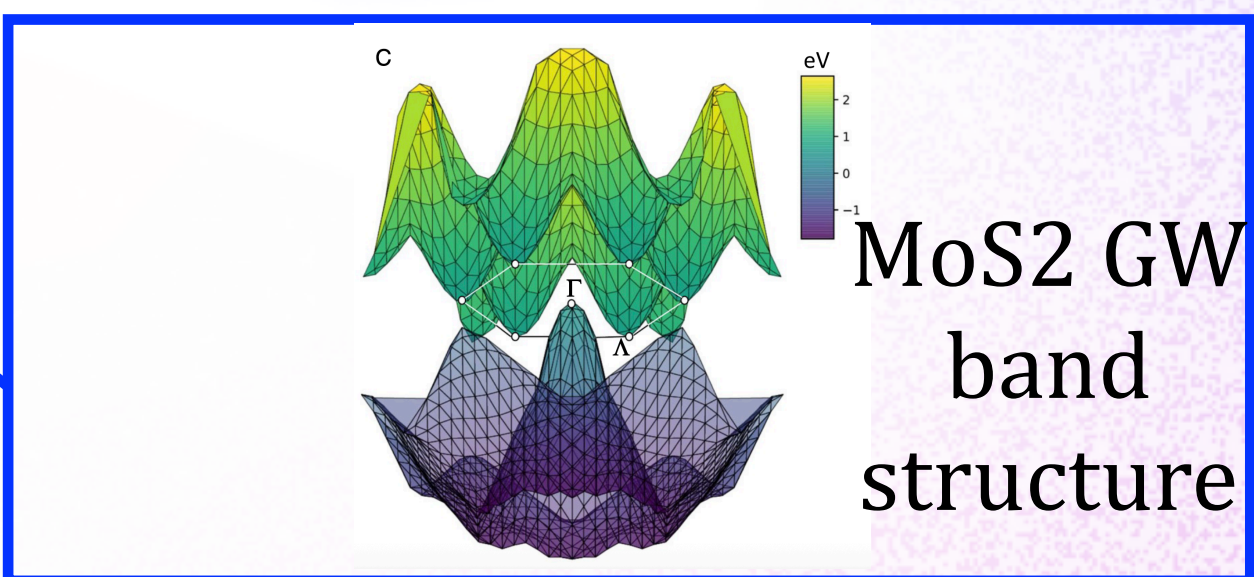
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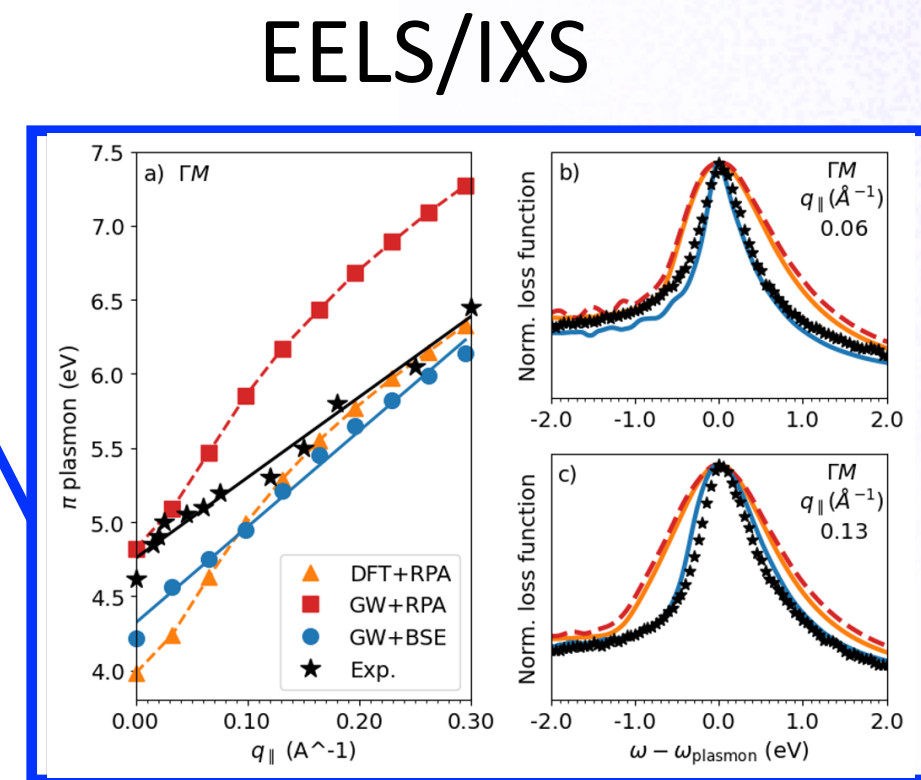
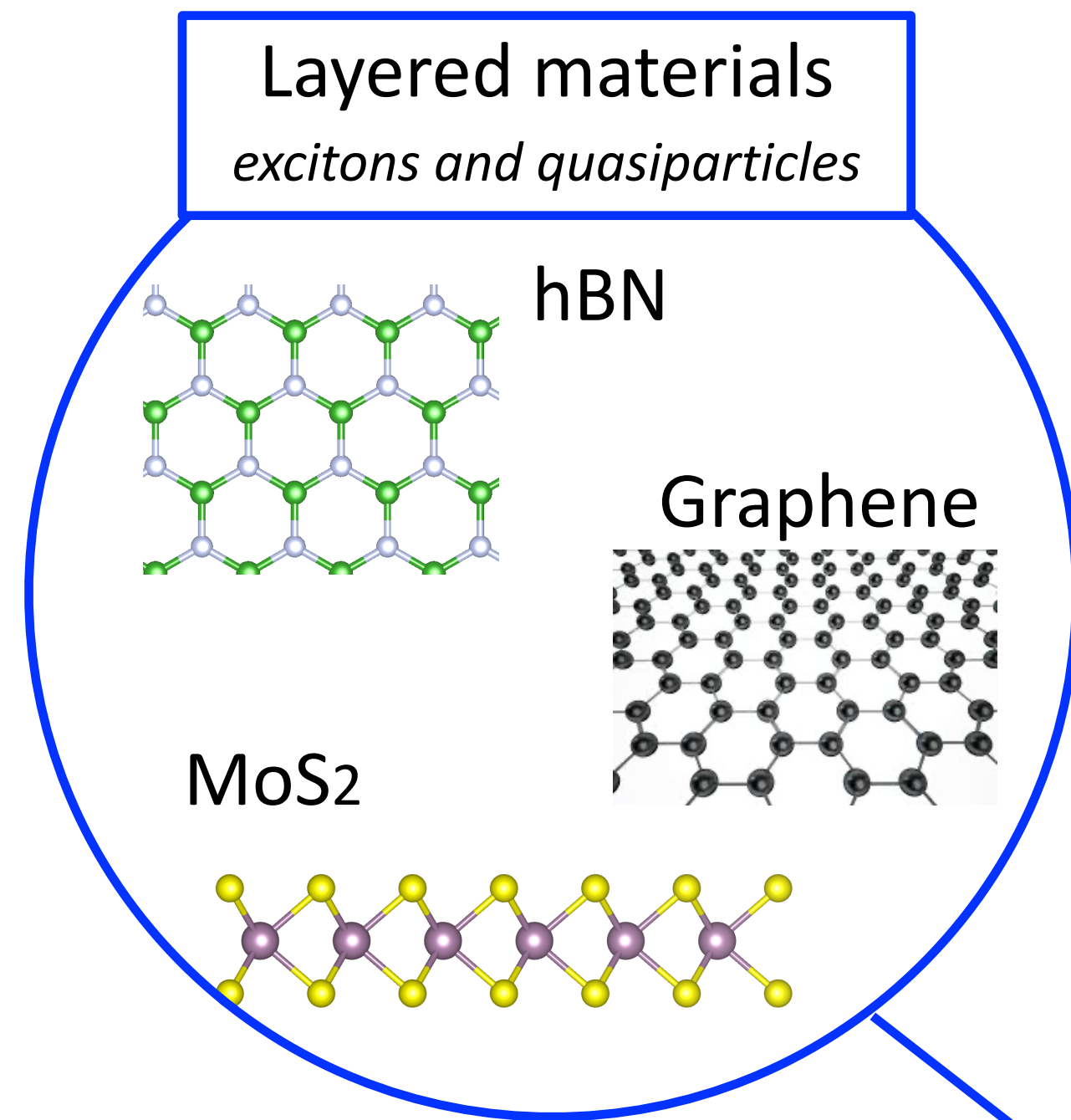




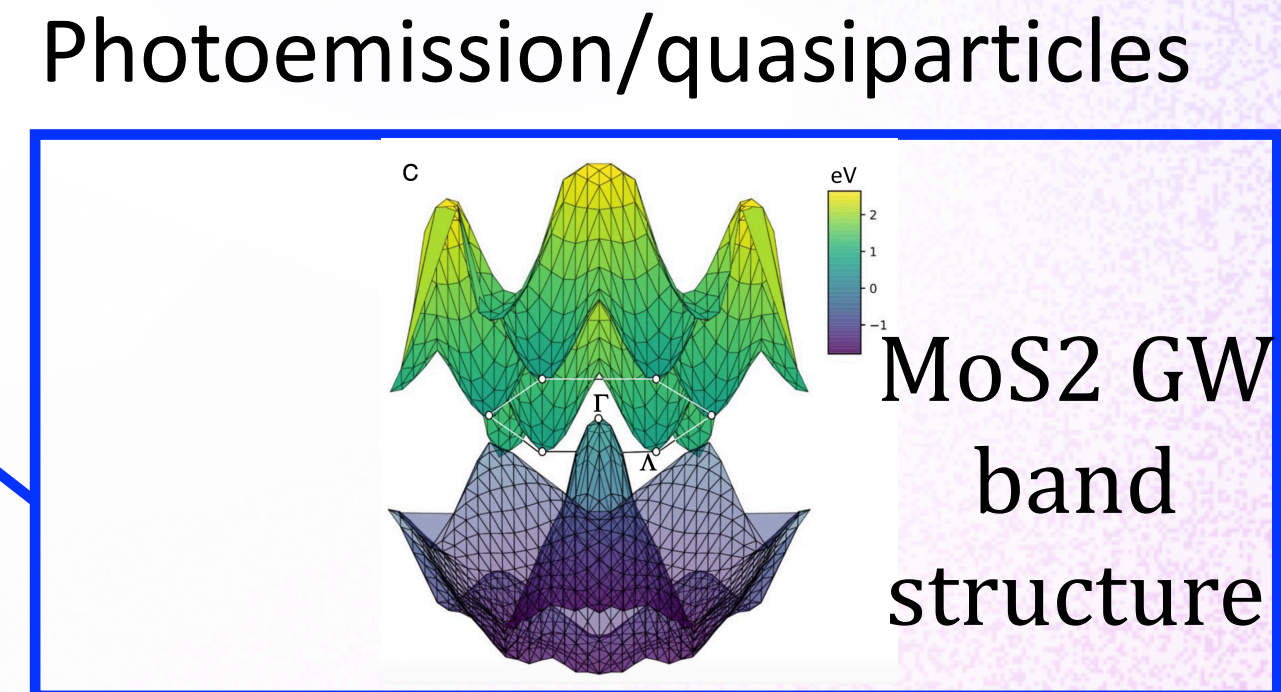
## Photoemission/quasiparticles



Ataei, Varsano, Molinari, Rontani PNAS (2021)

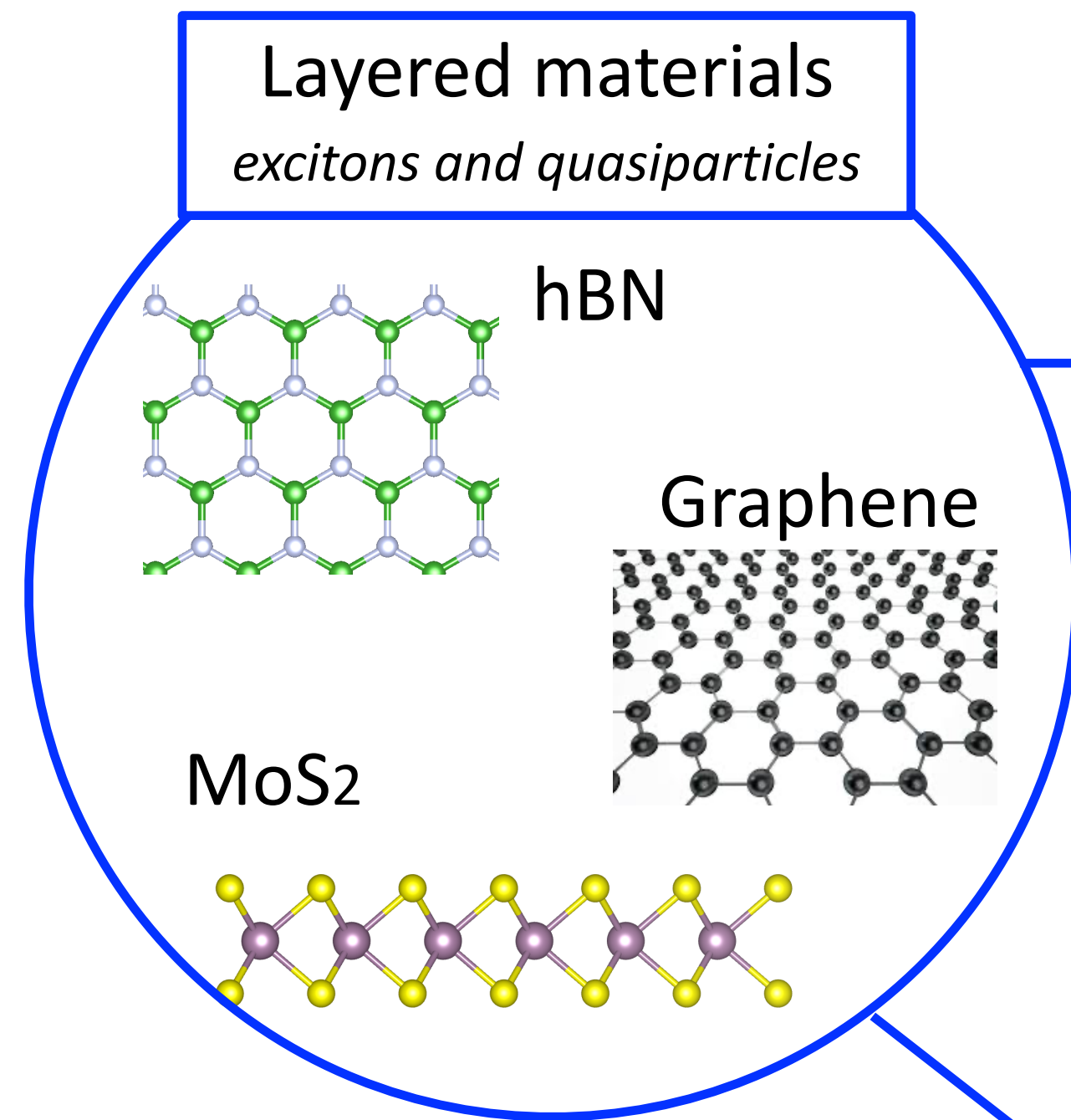


EELS free-standing graphene  
*Guandalini, Varsano, Ferretti...Nano Lett. (2023)*

