# Exciton interference in hexagonal boron nitride

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**Preprint available:**

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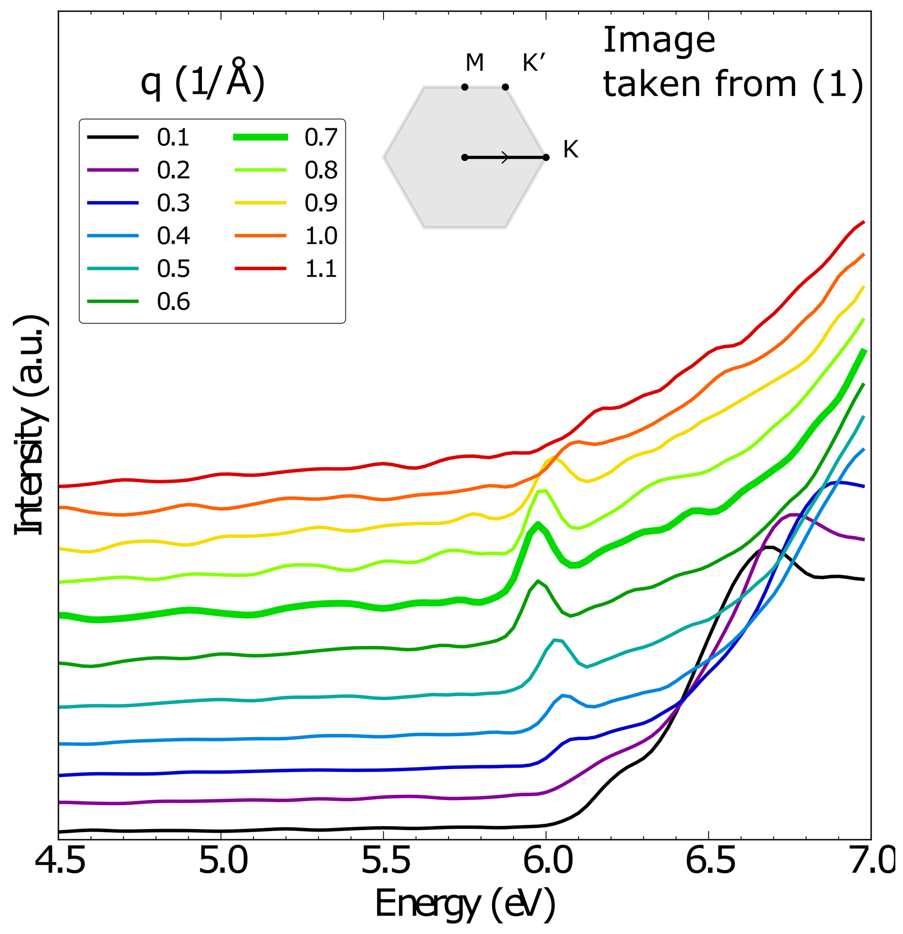
## High-accuracy electron energy loss (1)




High-accuracy electron energy loss spectroscopy (EELS) has been carried out on bulk-hBN along the ΓK direction (1).

Dispersive peak of excitonic nature.

**q=0.7$Å^{-1}$ : minimum energy & maximum intensity**

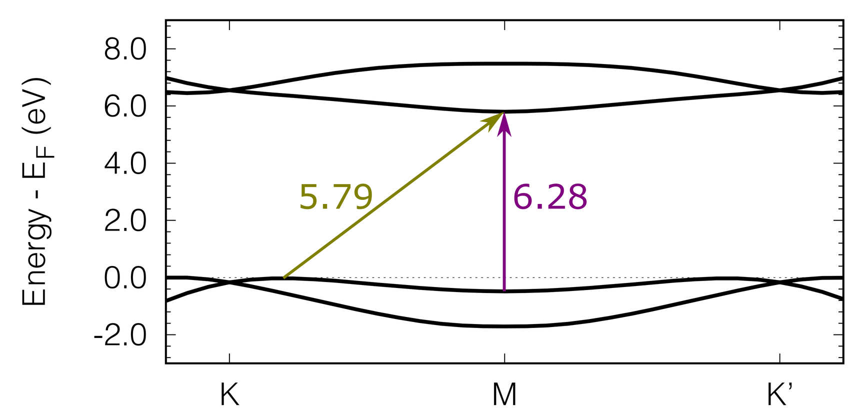
**q=1.1$Å^{-1}$ almost disappears**

(1) Scuster et al, arXiv:1706.04806v1 (2017)

