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Electron-phonon interaction as seen in diffuse and inelastic scattering

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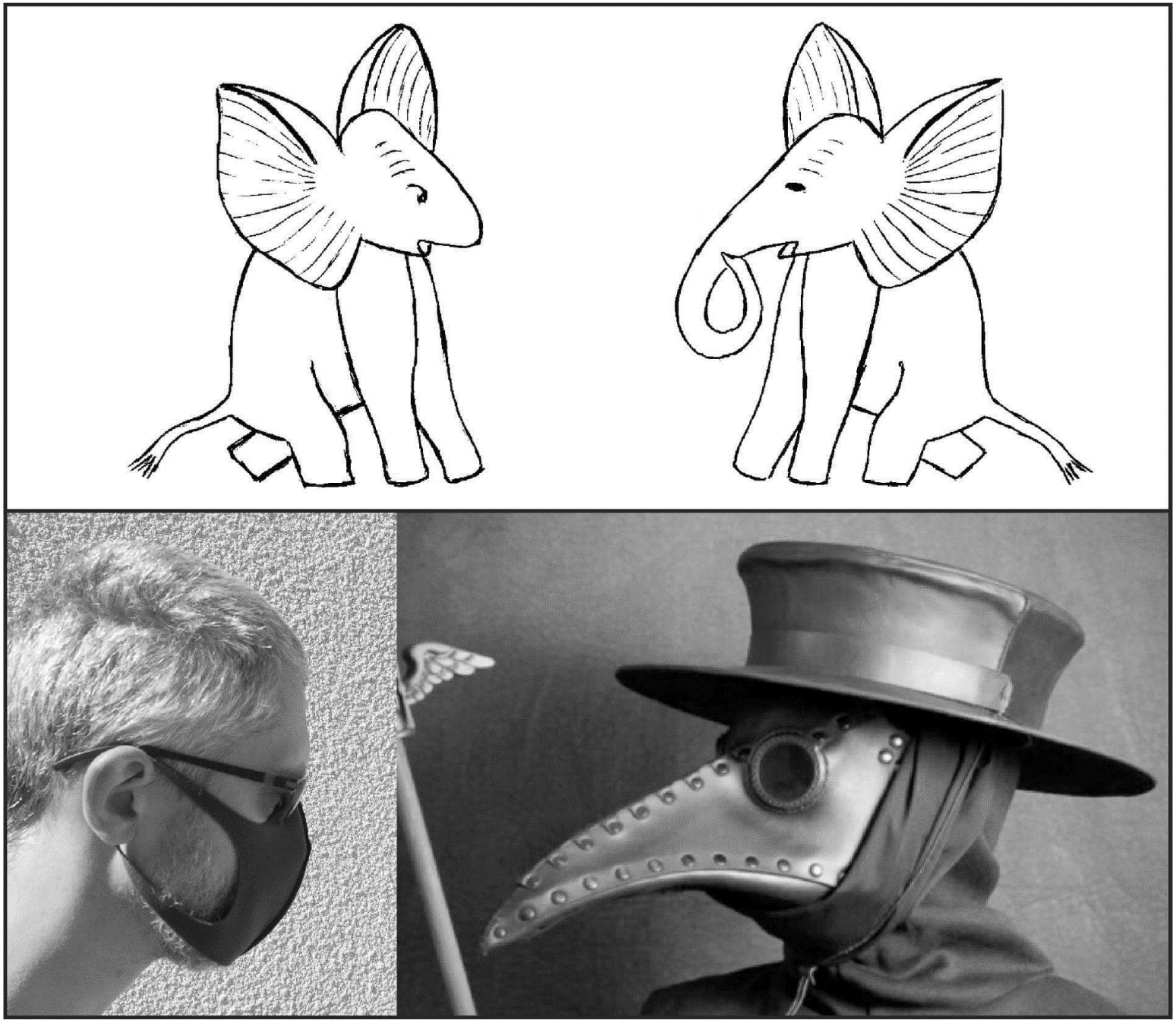
The Elephant’s Child et al.



Outline

- ✓ Diffuse and inelastic x-ray scattering
- ✓ Bad and good nesting with biased examples

TDS and lattice dynamics

TDS intensity ~1/ω^2

$$I(\vec{Q}) \propto \sum_{j=1}^{3N} \frac{1}{\omega_j} \coth\left(\frac{\hbar\omega_j}{2kT}\right) \left| \sum_{d=1}^{N} f_d(Q) \exp(-W_d(\vec{Q}) + i\vec{Q}\cdot\vec{d})(\vec{Q}\cdot\hat{\sigma}_d^j(\vec{q}))M_d^{-1/2} \right|^2$$

LE JOURNAL DE PHYSIQUE ET LE RADIUM. SÉRIE VIII, TOME X, MARS 1949.

DIFFUSION DES RAYONS X DANS L'ALUMINIUM PAR LES ONDES D'AGITATION THERMIQUE

Par PH. OLMER.
Assistant à la Faculté des Sciences de Paris.