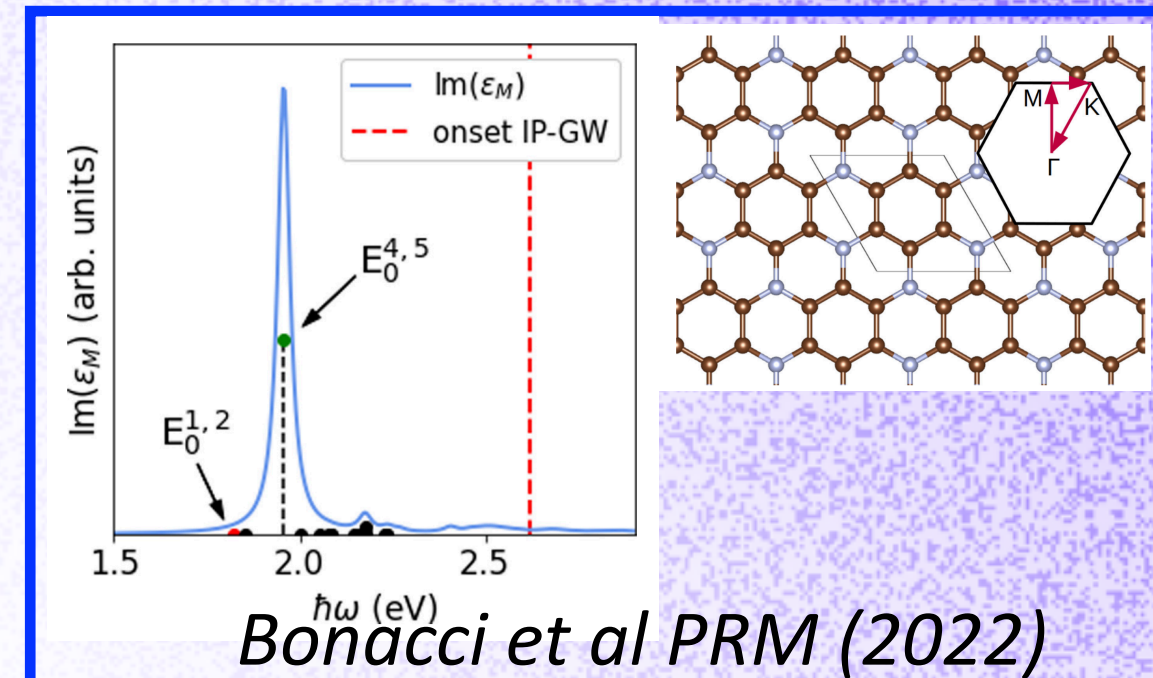


*Ataei, Varsano, Molinari, Rontani PNAS (2021)*

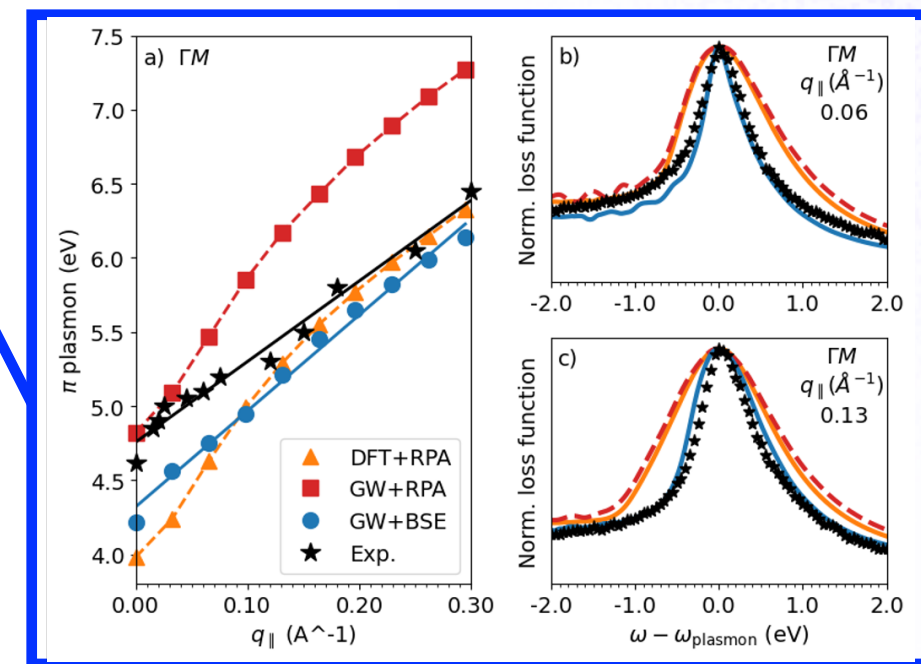
# Many Body technique for spectroscopy:



## Optical absorption: Excitons



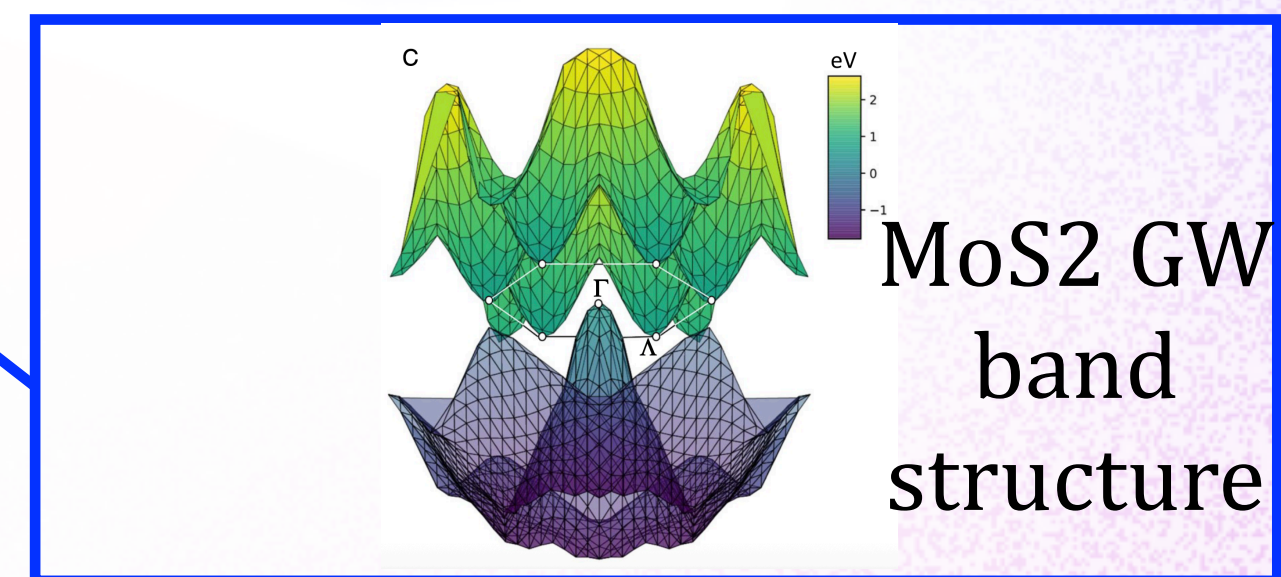
## EELS/IXS



## EELS free-standing graphene

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

## Photoemission/quasiparticles

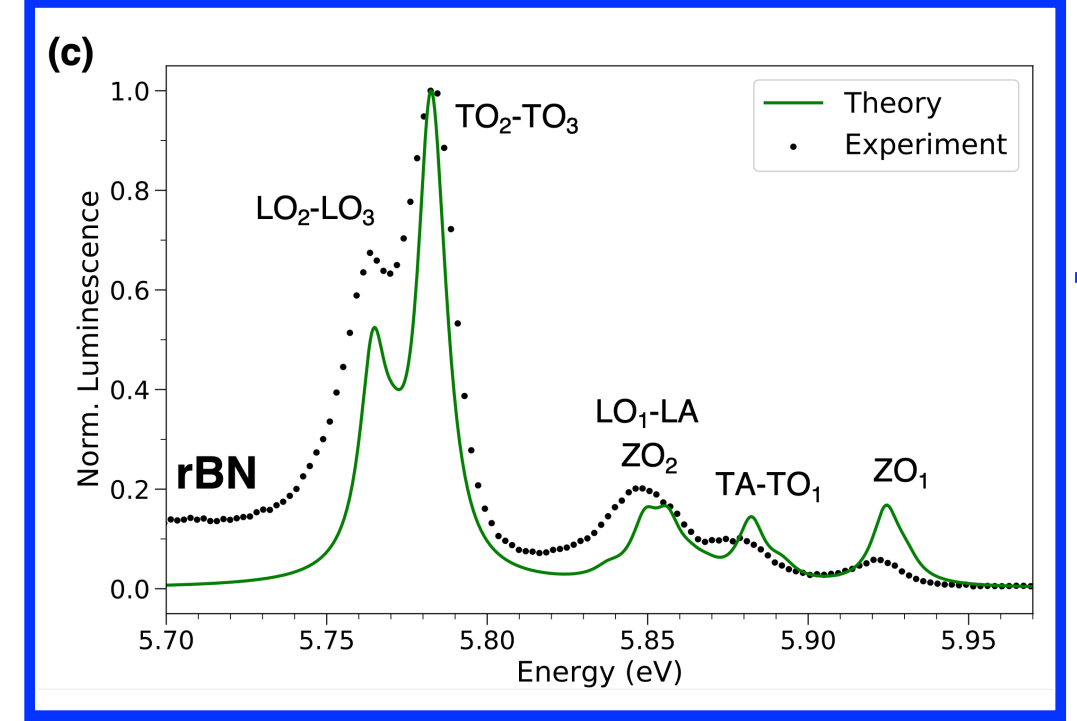


*Ataei, Varsano, Molinari, Rontani PNAS (2021)*

# Many Body technique for spectroscopy:

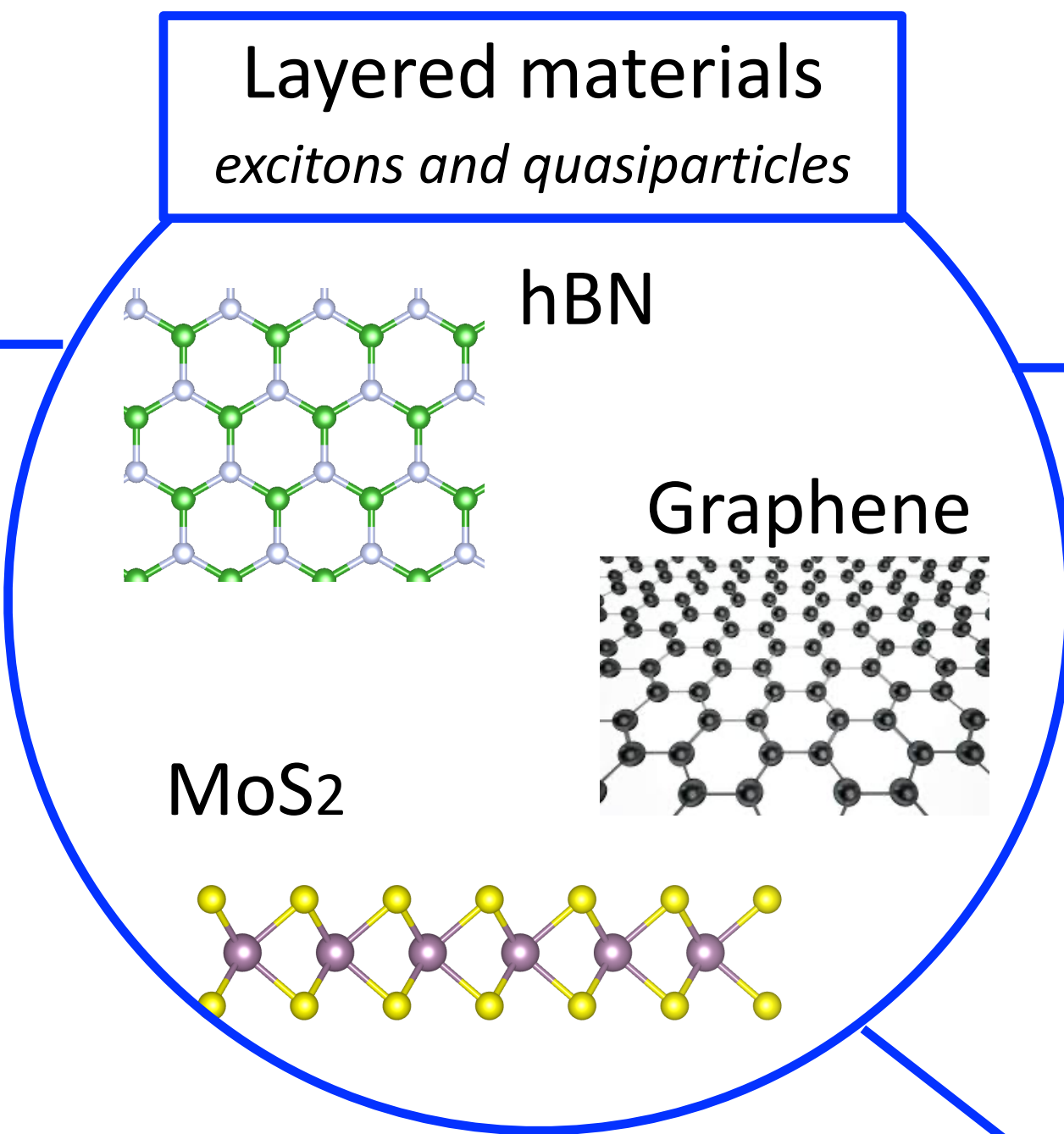


## Phonon-assisted luminescence

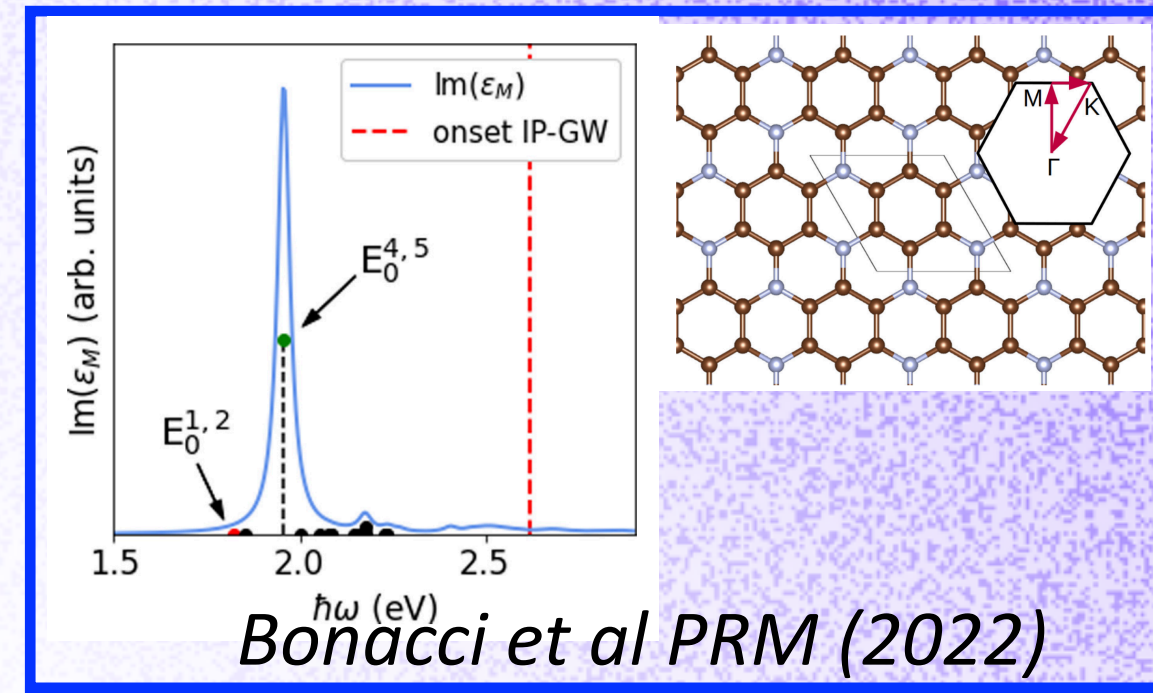


Zanfognini, Paleari, Molinari, Varsano ...PRL (2023)