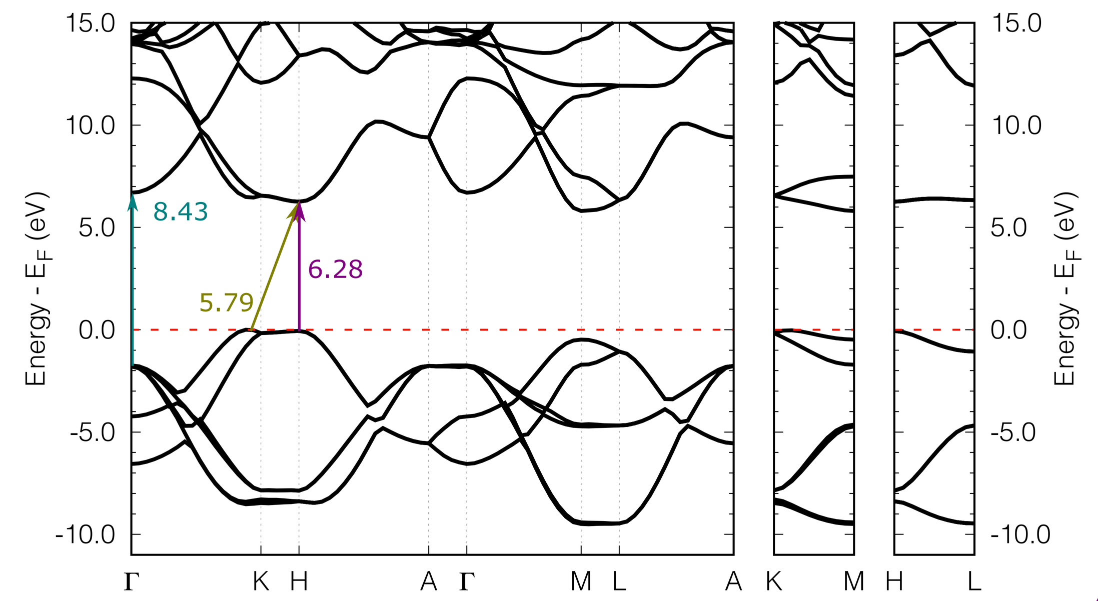
## Single-particle band structure: $G_0W_0$ at LDA

Band structure of bulk hBN (AA' stacking) has **indirect gap** between a **point close to *K* and *M*.** Established theoretical result.

| gap | LDA | $G_0W_0$ |
|---|---|---|
| direct at Γ | 6.42 | 8.43 |
| indirect ($\approx K \to M$) | 4.73 | 5.79 |
| smallest optical ($M$) | 4.46 | 6.28 |

