Modeling excitons in bulk and single-layer hBN

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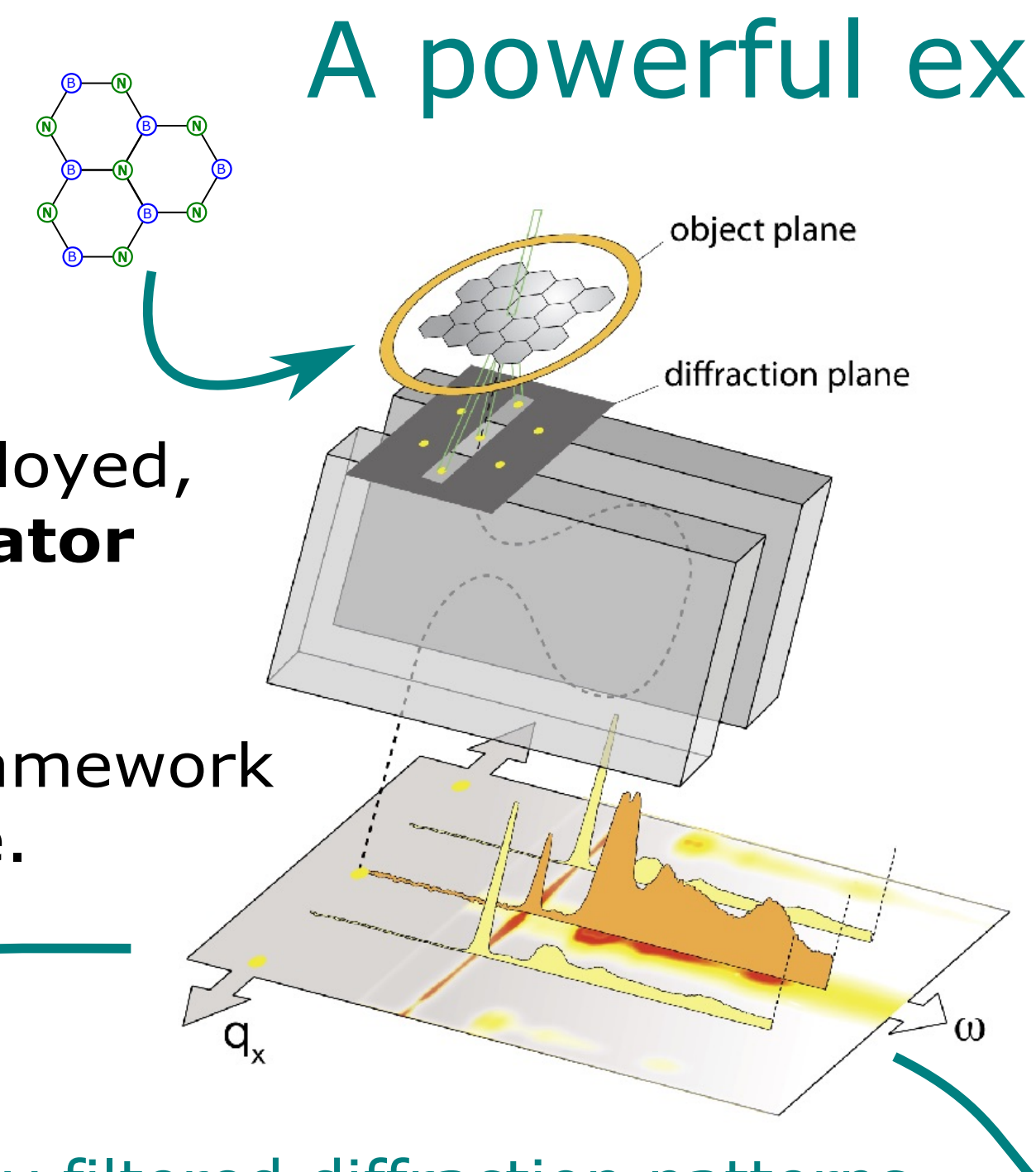
spectroscopic measurements and *ab-initio* simulations of bulk AA'

A powerful experimental setup



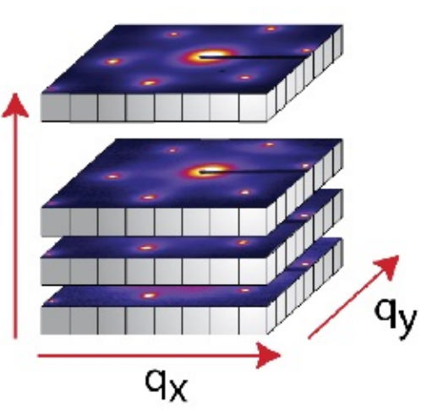
Depending on the filter employed, **monochromator or slit**, two different acquisition framework are accessible.

The **energy-filtered transition electron microscope** permits the acquisition of electron energy loss spectra (EELS) in the form of a ***datacube***.