## Layered materials excitons and quasiparticles

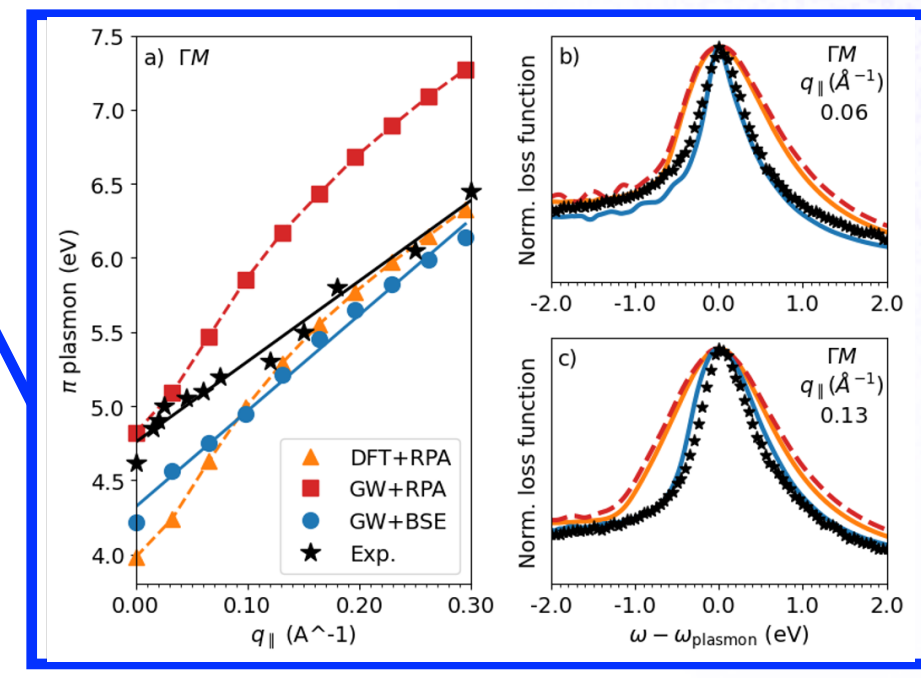


## Optical absorption: Excitons



Bonacchi et al PRM (2022)

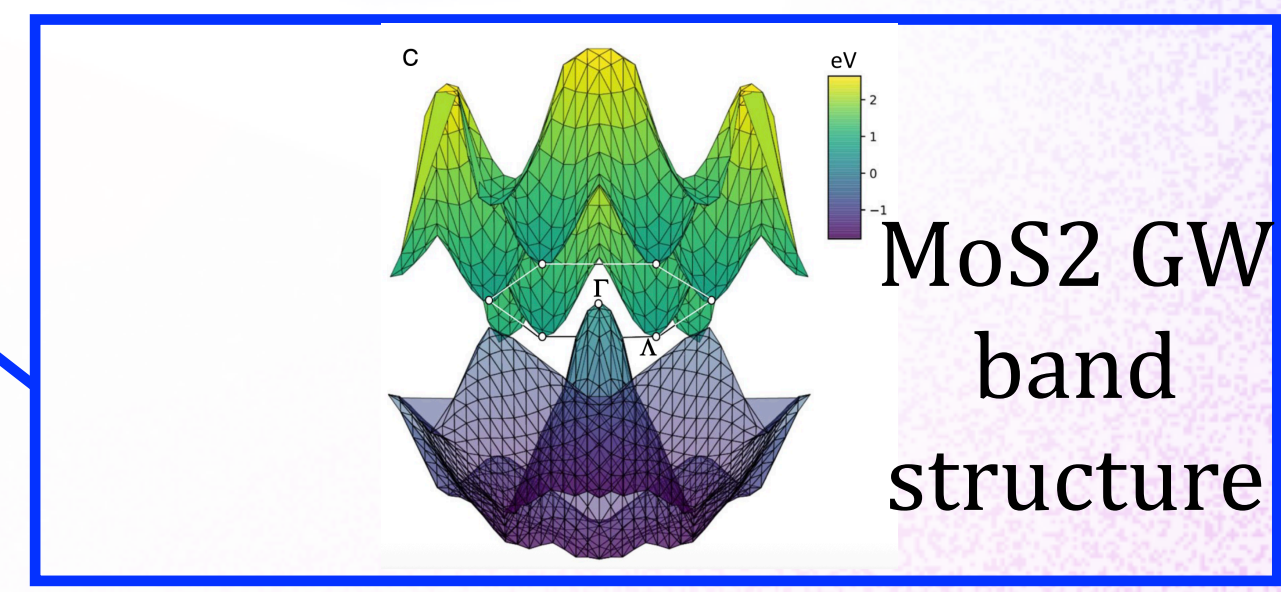
## EELS/IXS



## EELS free-standing graphene

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

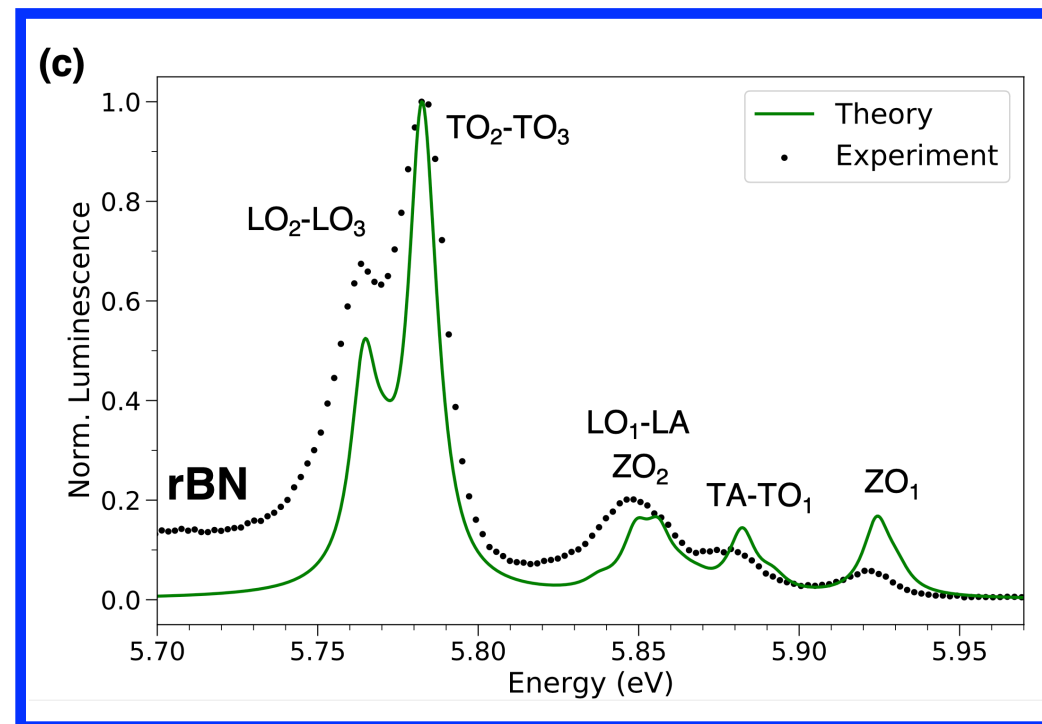
## Photoemission/quasiparticles



Ataei, Varsano, Molinari, Rontani PNAS (2021)

# Many Body technique for spectroscopy:

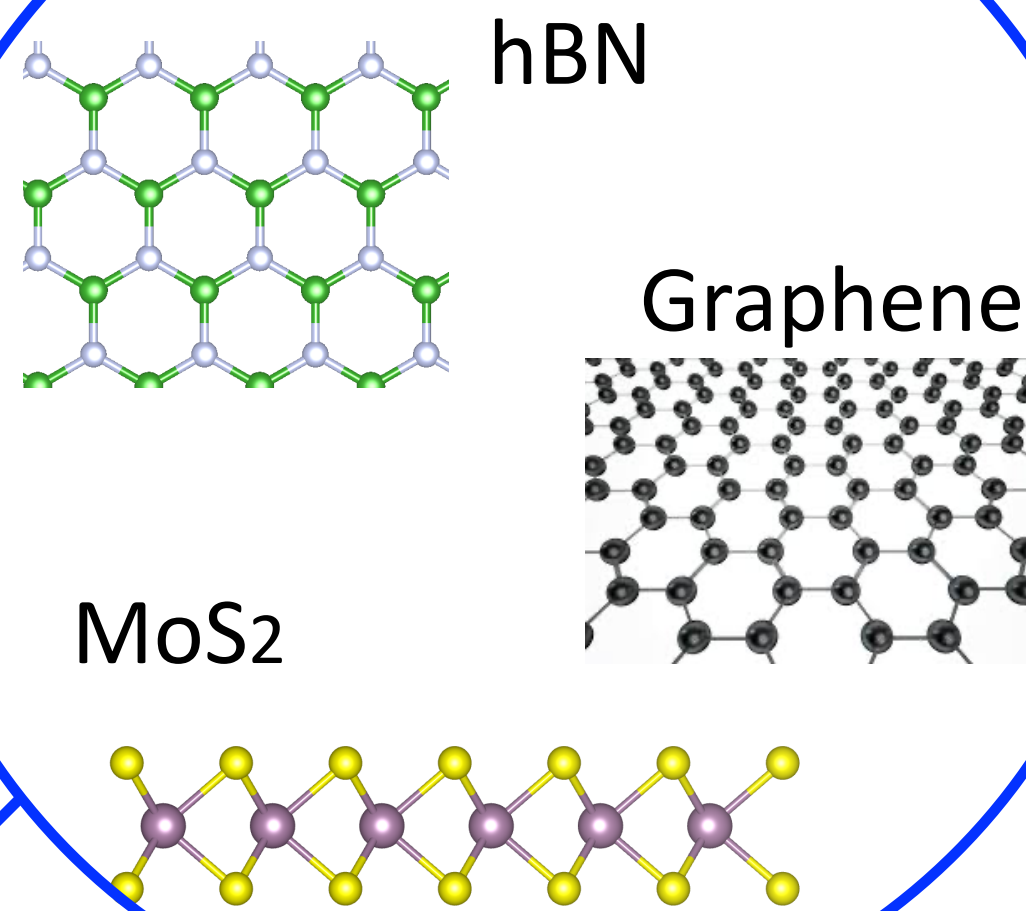
## Phonon-assisted luminescence



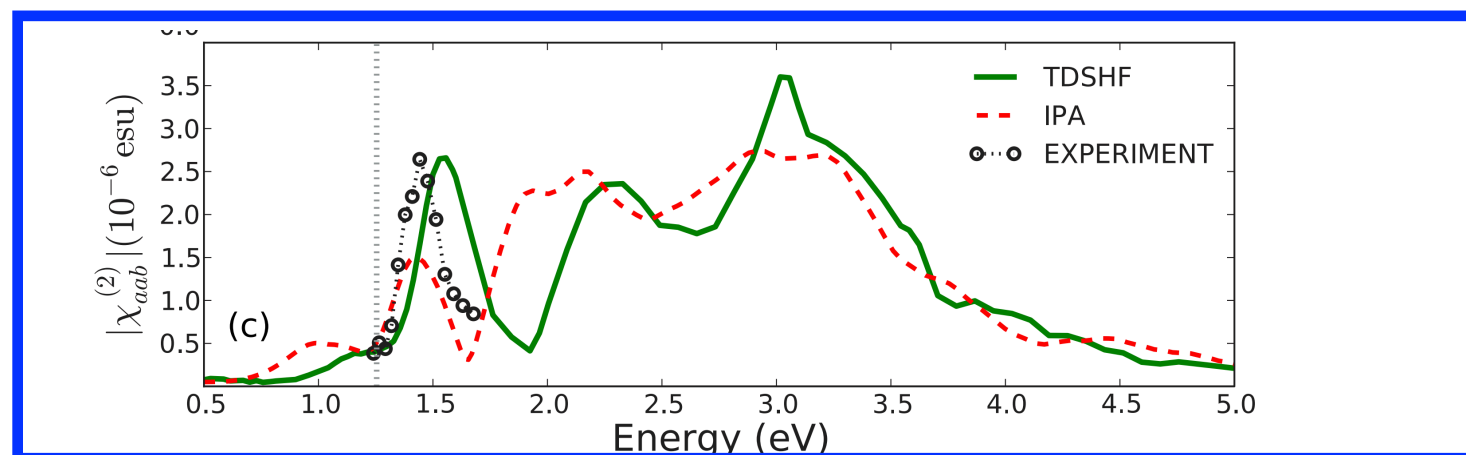
Zanfagnini, Paleari, Molinari, Varsano ...PRL (2023) See P2.36: Fulvio Paleari

## Layered materials

excitons and quasiparticles

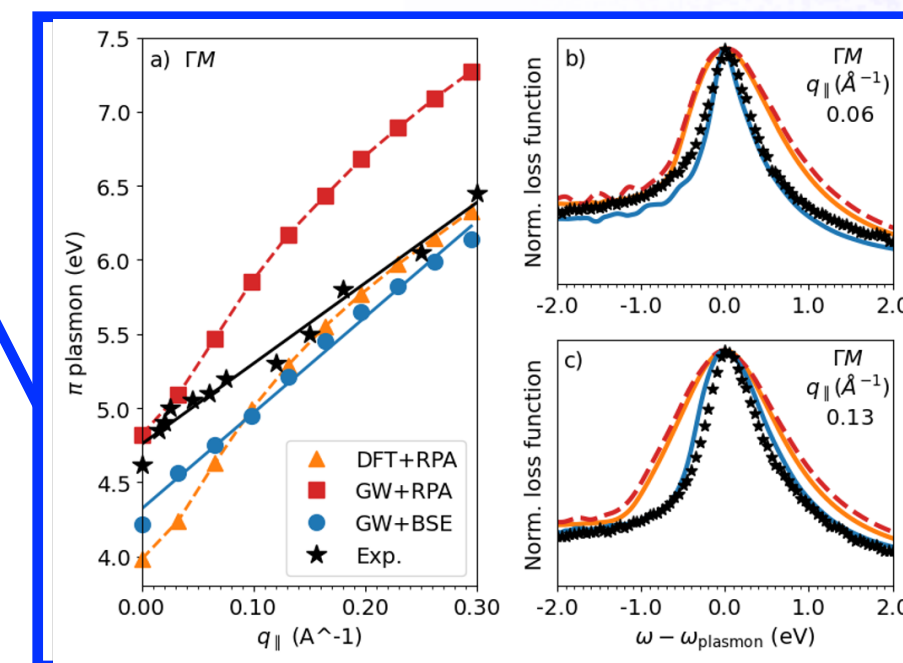


## High-harmonic generation



PRB 89, 081102(R) (2014)