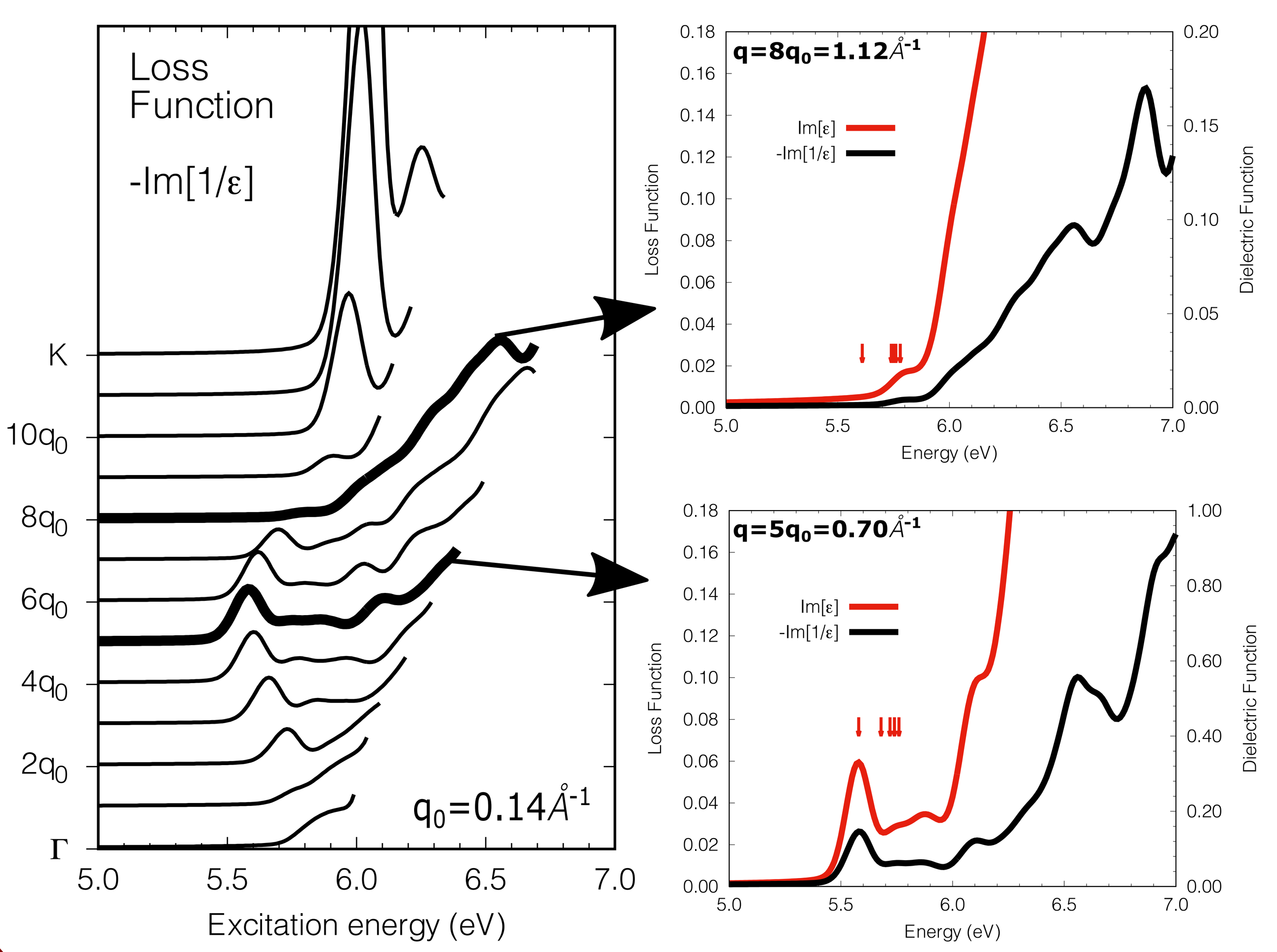



**Computational details:**
- contour deformation
- nbands=600
- cutoff wfn.=816 eV
- cutoff mat.dim.=816 eV
- Γ-centered 6x6x4




## GW-BSE Excitonic spectra and dispersion

### GW-BSE spectra along ΓK




An additional **shift of 0.4 eV** to align to experiments for the **lack of self-consistency in GW.**

The GW-BSE dispersion of the loss function **perfectly reproduces** the experimental dispersion of the peak.

The intensity of the loss function is **maximum at q=5q0** and **mnimum at q=8q0**
Intensity and dispersion of loss function follow the peaks of the **dielectric function.**