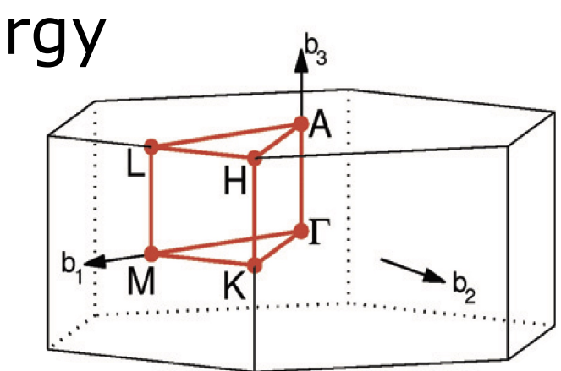
ab-initio EELS within the **random phase approximation** (RPA) reproduces correctly **in-plane excitations**.

energy filtered diffraction patterns

horizontal slices

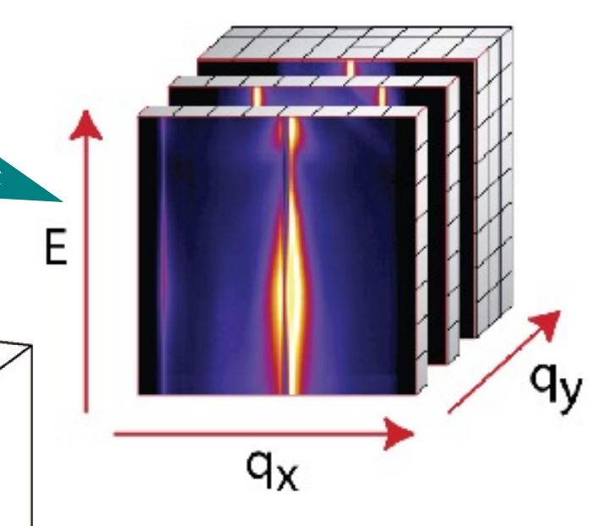


losses of a given energy are mapped on planes of the reciprocal-space.