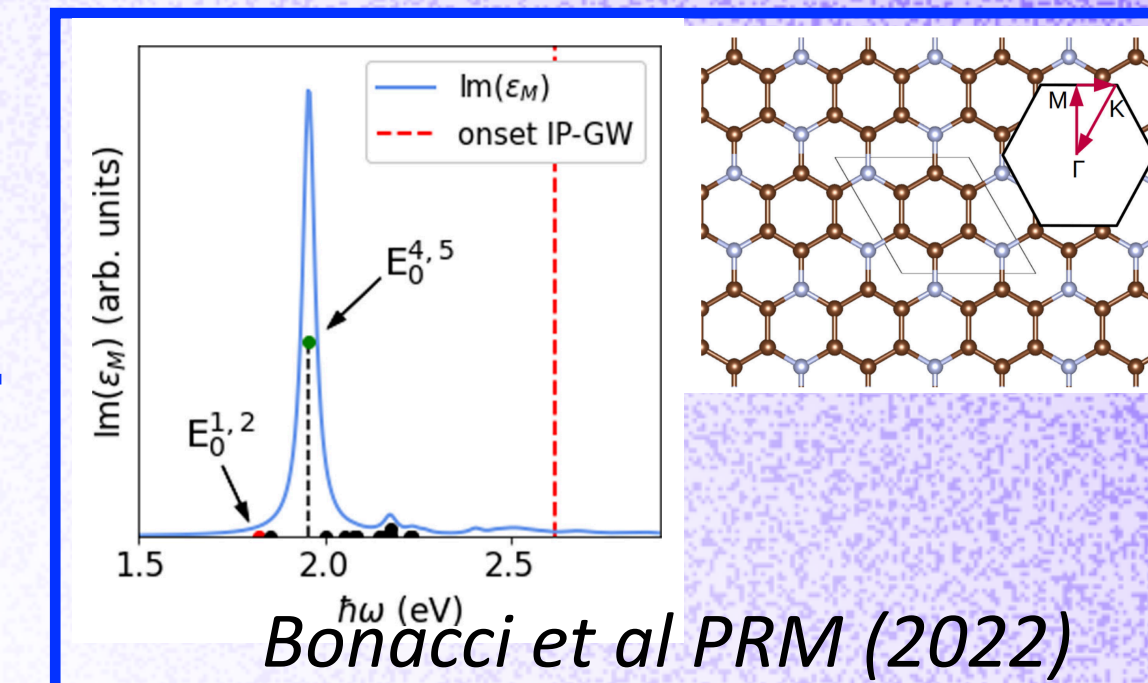
## EELS/IXS



EELS free-standing graphene

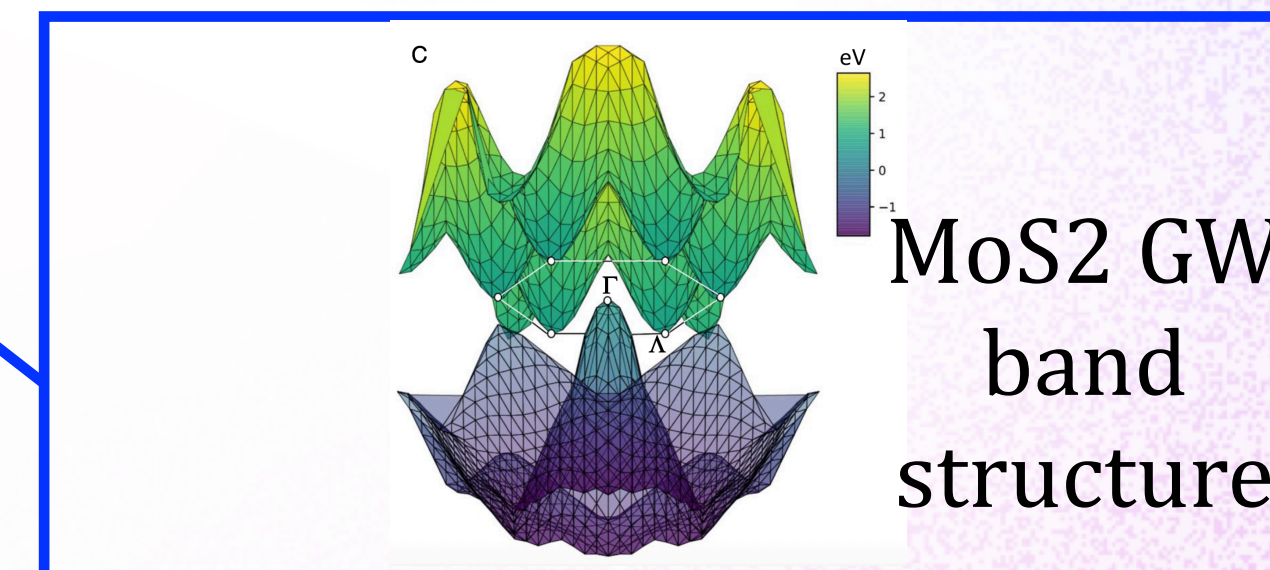
Guandalini, Varsano, Ferretti...Nano Lett. (2023)

## Optical absorption: Excitons



Bonacchi et al PRM (2022)

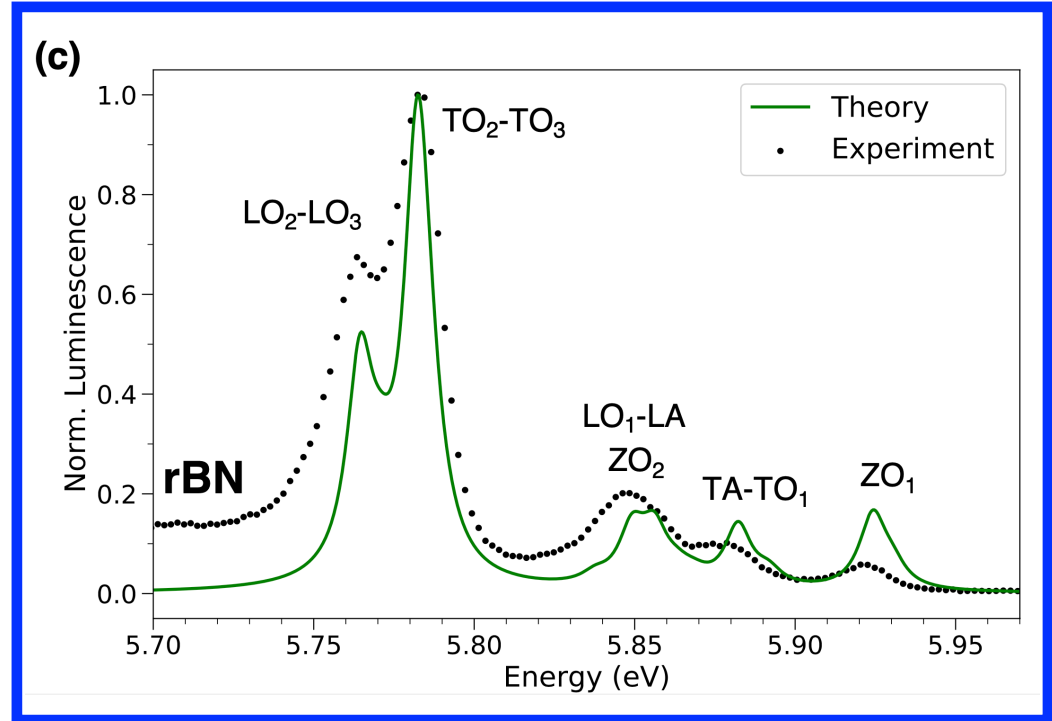
## Photoemission/quasiparticles



Ataei, Varsano, Molinari, Rontani PNAS (2021)

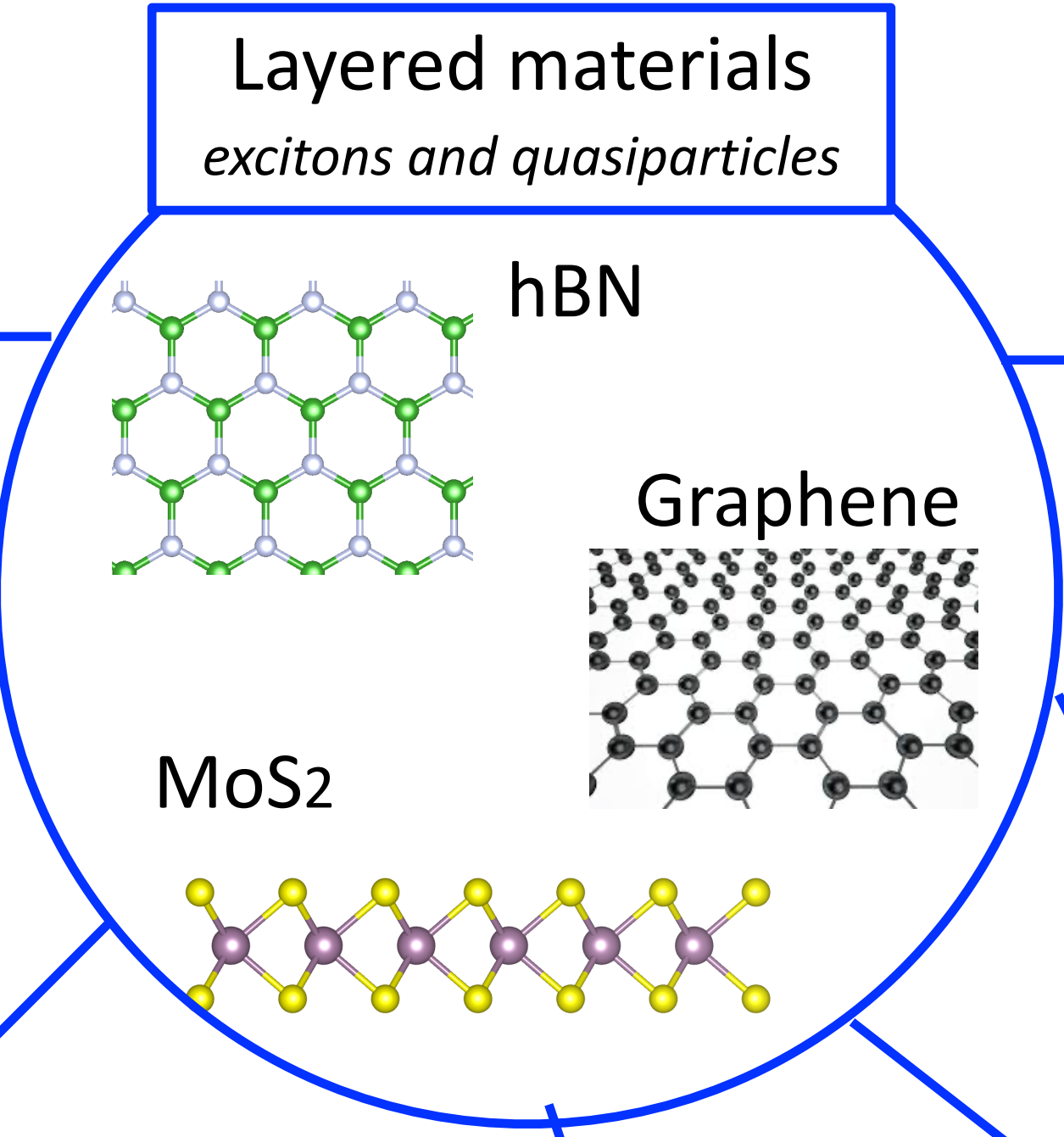
# Many Body technique for spectroscopy:

## Phonon-assisted luminescence

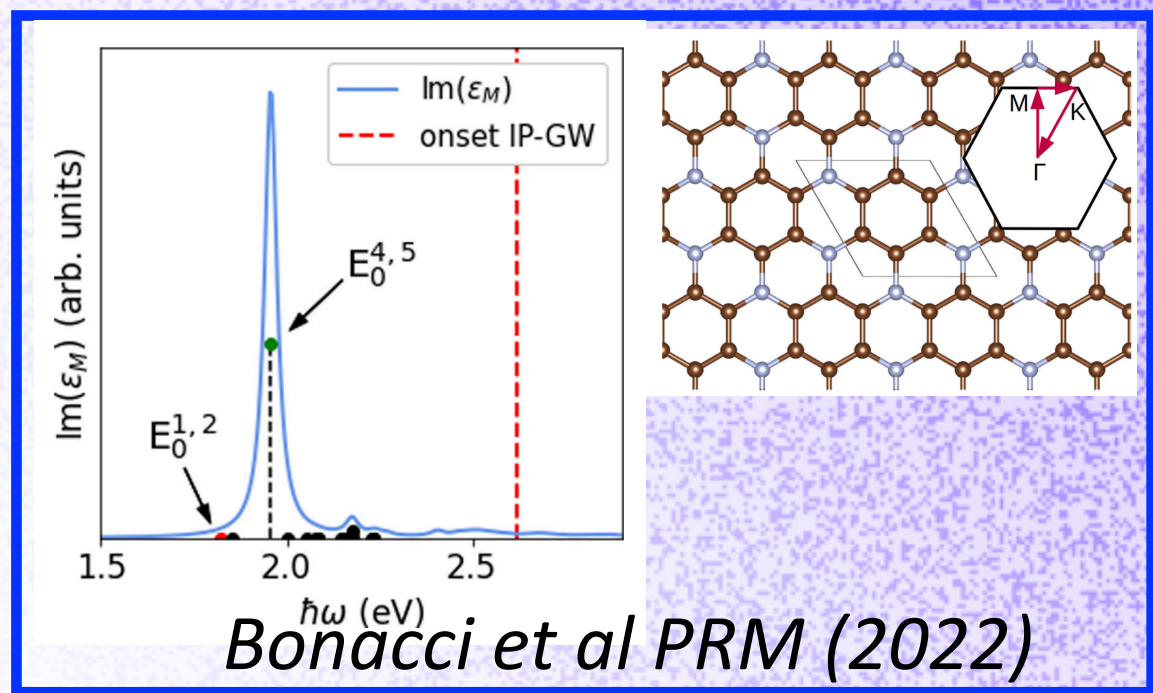


Zanfrognini, Paleari, Molinari, Varsano ...PRL (2023) See P2.36: Fulvio Paleari

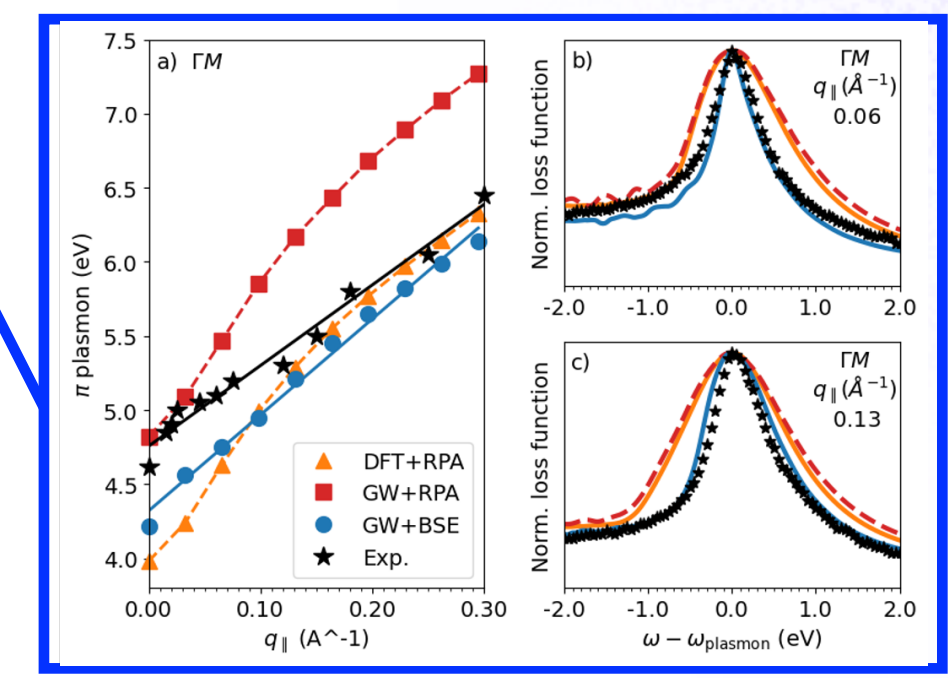
## Layered materials excitons and quasiparticles