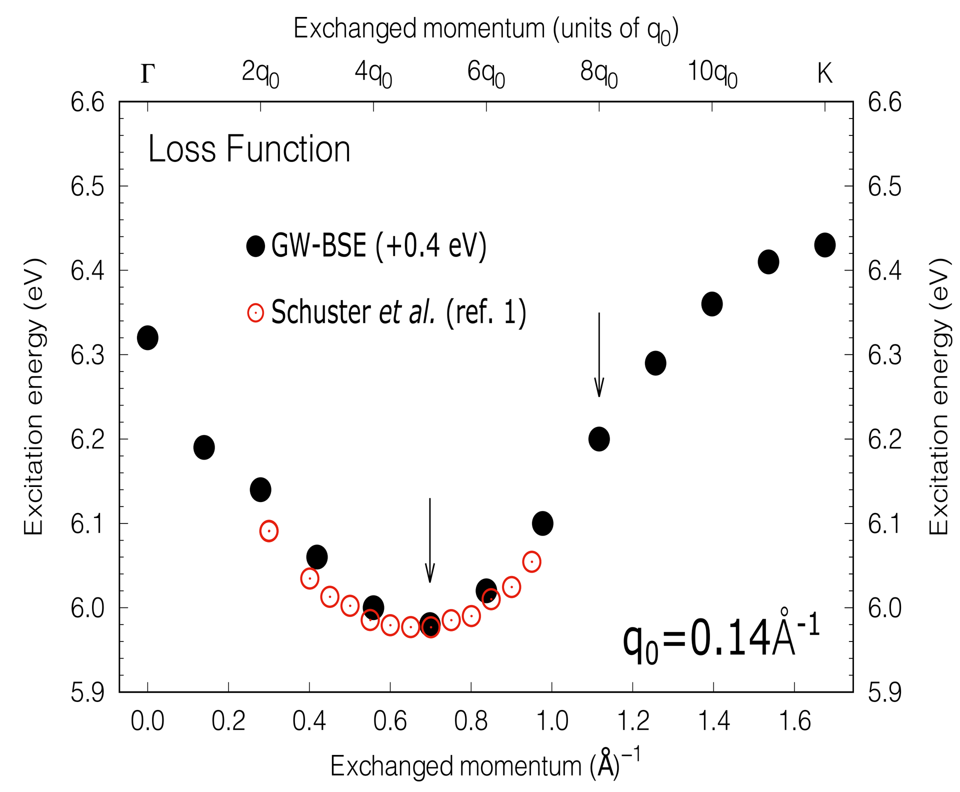
**What is the origin of these intensity variations?**
Answer by decomposing the spectral intensity in **contributions from the IP-transitions.**

peak intensity — IP-transition matrix element

$$\epsilon(\mathbf{q},\omega) \propto \sum_\lambda \frac{I_\lambda(\mathbf{q})}{E_\lambda(\mathbf{q}) - \omega + i\eta} \qquad I_\lambda(\mathbf{q}) = \left|\sum_t \tilde{\rho}_t(\mathbf{q}) A_t^\lambda(\mathbf{q})\right|^2 = \left|\sum_t M_t^\lambda(\mathbf{q})\right|^2$$

independent-particle transition index $t = (V, \mathbf{k}) \to (C, \mathbf{k}+\mathbf{q})$

### Loss function dispersion




**Computational details:**

| screening | Bethe-Salpeter |
|---|---|
| nbands = 350 | nbands = 6+3 |
| mat.dim. = 120 eV | mat.dim. = 80 eV |
| cutoff wfn.=200 eV | cutoff wfn.=110 eV |

Γ-centered 36x36x4

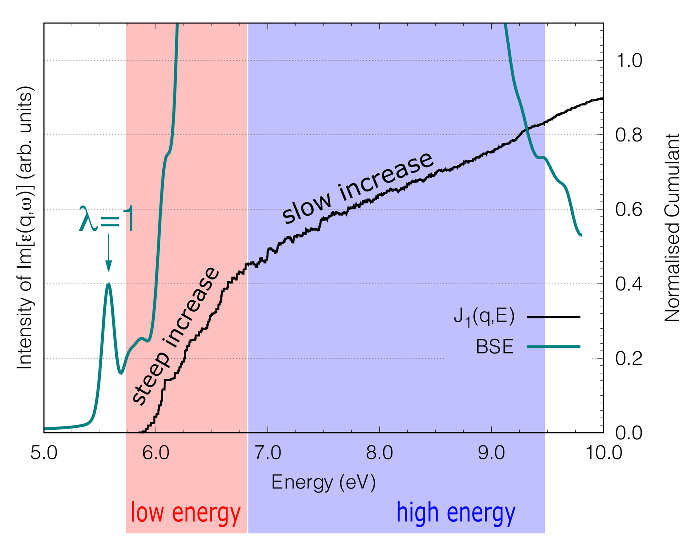
## Analysis of the peak intensity: Decomposition of IP-transitions