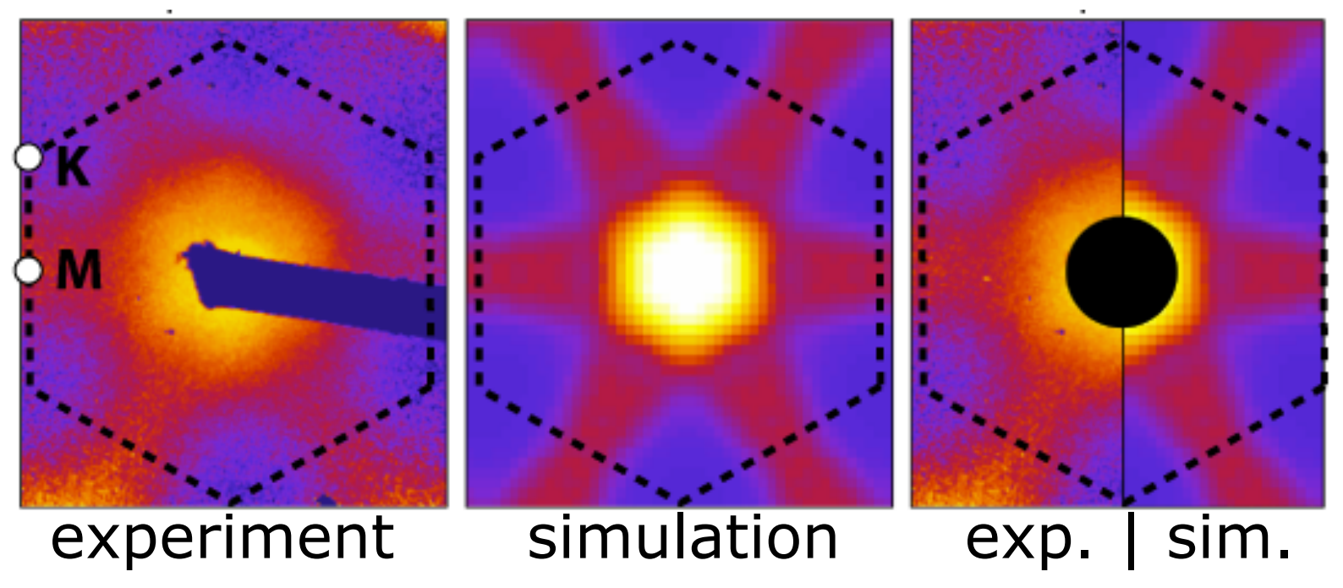
selecting the direction with a slit

vertical slices: ω-q maps

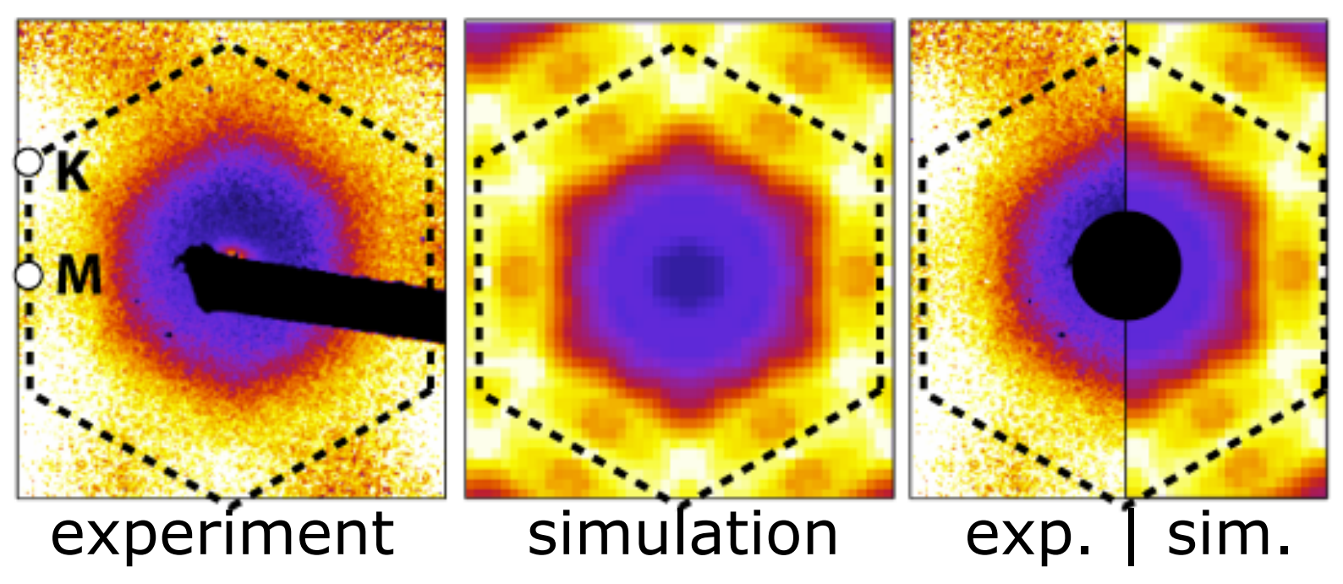


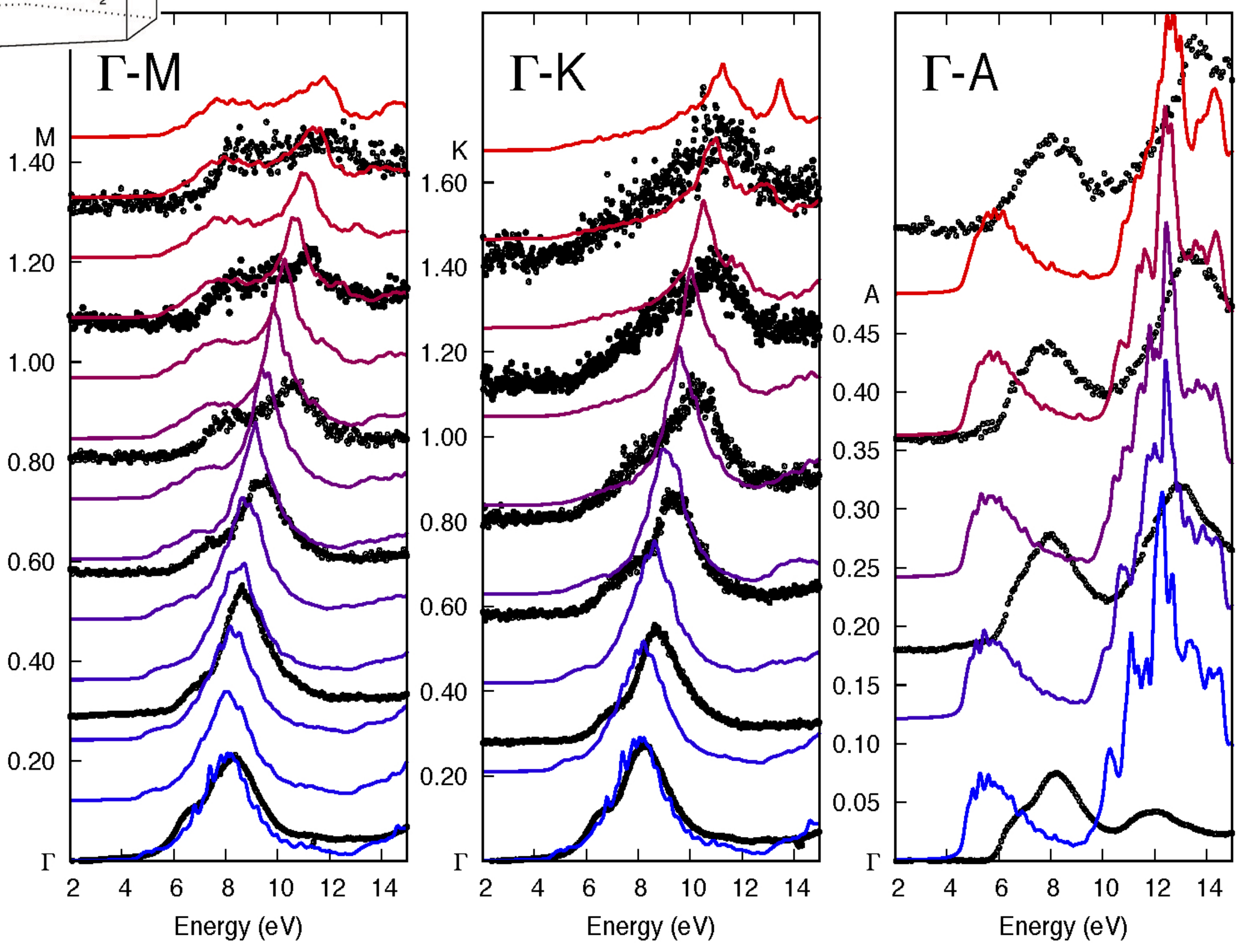
The loss function is recorded simultaneously for several transferred momenta.