## Optical absorption: Excitons



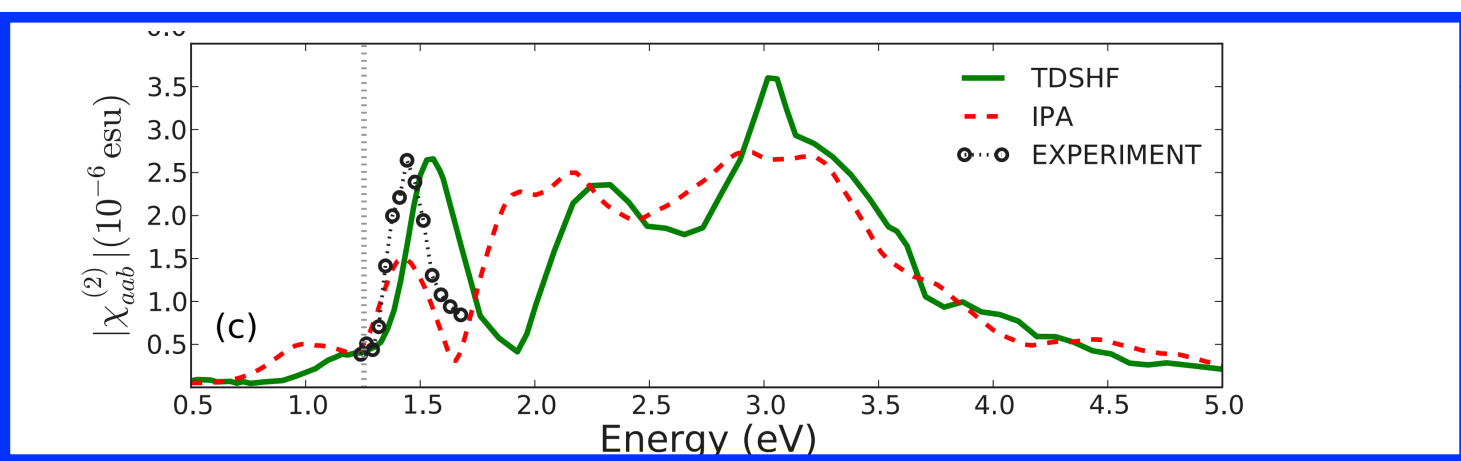
## EELS/IXS



## EELS free-standing graphene

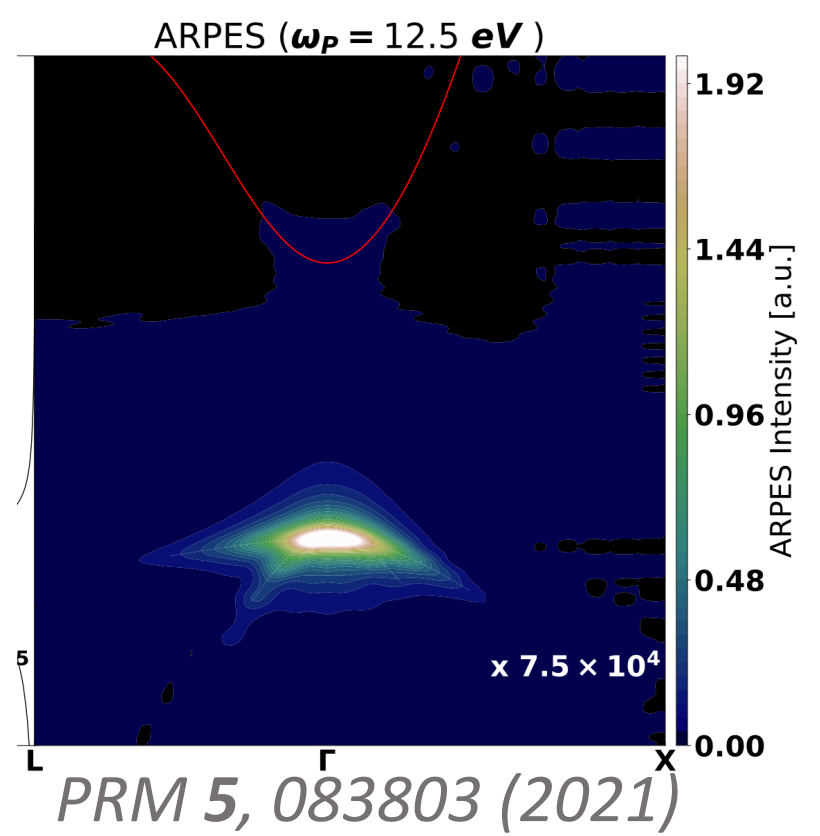
Guandalini, Varsano, Ferretti...Nano Lett. (2023)

## High-harmonic generation

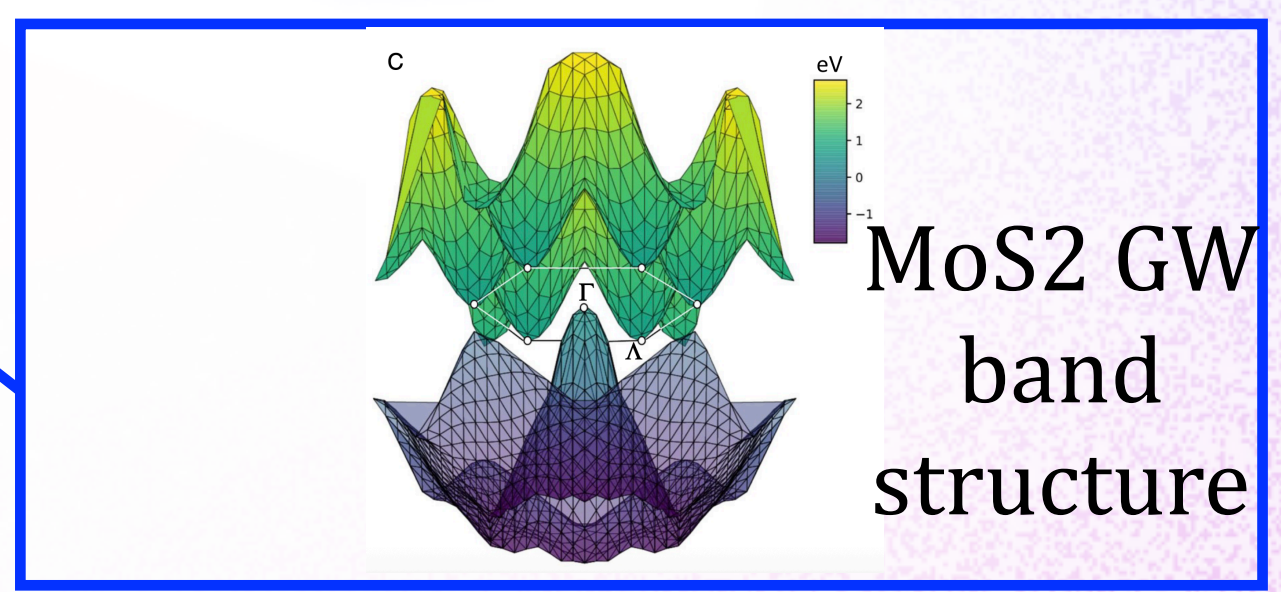


PRB 89, 081102(R) (2014)

## Time-resolved spectra

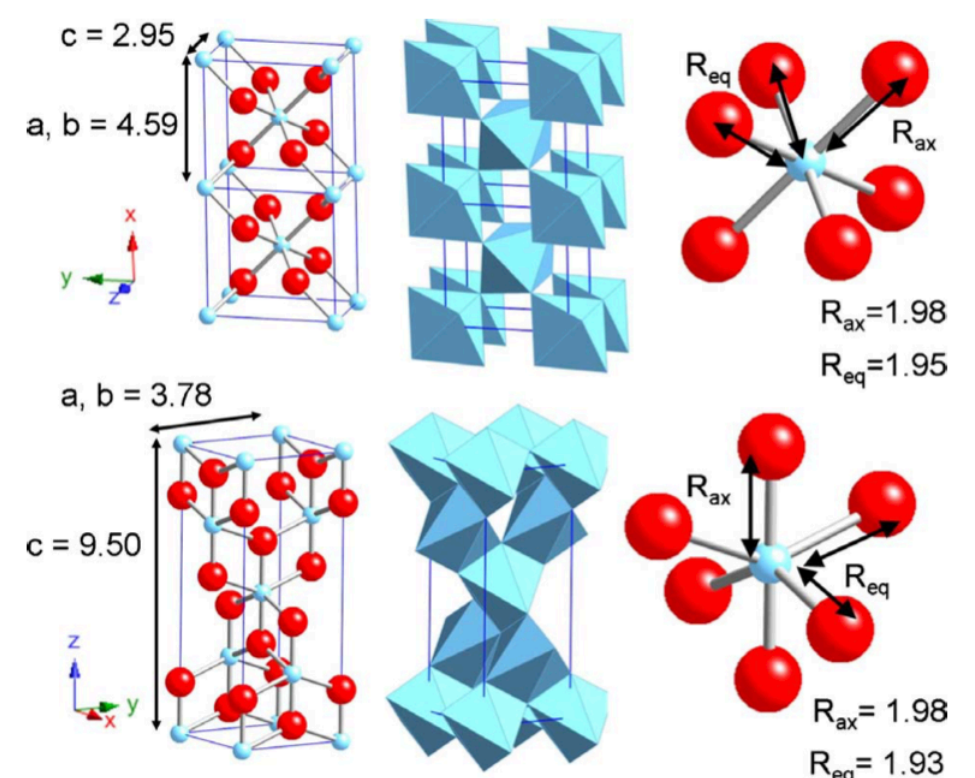


## Photoemission/quasiparticles



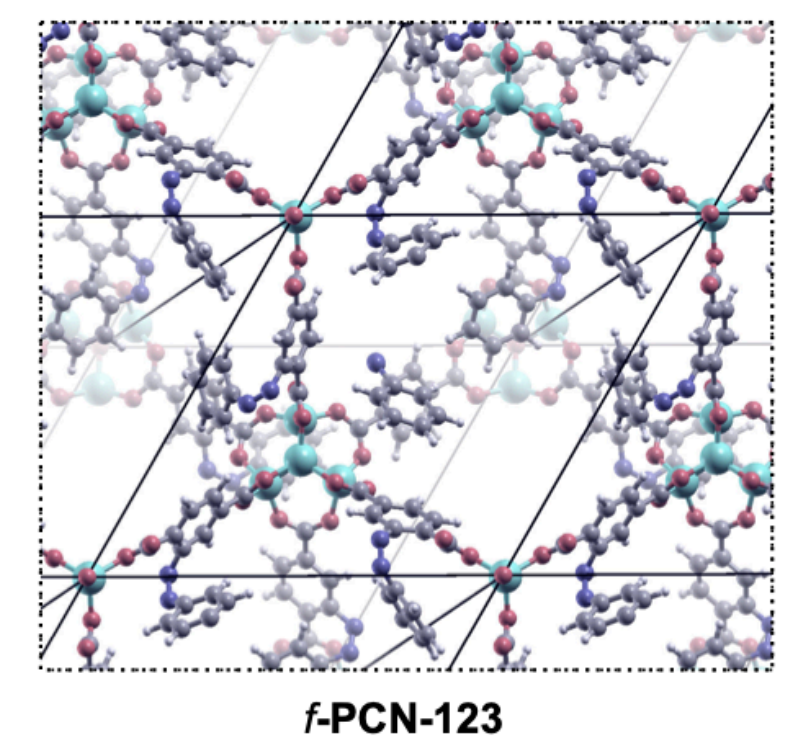
Ataei, Varsano, Molinari, Rontani PNAS (2021)