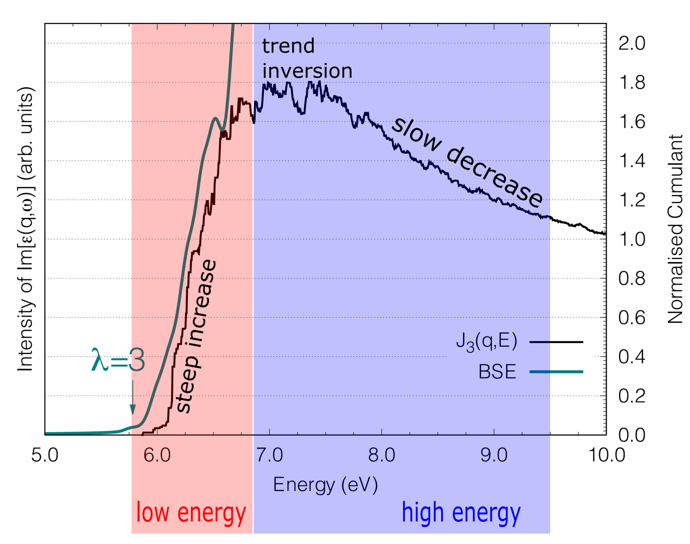
### Analysis of q=5q0 = 0.7$Å^{-1}$ — Analysis of q=8q0 = 1.12$Å^{-1}$

**Normalized cumulant weight**

$$\mathcal{J}_\lambda(\mathbf{q},E) = \frac{1}{I_\lambda(\mathbf{q})}\left|\sum_{t:E_t\le E} M_t^\lambda(\mathbf{q})\right|^2$$

Information abaout the building-up of the excitonic peak.

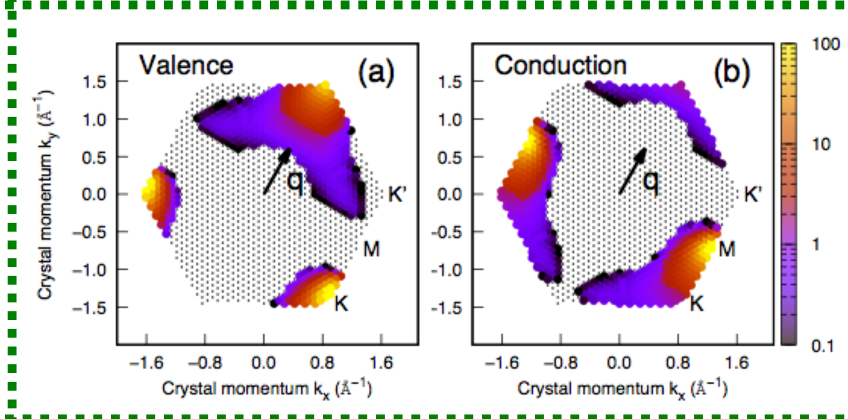
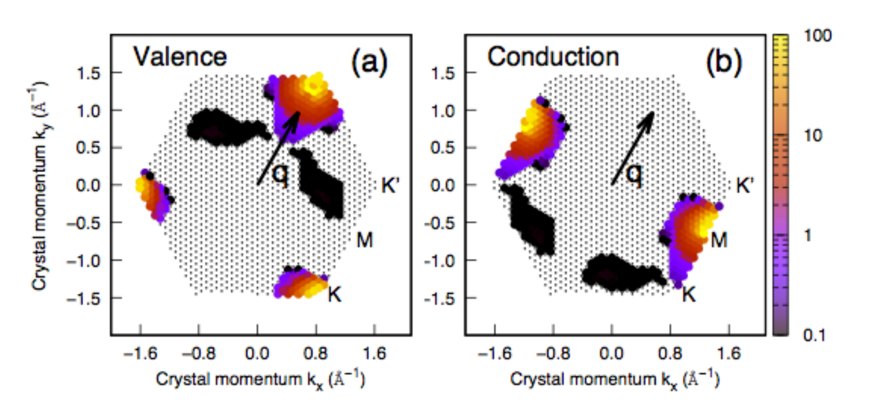



**Positive phase; group *KM***

$\mathrm{Re}[M_t^\lambda(\mathbf{q})] > 0 \quad \& \quad \mathrm{Im}[M_t^\lambda(\mathbf{q})] > 0$