cut at 8 eV

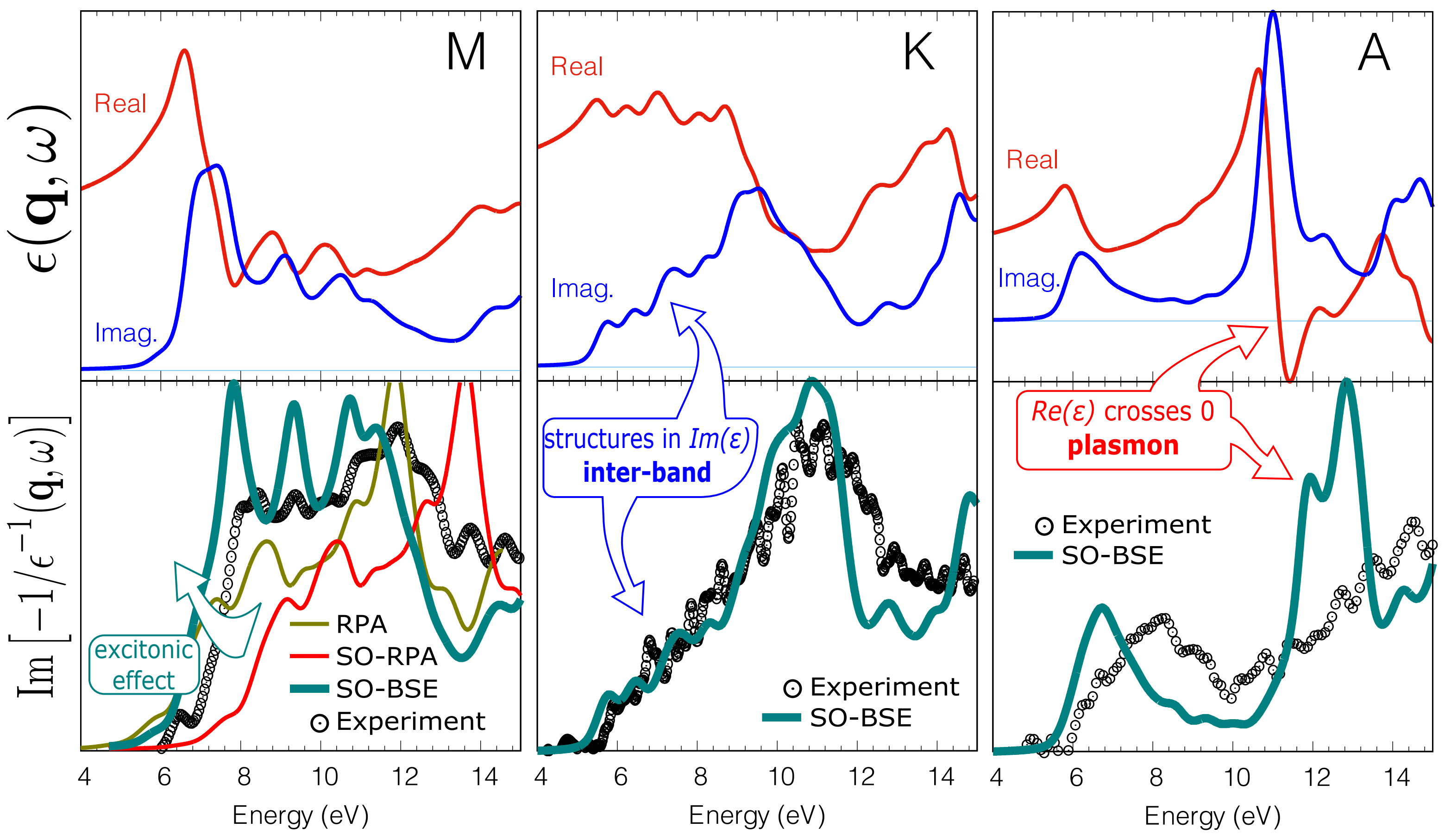


cut at 12 eV





Analysis of the excitations



Solving the **Bethe-Salpeter equation** (BSE) accounts quantitatively for **excitonic effects** in the **complex dielectric function** at **different momenta**.

The comparison between different levels of the theory and of different quantities allow for **thorough analysis** and **great insight**.

details and references

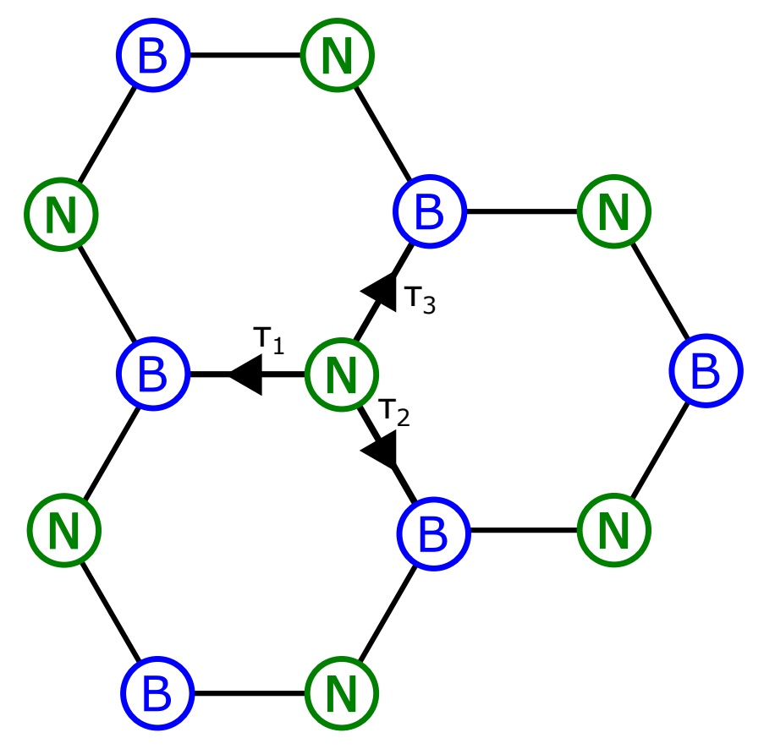
RPA calculations	**BSE calculations**
code: GPAW	code: GPAW
k-point grid: 24x24x8 Γ-centered	k-point grid: 12x12x4(8) Γ-centered
N. bands: 20	N. bands: 20, 6 valence + 8 conduction
cutoff: 60 eV	cutoff: 60 eV
	scissor operator: 1.73 eV