# Which systems you can deal with:

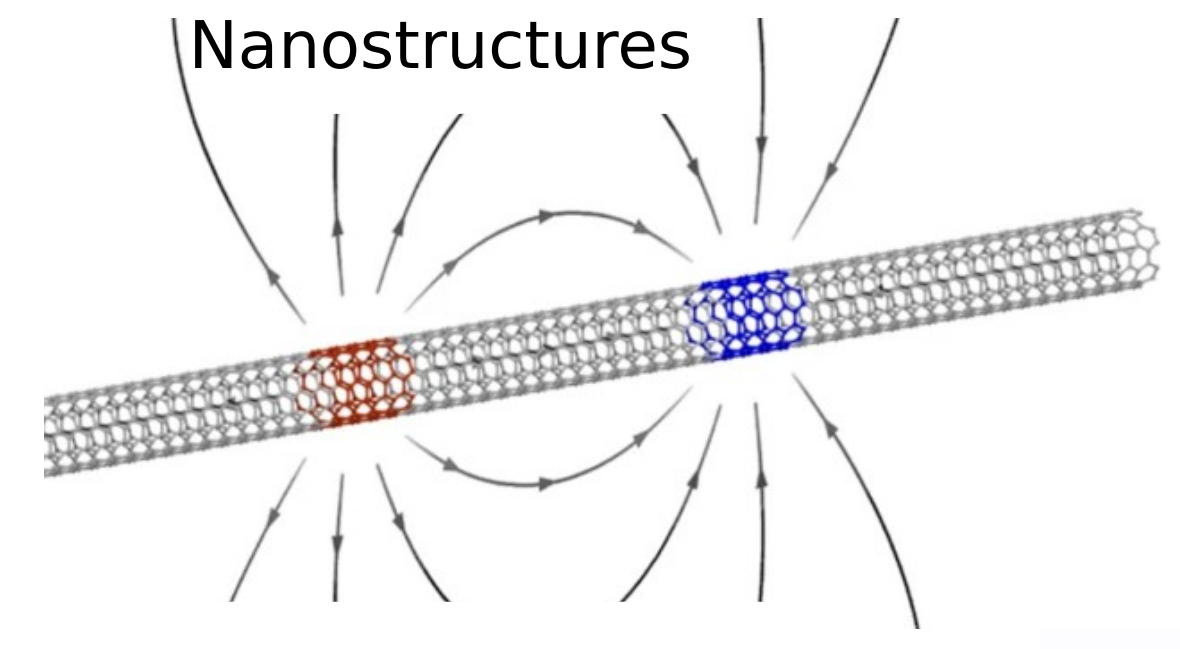


L. Chiodo et al. Phys. Rev. B (2010)

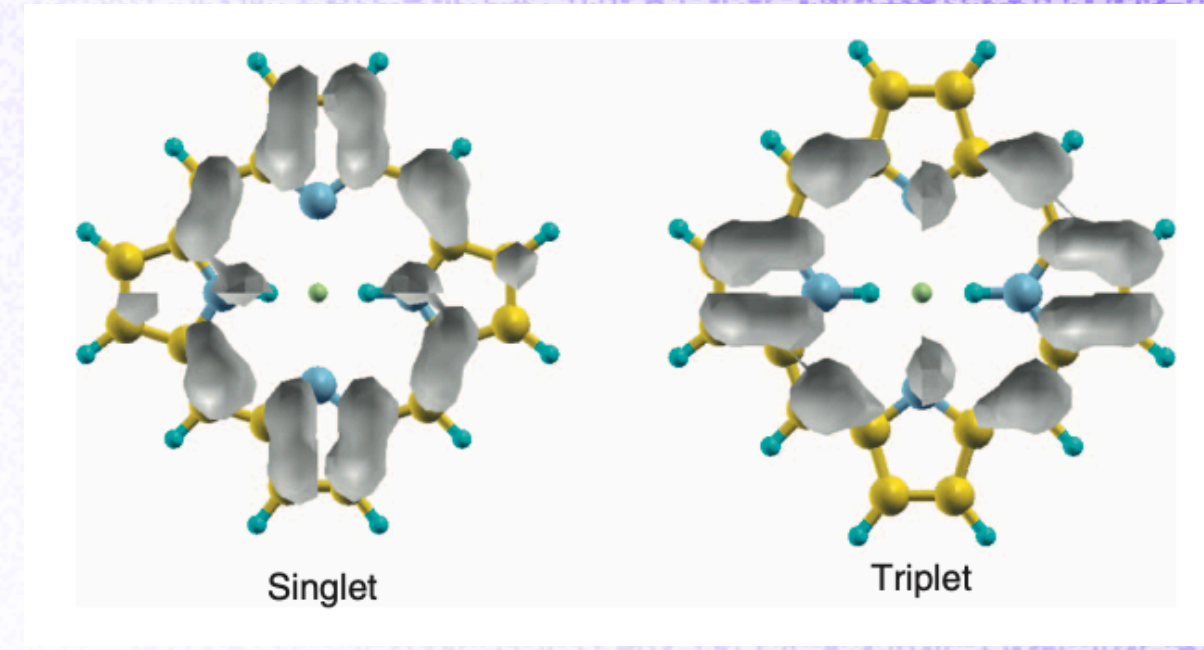
## MOFs



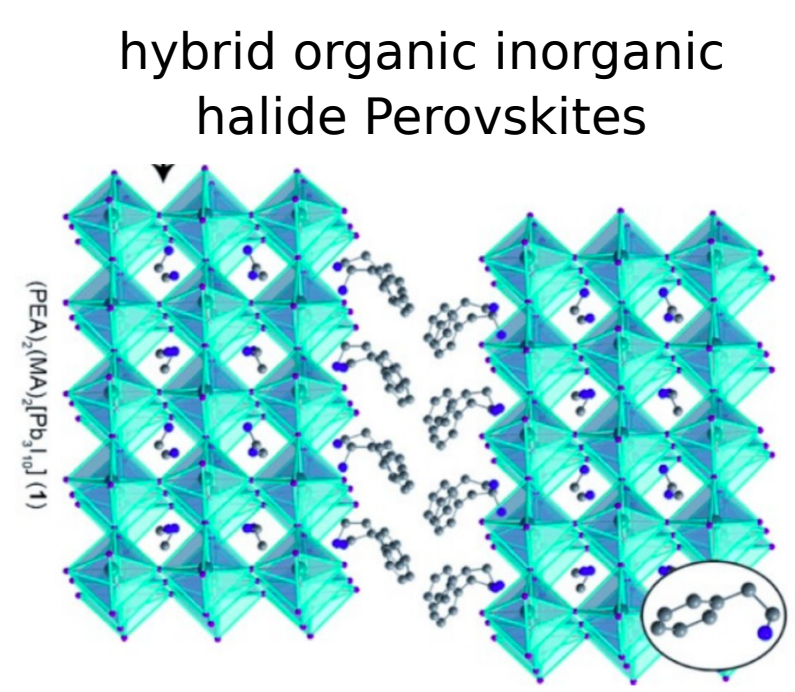
A. Rajan et al J. Phys. Chem. Lett. (2021)



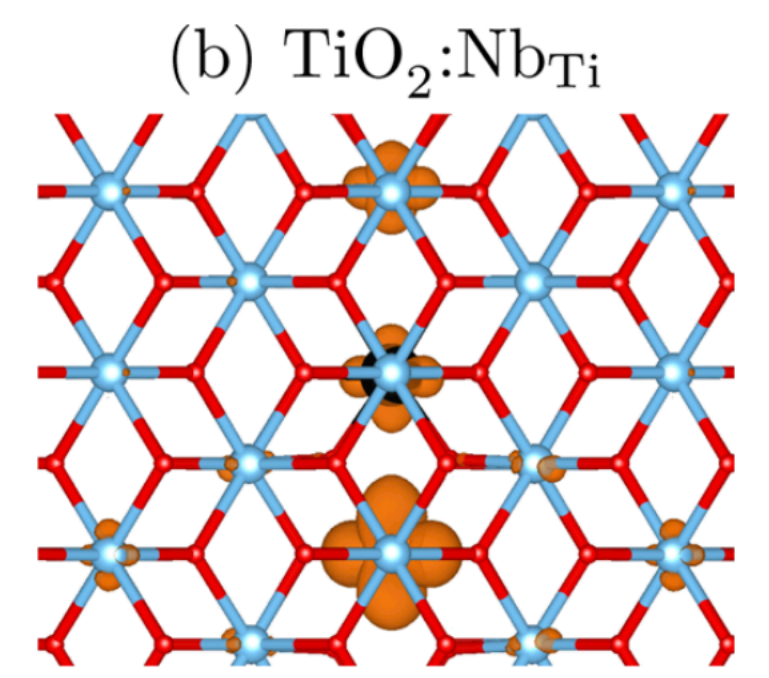
C. Attaccalite et al, Phys. Rev. B 95, 125403 (2017)  
 D. Varsano, D. Sangalli et al. Nature Comm. 8, 1461 (2017)



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

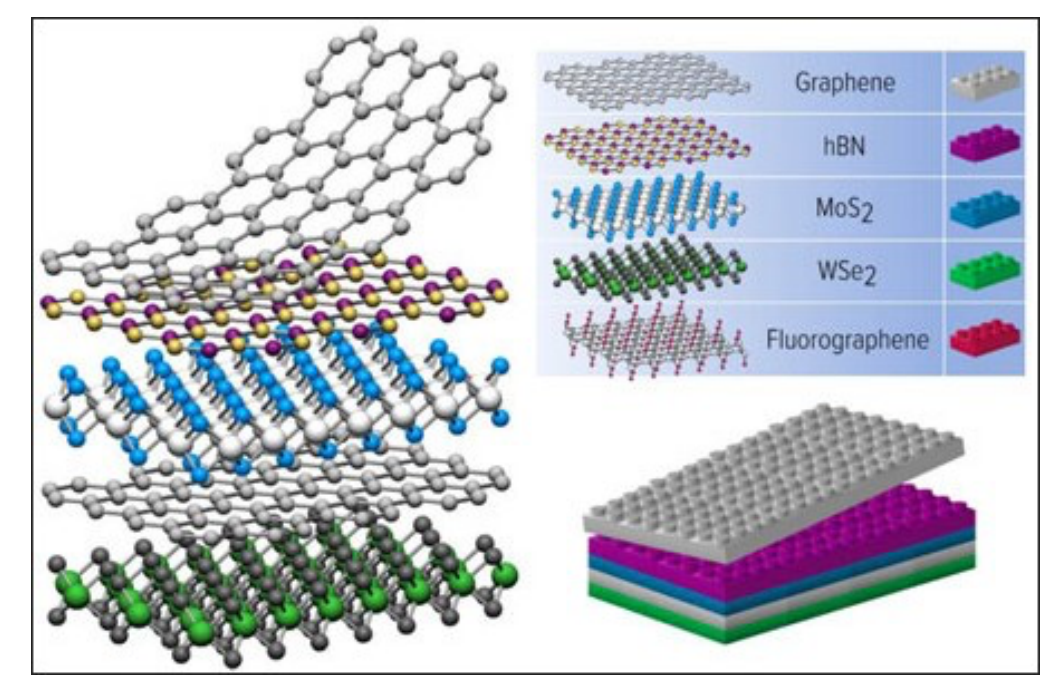


M. Palumbo et al. ACS Energy Letter (2020)

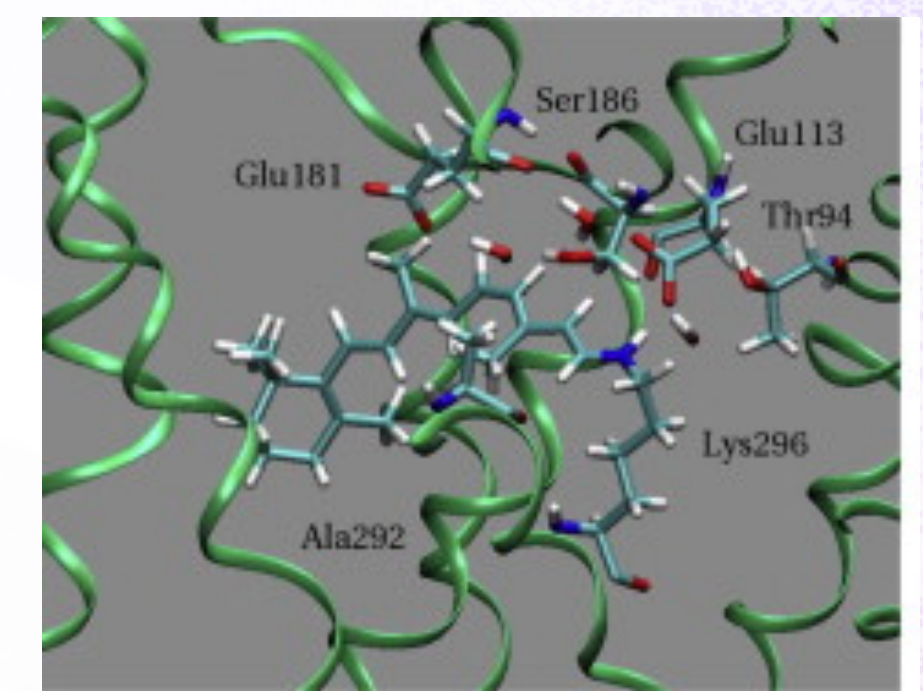


M. Atambo et al. Phys. Rev. Mat (2019)

## 2D materials and heterostructures



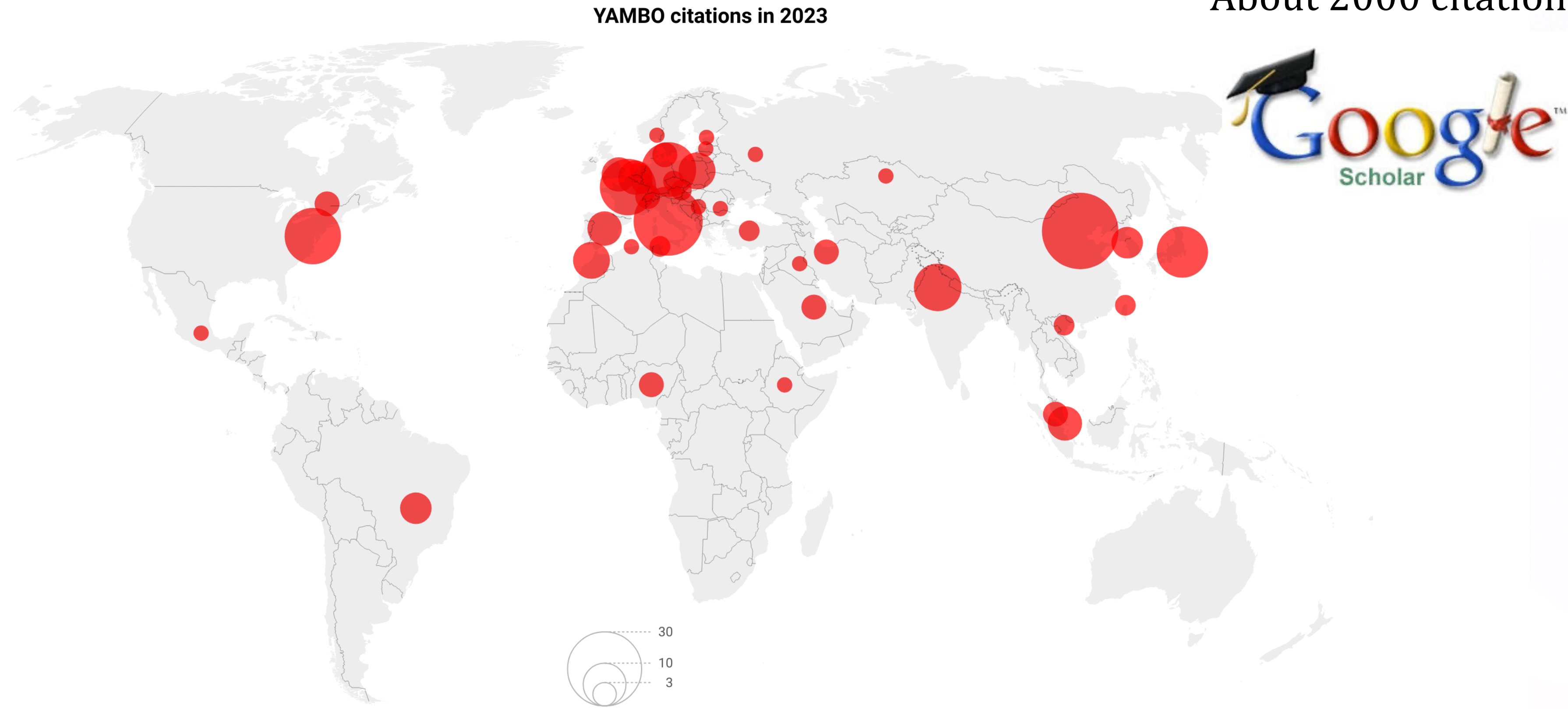
A Molina-Sánchez et al. Nano Lett. (2017)