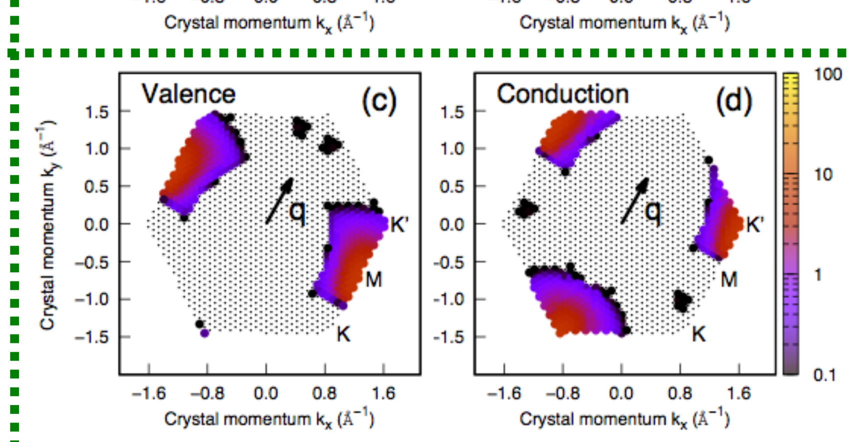
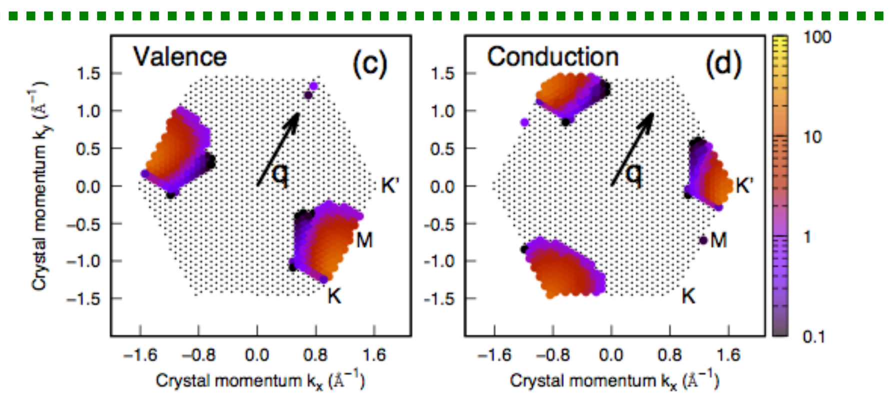
Band-contracted map of the IP-transitions $\left|\sum_{V,C} M_t^\lambda(\mathbf{q})\right|^2$


**Negative phase; group *MK'***

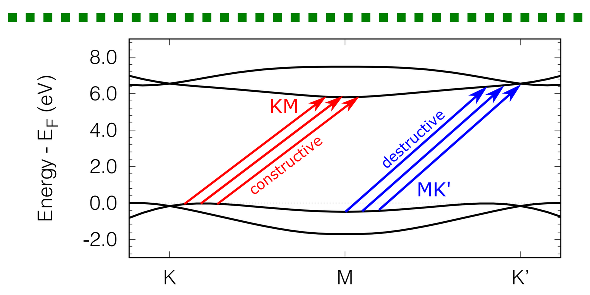
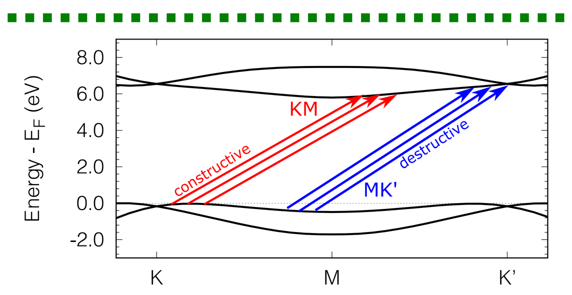
$\mathrm{Re}[M_t^\lambda(\mathbf{q})] < 0 \quad \& \quad \mathrm{Im}[M_t^\lambda(\mathbf{q})] < 0$

Band-contracted map of the IP-transitions $\left|\sum_{V,C} M_t^\lambda(\mathbf{q})\right|^2$


**Sketch of IP-transitions**

At $5q_0$ *KM* dominates: higher number and intensity.
At $8q_0$ the two groups are competing.


## Conclusions

- The GW-BSE dispersion of the peak of the loss function **perfectly reproduces experimental data** (1).

- Transitions can be **classified in groups** depending on the **phase** of $M_\lambda^t(\mathbf{q})$.

- **Competition between two groups of transitions** (*KM* and *MK'* groups). *KM* dominates at q=0.7Å-1; the two groups **interfere destructively** at q=1.1Å-1.

- Intriguing **valleys physics**.

- **General** framework and analysis tools, **applicable to any study** of excitonic properties.

- Possible way to redefine an **optimized basis** for excitons.