Paper submitted. See also *arXiv:1701.05119*

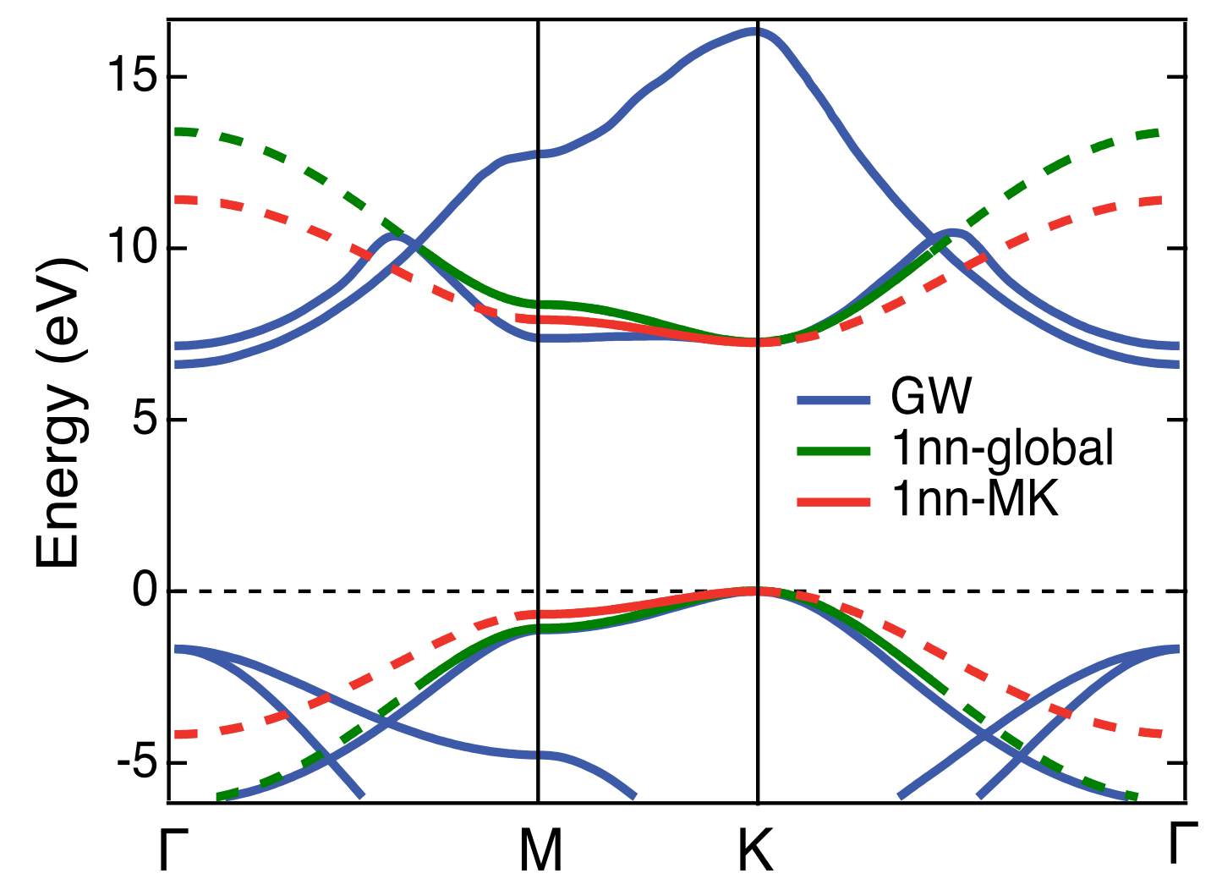
single-layer with simple tight-binding model

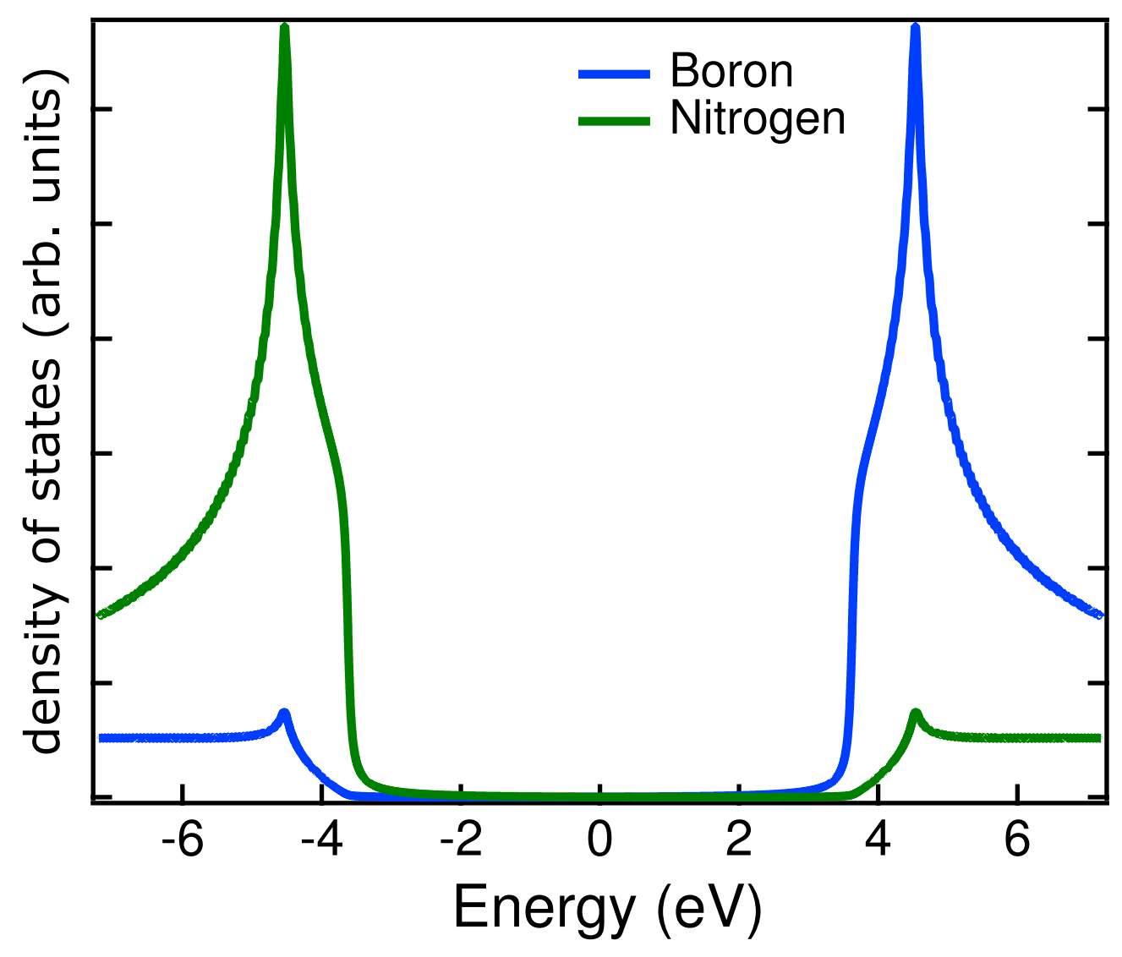
The single-layer is an **ideal system for a tight-binding model** because of the relatively simple band structure close to the gap.