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

# Yambo Impact

About 2000 citations

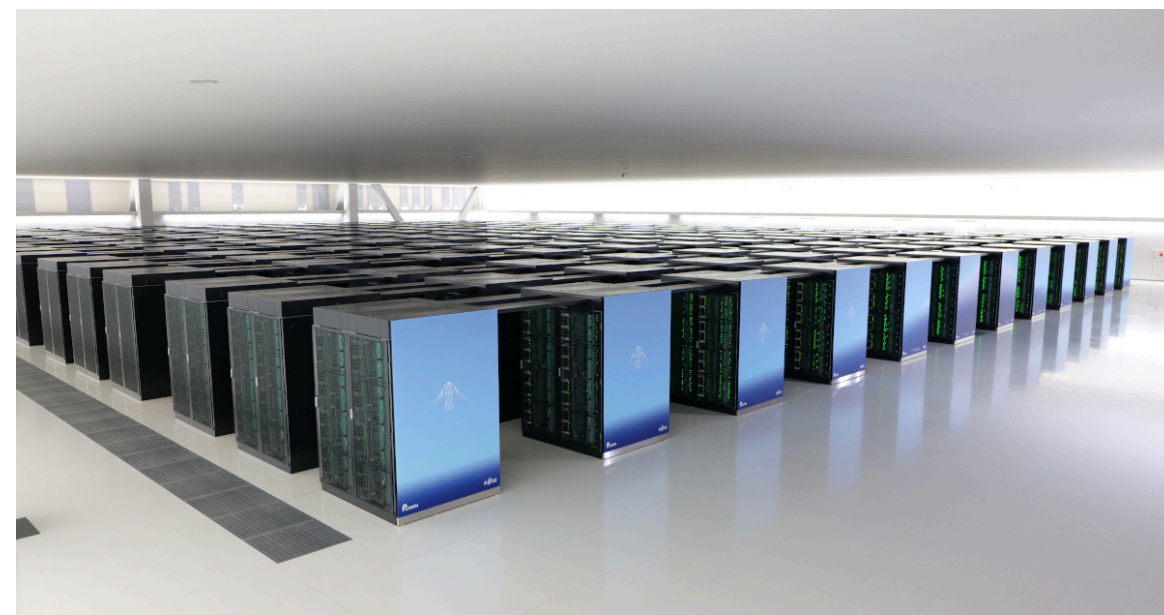


A. Marini, C. Hogan, M. Gruning, D. Varsano, *Comp. Phys. Comm.* **180**, 1392 (2009)

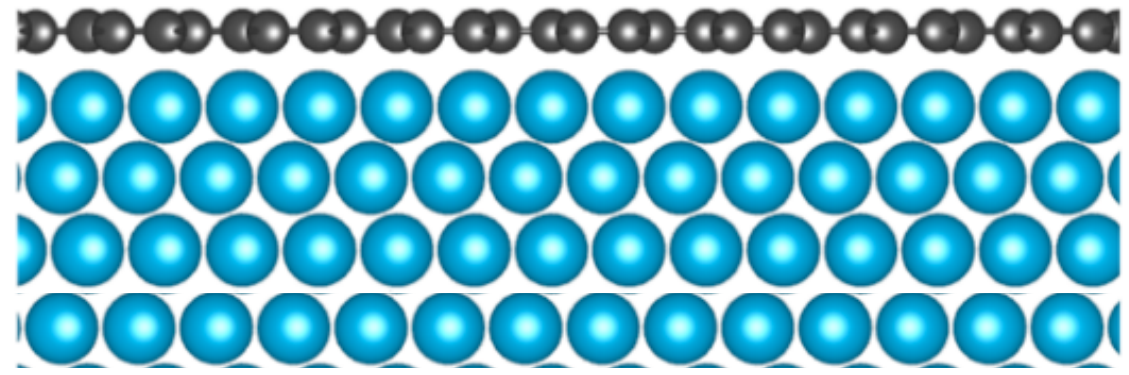
D. Sangalli, et al, *J. Phys.: Condens. Matter.* **31**, 325902 (2019)

# The Yambo code:

Ported in most of EuroHPC machines:



- Yambo **SPACK recipes** updated to support NVIDIA GPU systems
- **Yambo already validated and/or deployed** on several EuroHPC machines, including:
  - Leonardo (booster + DCGP)
  - LUMI-G, LUMI-C
  - Karolina
  - Meluxina
  - Vega
- **Most architectures** relevant to **EuroHPC** covered, including
  - INTEL, AMD host CPU
  - NVIDIA, AMD, INTEL GPUs
  - ARM-based hosts (eg Graviton 3)

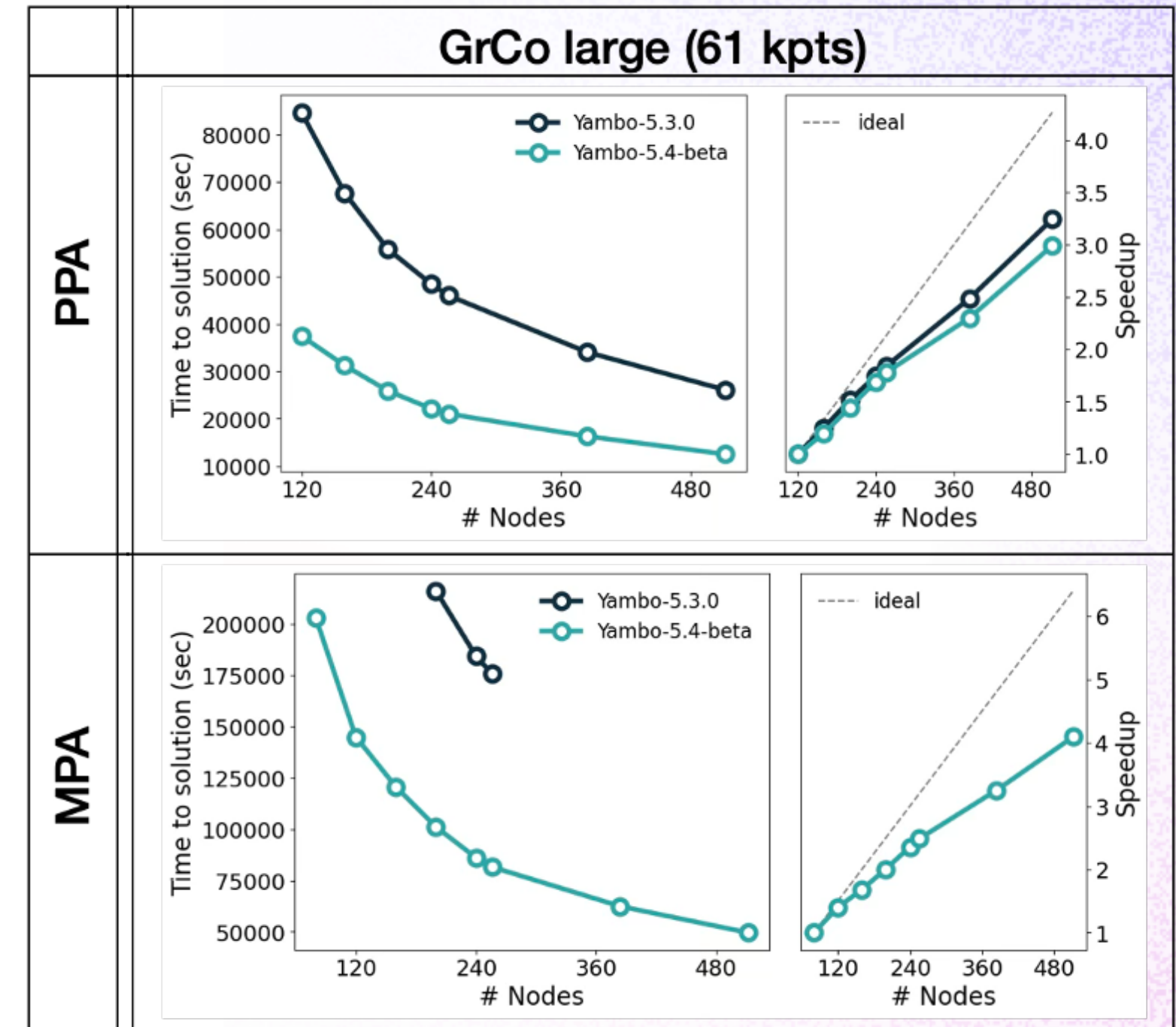
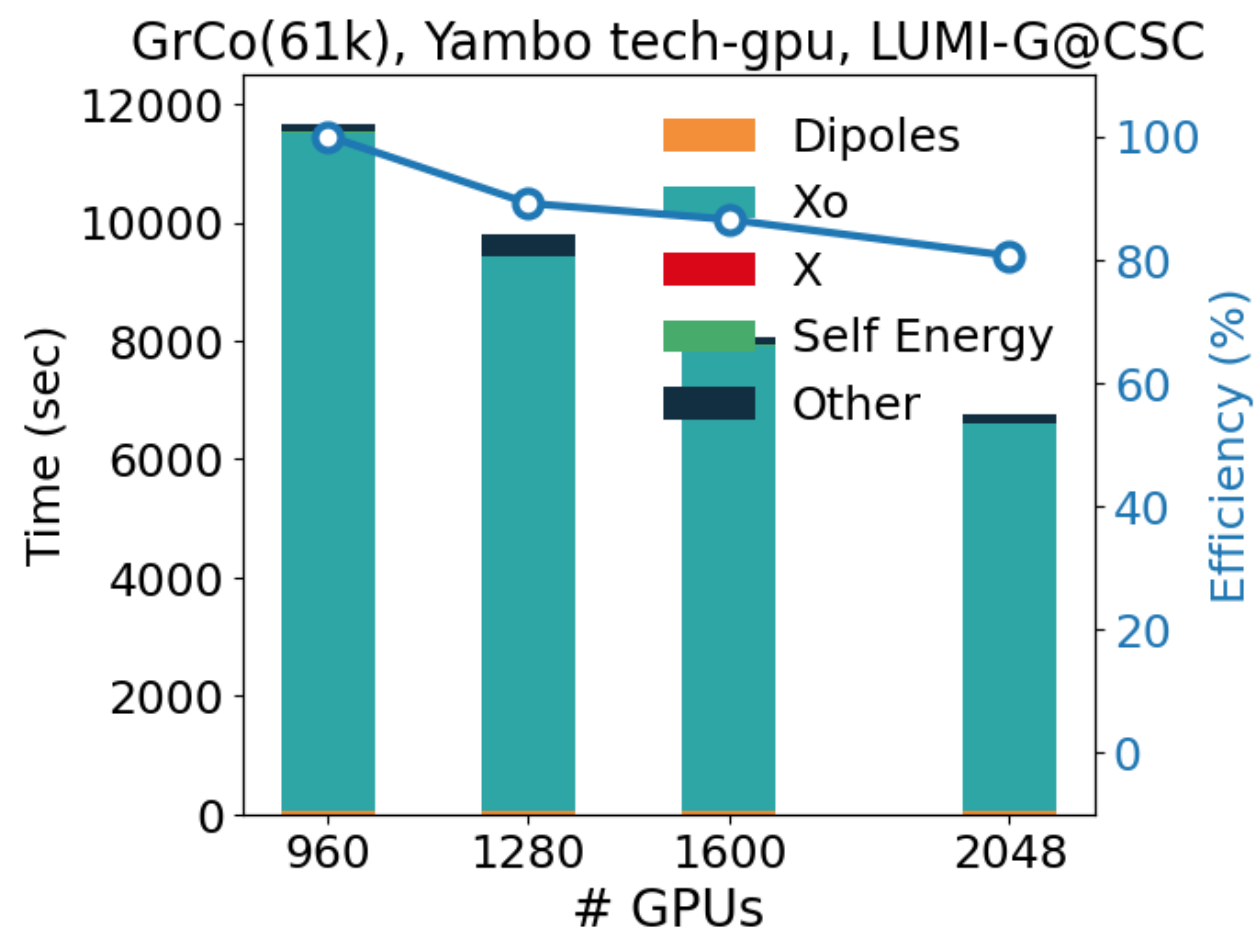
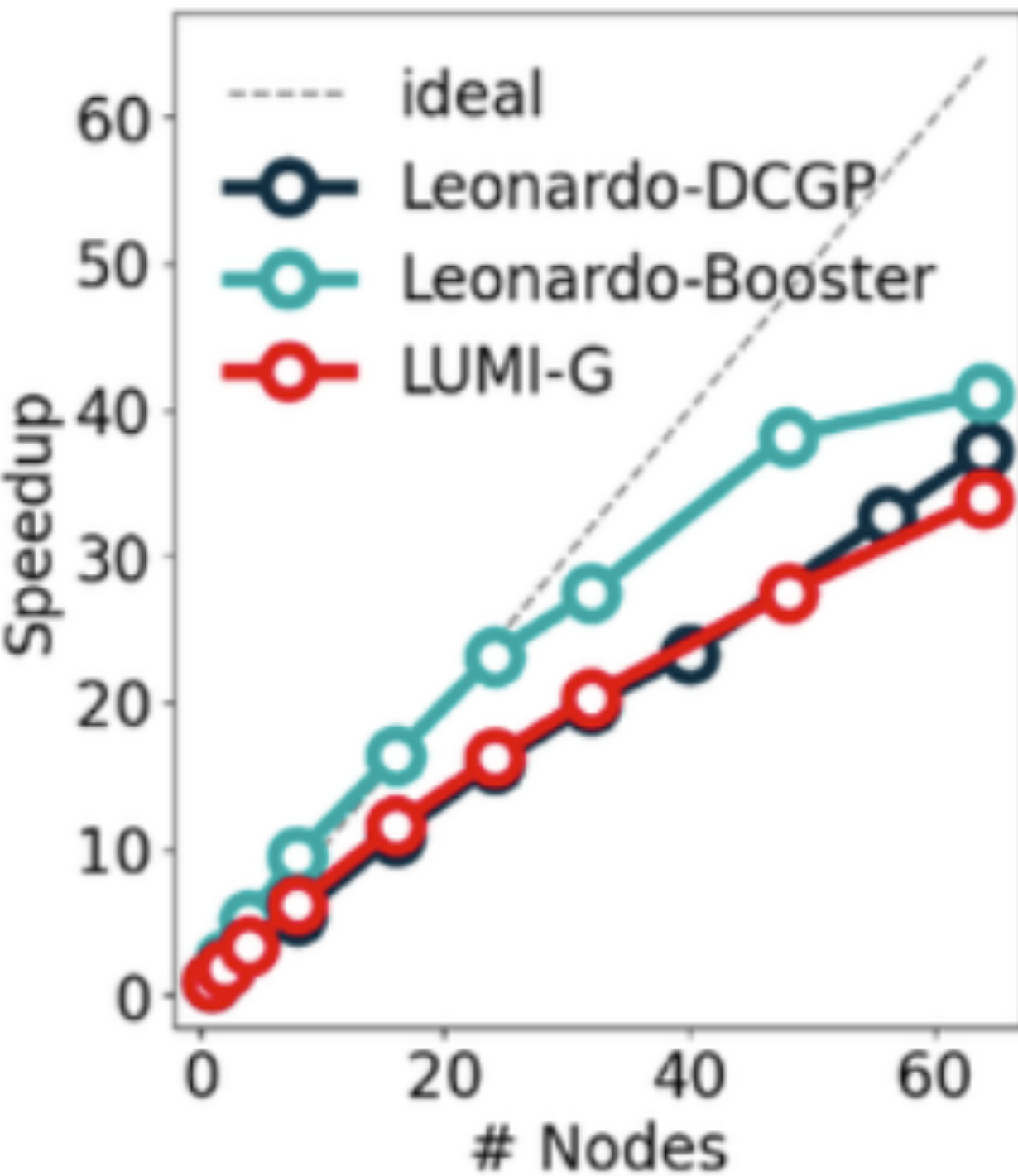
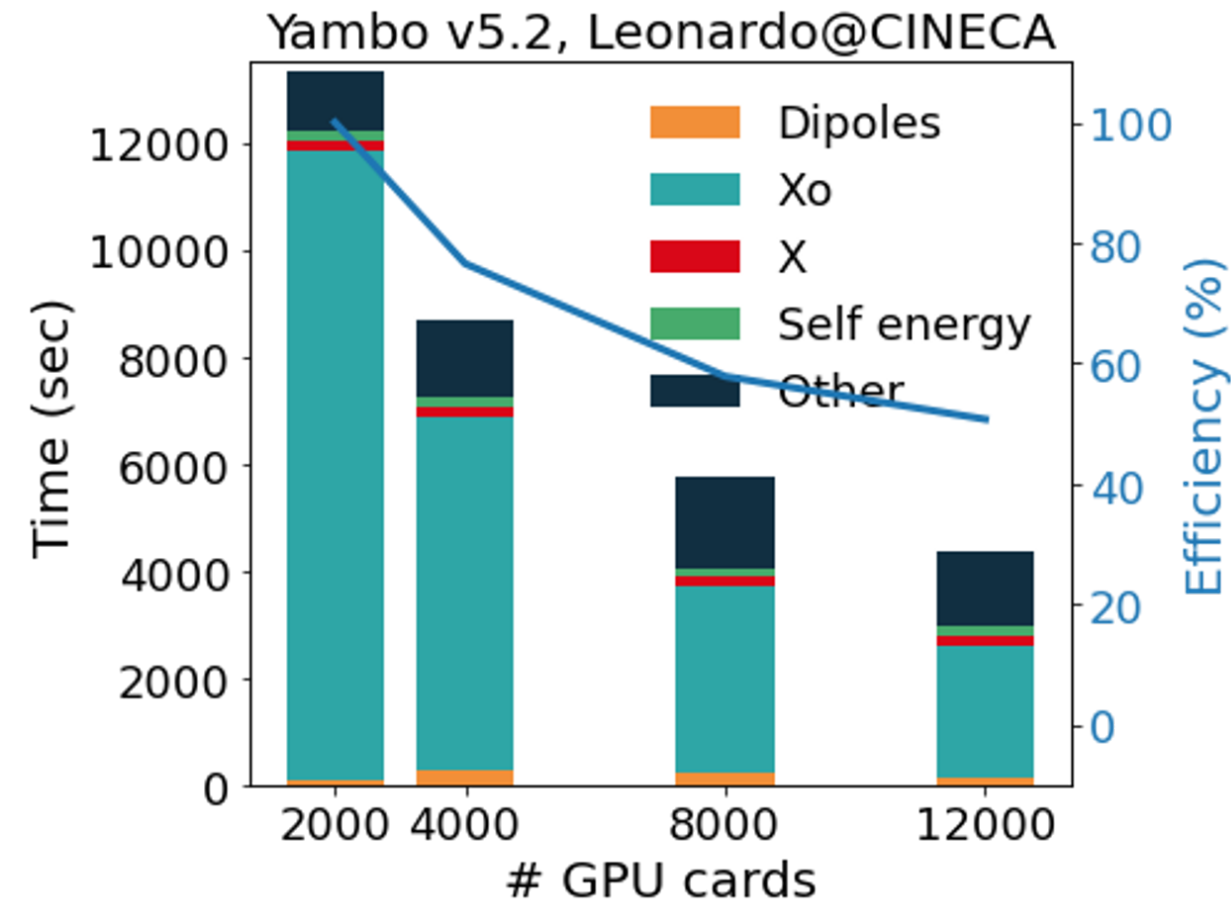