single-particle properties



Two parameters are enough to give a good description of single-particle properties:
1) the hoping integral T, adjusted on the **band dispersion** and
2) the difference of in-site energies, parametrised from **the gapwidth**.



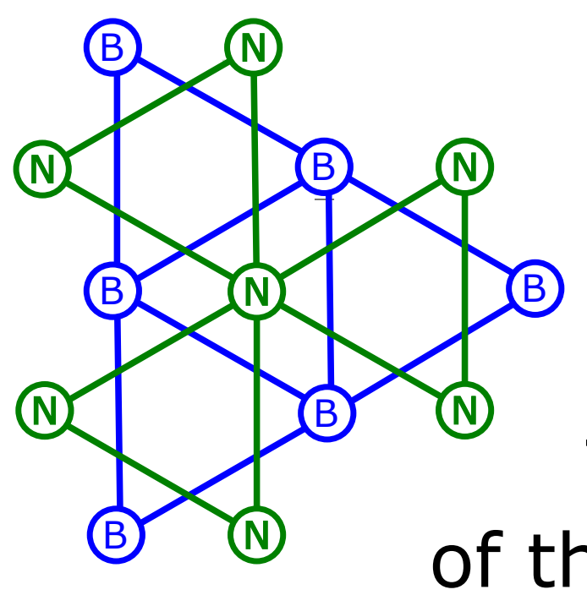


Paper in preparation

On the tight-binding model see also *Phys. Rev. B 94, 125303 (2016)*
On the dispersion see also *Phys. Rev. Lett. 116, 066803 (2016)*

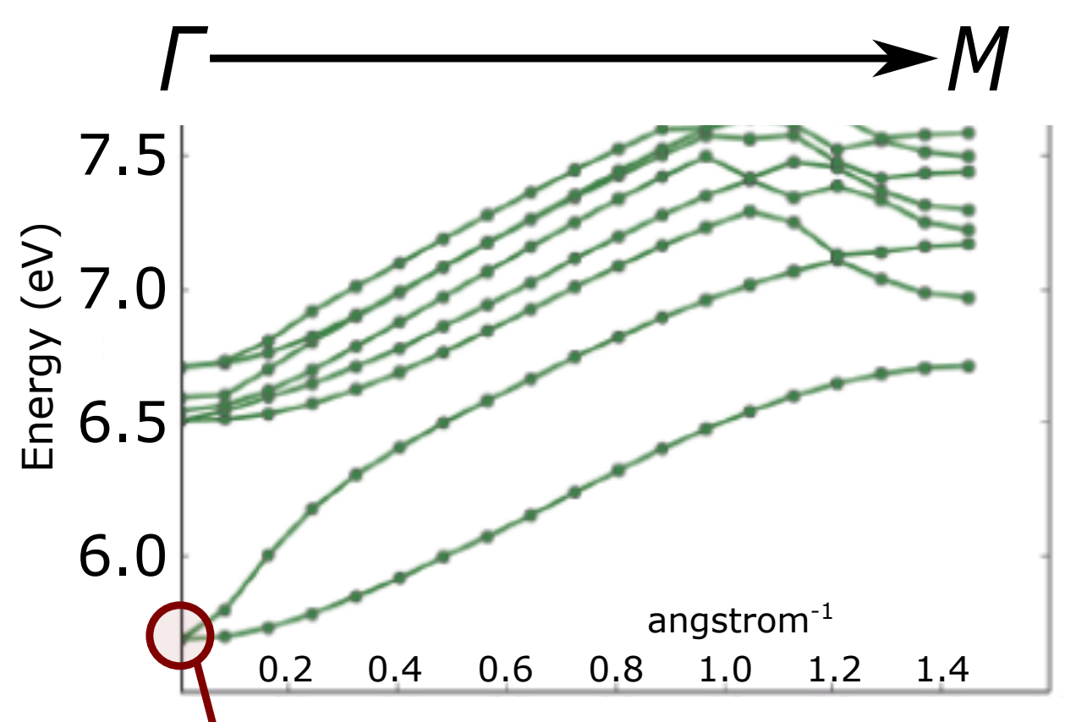
two-particle neutral excitations (excitons)

Two intercalated triangular lattices.
1) electrons move on π^* orbitals of B,
2) holes move on π orbitals of N.
The model predicts **excitonic features** (wavefunction, dispersion ...) in close agreement with BSE.

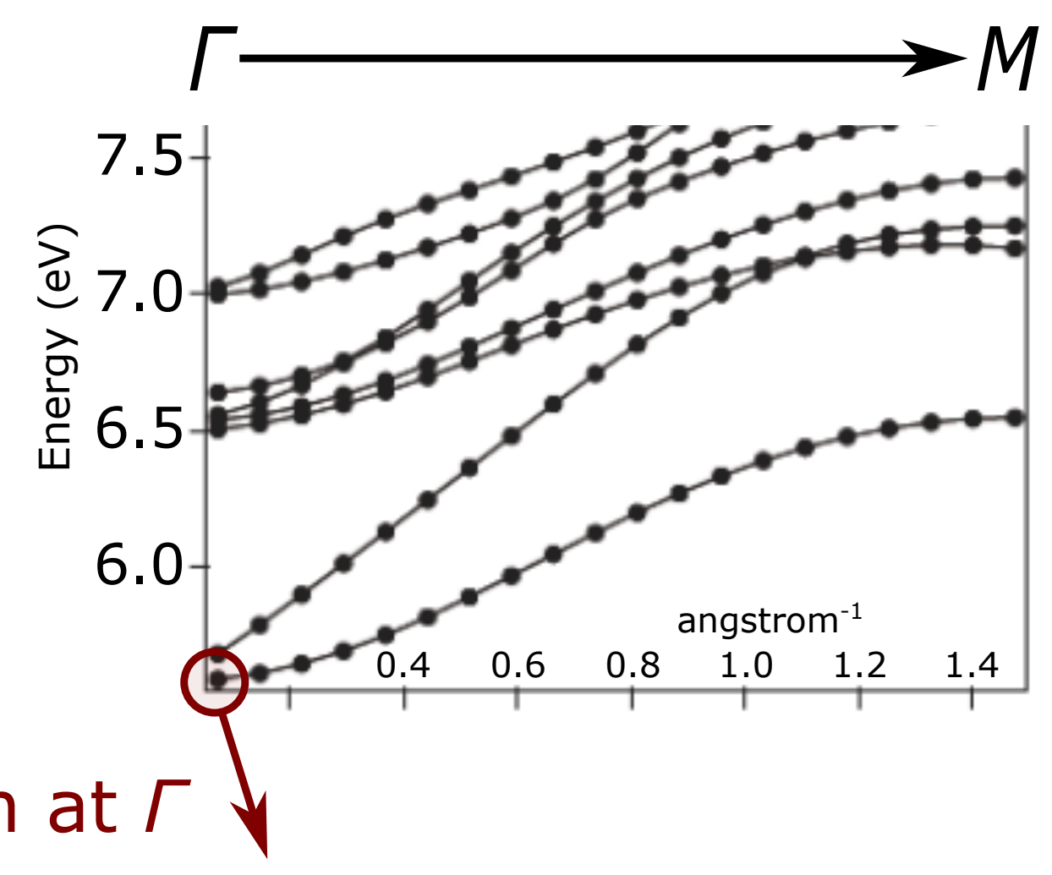


The **simplicity** of the tight-binding framework and its formulation in **real-space** permit **clear and insightful** interpretations