Quasiparticle correction of Graphene / Cobalt interface



**Leonardo @ CINECA:**  
4 Nvidia A100 next / node

**runs:** up to 3000 nodes about 87% of the whole machine (3456 nodes)



## 2023

- Asesma 2023 Kigali (Rwanda)
- Yambo 2023 Rome (Italy)
- Rasesma 2023 Nairobi (Kenya)

## 2024

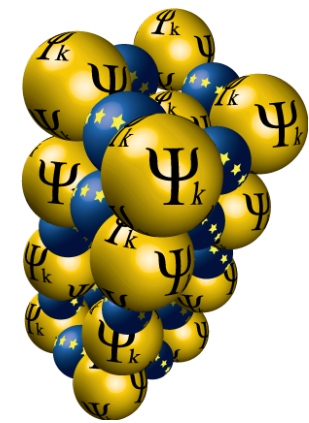
- Workshop on High Performance Computing for Materials Characterization, Design and Discovery Barranquilla (Colombia)
- MAX@ENCCS school
- Yambo@Aiida plugin school

## 2025

- Modena (Italy) May 2025

## 2026

- Kobe (Japan) Jan 2026



Collaboration with renowned institutions and competence centres.

Colombia 2024



Rome 2023



Modena 2025



# Many-Body Perturbation Theory and Excited-State Simulations

## What you will learn:

MBPT Theoretical Foundation:

Linear Response

GW approximation

Absorption spectroscopy and Bethe Salpeter Equation

## Learning Objectives:

How to obtain meaningful results

Awareness of the used approximations

Main algorithms

Accuracy and limitations of the methods

Performance and best practices

Automations and post processing

## How MBPT can be useful for your own research:

**Don't hesitate to ask questions: after the lectures, and during hands-on sessions**



# Program:

## Day 1 :

D. Varsano: **Yambo & MBPT**

C. Cardoso: **Linear Response Theory**

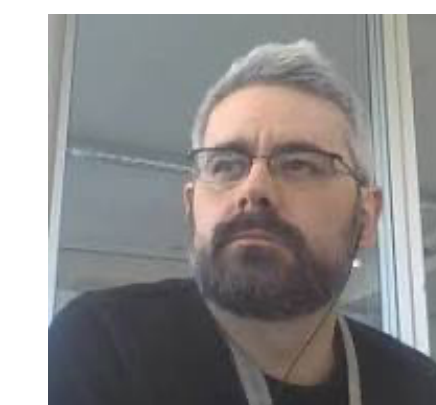
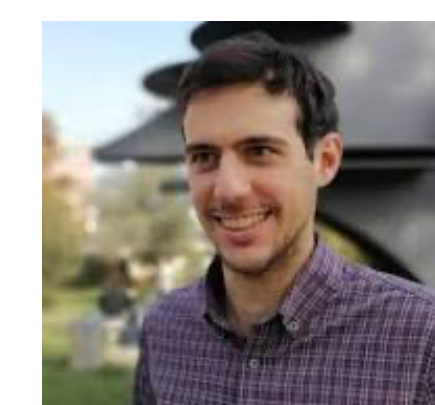


## Day 2 :

A. Ferretti: **Many Body Perturbation Theory and the GW approximation**

G. Sesti : **GW in production: algorithms and approximations**

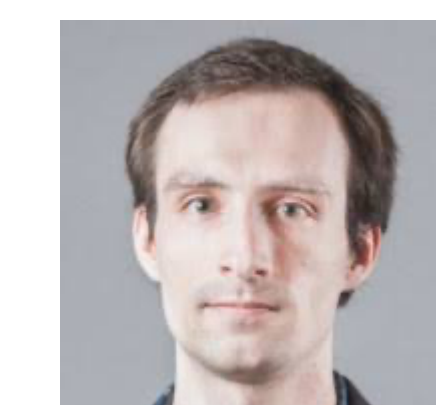
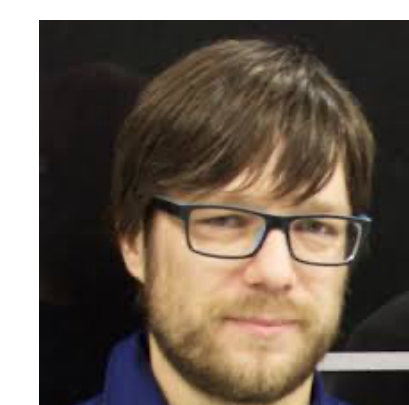
N. Spallanzani : **Parallel strategies and GPU porting**



## Day 3 :

F. Paleari : **The Bethe-Salpeter equation and BSE solvers**

L. Riha/F. Vaverka :



## Hands on:

Practical Sessions with Yambo: **First steps: a walk through from DFT to optical properties**

Practical Sessions with Yambo: **A tour into the GW approximation**

Practical Sessions with Yambo: **Optical absorption and Exciton Analysis**



## Take Home Messages:

- **Density Functional Theory (DFT)** is the workhorse for ground-state electronic structure calculations, enabling accurate predictions of structural and total-energy properties.
- **DFT is not a theory of excited states:** Kohn–Sham eigenvalues generally lack a rigorous interpretation for spectroscopic quantities.
- **Many-Body Perturbation Theory (MBPT)**—most commonly within the **GW and Bethe–Salpeter Equation (BSE)** frameworks—provides an accurate description of electronic and optical excitations.
- In MBPT, the **one-particle Green’s function** is the central object, yielding **quasiparticle energies and lifetimes** directly comparable to spectroscopy.
- Quasiparticle energies are obtained by solving a **nonlinear equation** involving the **self-energy  $\Sigma(\omega)$** , a non-local and dynamical potential, usually approximated as GW.

## Take Home Messages:

- **MBPT calculations are significantly more computationally demanding than DFT**, typically restricting applications to systems about **one order of magnitude smaller**.
- Today, MBPT (**G0W0**) is feasible for **medium-size systems**, thanks to scalable algorithms and **HPC architectures**, including hybrid CPU/GPU platforms; **exascale computing is a game-changer**.

**DFT tells us where the electrons “are”; MBPT tells us how they are observed.**

# Useful Links:



<https://wiki.yambo-code.eu>

<https://yambo-code.github.io/yambo-wiki/>



## Instruction for the tutorials

- 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

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

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

**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)

**nk, n'k' ranges where GW/ $\Sigma_c$  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>

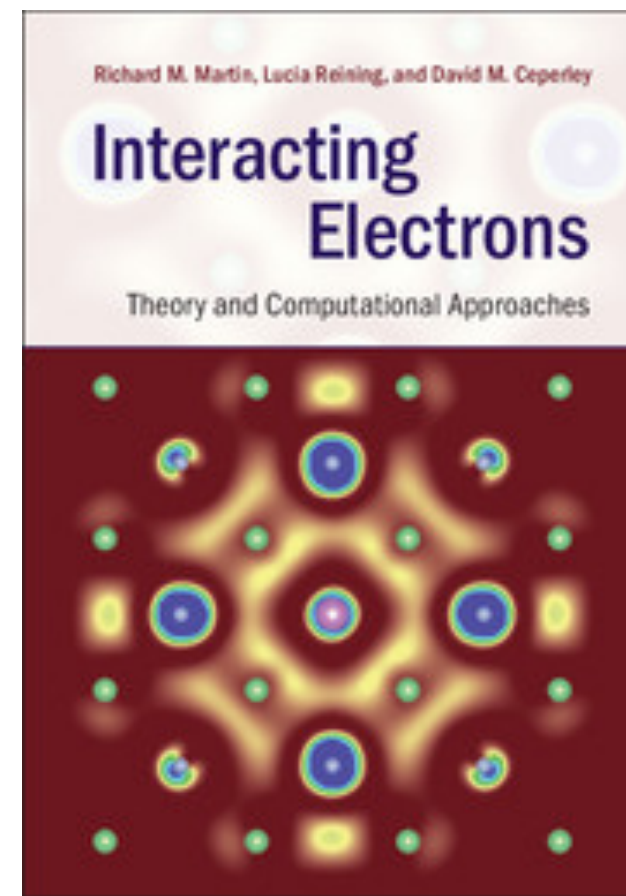


<https://yamboschools.slack.com/archives/C0B2GUHL5C0>

SUBFORUMS		STATISTICS
<p><b>Announcements and Job offers</b> A subforum where you can post Announcements and Job offers related with the Yambo code. Moderators: <b> Davide Sangalli, andrea.ferretti, myrta gruning, andrea marini, Daniele Varsano, Conor Hogan</b></p>		Topics: 13 Posts: 24
<p><b>Compilation</b> 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: <b> Davide Sangalli, andrea.ferretti, myrta gruning, andrea marini, Daniele Varsano, Conor Hogan, Nicola Spallanzani</b></p>		Topics: 219 Posts: 1499
<p><b>Importing core databases (a2y, p2y and e2y)</b> Forums dealing with all aspects related to conversion of data from Abinit, PWscf or ETSF-io into the native Yambo core databases. Moderators: <b> andrea.ferretti, Conor Hogan</b> Subforums: <a href="#">PW</a>, <a href="#">Abinit</a></p>		Topics: 96 Posts: 513
<p><b>Running Yambo</b> 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: <a href="#">Linear Response and Screening in reciprocal space</a>, <a href="#">GW calculations</a>, <a href="#">Bethe Salpeter</a>, <a href="#">Electron-Phonon effects (yambo_ph)</a>, <a href="#">Non linear optics (yambo_nl)</a>, <a href="#">Real time propagation (yambo_rt)</a>, <a href="#">Other issues</a></p>		Topics: 1100 Posts: 6576
<p><b>Post Processing (ypp)</b> Anything regarding the post-processing utility (e.g. excitonic wavefunction analysis) is dealt with in this forum. Moderators: <b> Davide Sangalli, andrea marini, Daniele Varsano</b></p>		Topics: 225 Posts: 1265
<p><b>Yambo-py</b> 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: <b> amolina, palful, mbonacci</b></p>		Topics: 69 Posts: 219
<p><b>Technical Issues</b> Various technical topics such as parallelism and efficiency, netCDF problems, the Yambo code structure itself, are posted here. Moderators: <b> Davide Sangalli, andrea.ferretti, myrta gruning, andrea marini, Daniele Varsano, Conor Hogan, Nicola Spallanzani</b></p>		Topics: 110 Posts: 618
<p><b>Yambo old versions</b> You can find here problems arising when using old releases of Yambo (&lt; 5.0). Issues as parallelization strategy, performance issues and other technical aspects. Moderators: <b> Davide Sangalli, andrea.ferretti, myrta gruning, andrea marini, Daniele Varsano, Conor Hogan</b></p>		Topics: 251 Posts: 1425

## 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:

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

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

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

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

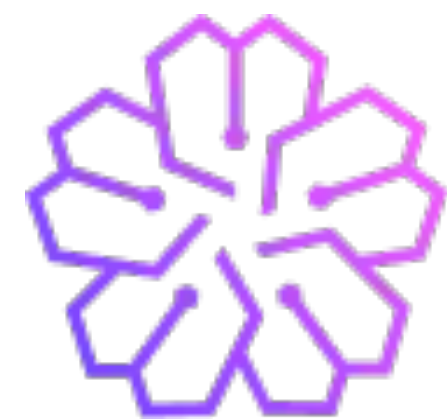
### Yambo code implementation:

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:



HANAMI

**EU-Japan Alliance in HPC**



**MaX (Materials design at the eXascale)**



Thank you for your attention