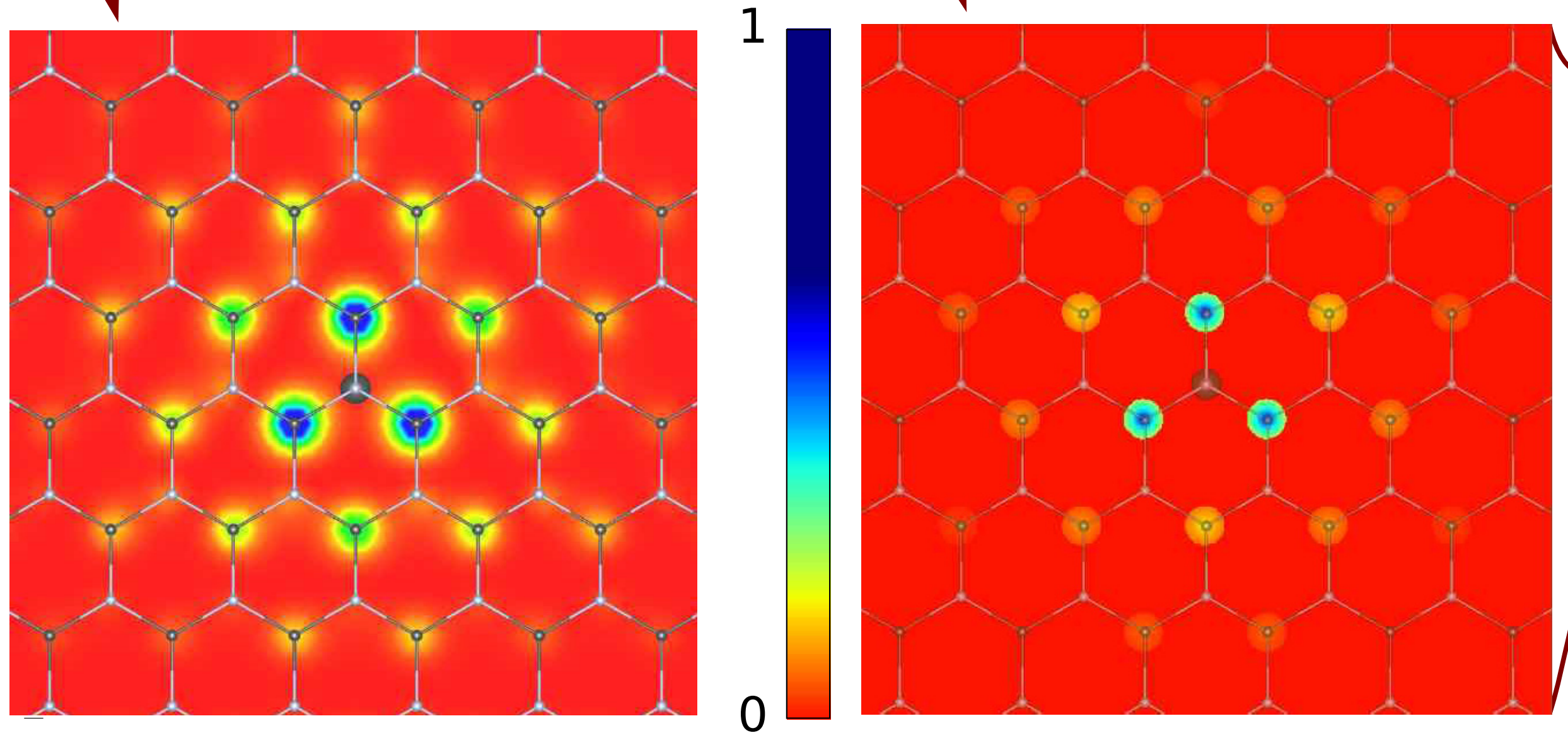
BSE dispersion



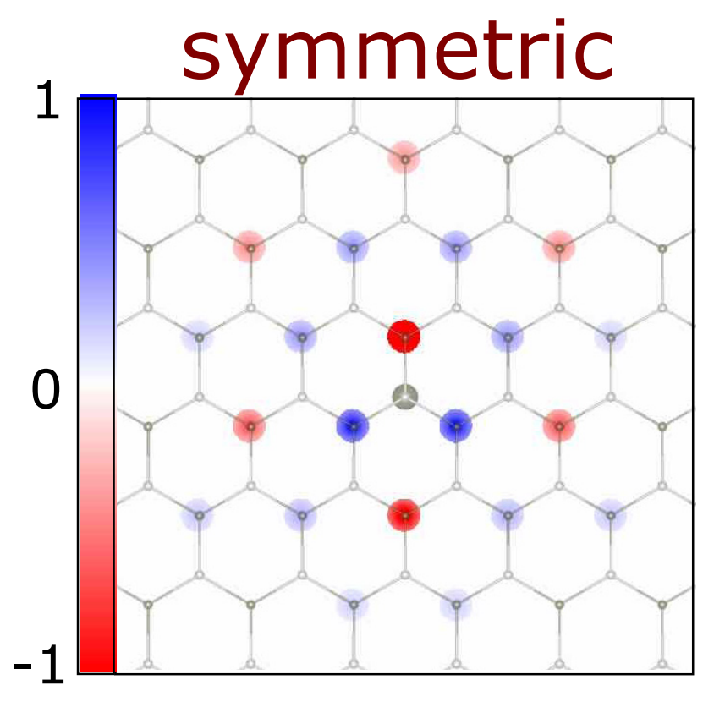
tight-binding



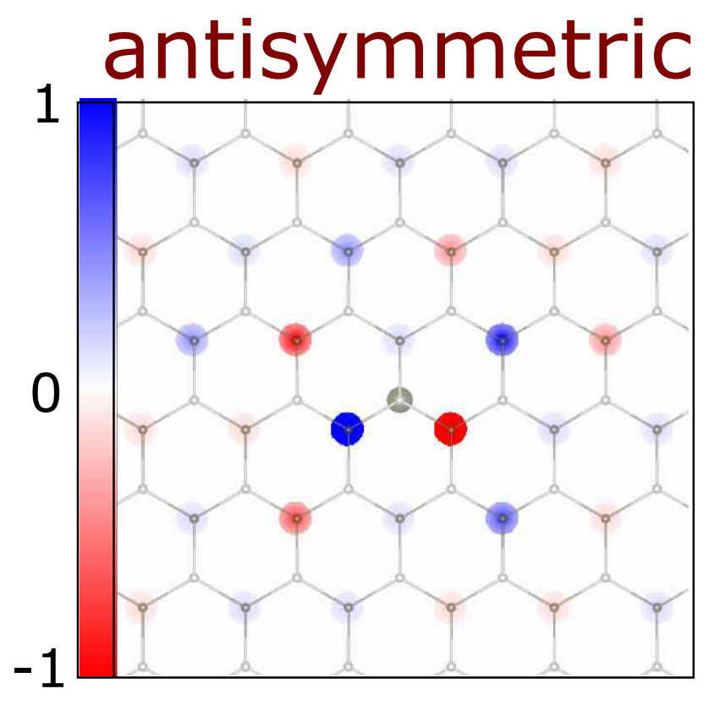
excitonic wave function at Γ



symmetric



antisymmetric



Conclusions and future development

- The **energy-filtered transition electron microscope** is a powerful technique providing accurate information on the electronic structure, especially conceived for the investigation of **electronic excitations at small *q***.
  Thanks to its simplicity, the experimental setup is **particularly suited for 2D systems**.
- The *ab-initio* simulations have been validated rigorously against experiment in AA' bulk hBN,
  the tight-binding model has been parametrised using *ab-initio* calculations and validated against BSE results on the single-layer hBN.
- The two theoretical approaches can be combined in a **promising and versatile strategy:**
  1) First one performs accurate ***ab-initio* simulations on benchmark systems** (bulk, single-layer, building blocks...);
  2) Then one **optimizes the parameters of the tight-binding** model using the results of the benchmark simulations;
  3) Finally one applies the tight-binding model to more **complex structures** (allotropes, heterostructures, defects, impurities....).