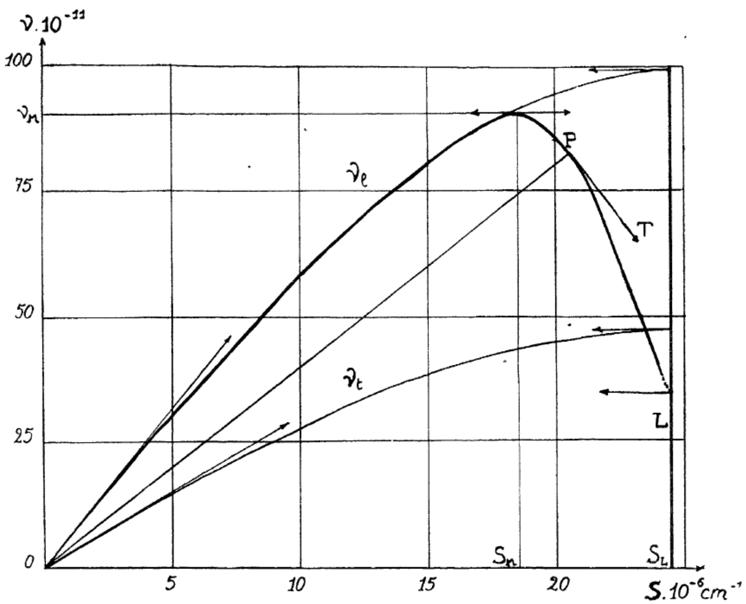


Fig. 13.

X-ray tube + point detector since 1948

ID28 hardware

beamlines

JOURNAL OF SYNCHROTRON RADIATION

ISSN 1600-5775

A new diffractometer for diffuse scattering studies on the ID28 beamline at the ESRF

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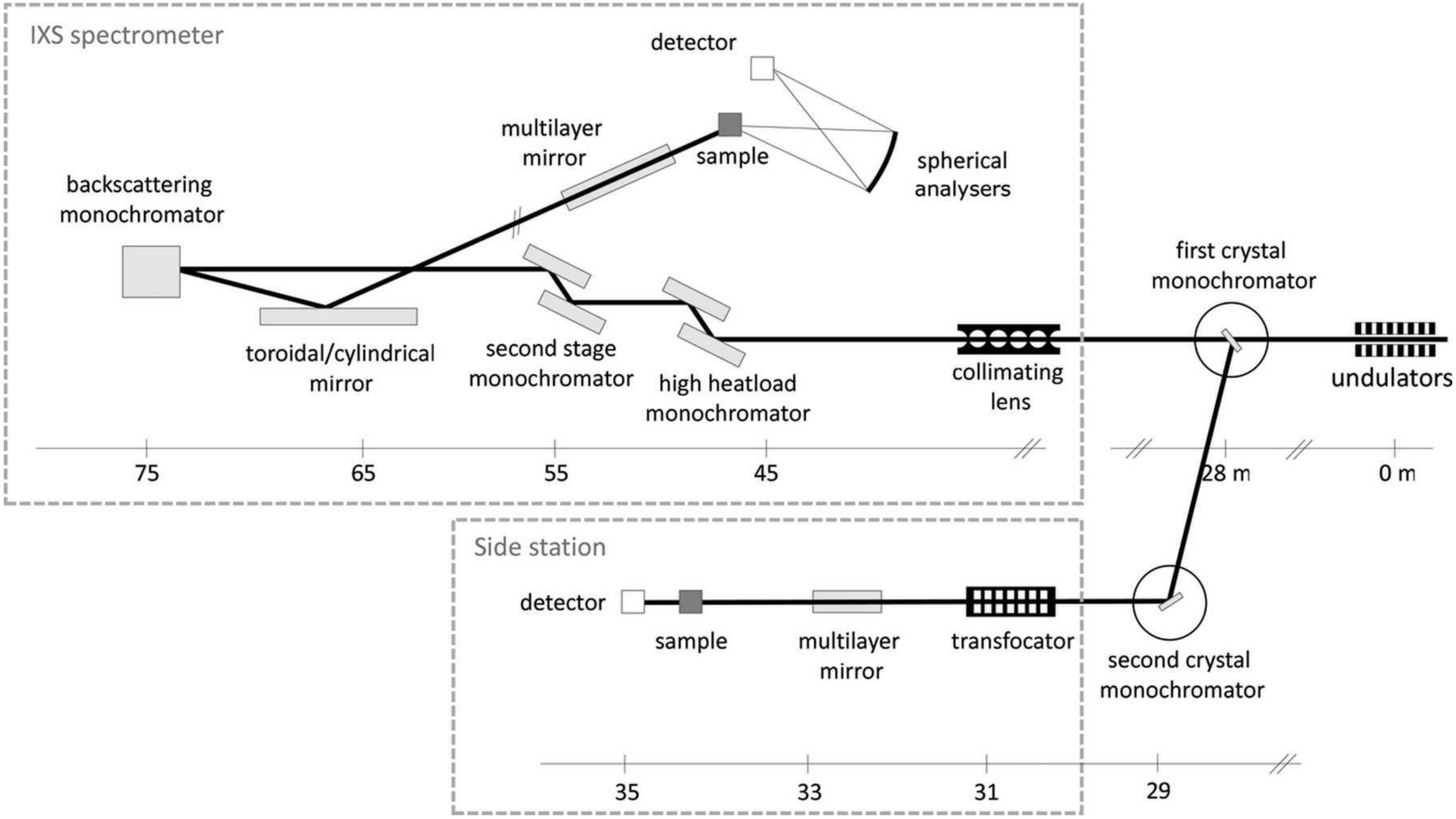
Diffuse scattering:

- Roadmaps for IXS measurements
- Identification of diffuse features
- Validation of lattice dynamics/disorder models



New ID28 diffractometer

C(311)[splitter]-Si(422) monochromator

0.52-0.98 Å

flux ~10^{12} ph/s @ 17.8 keV

focal spot down to 20x40 μm

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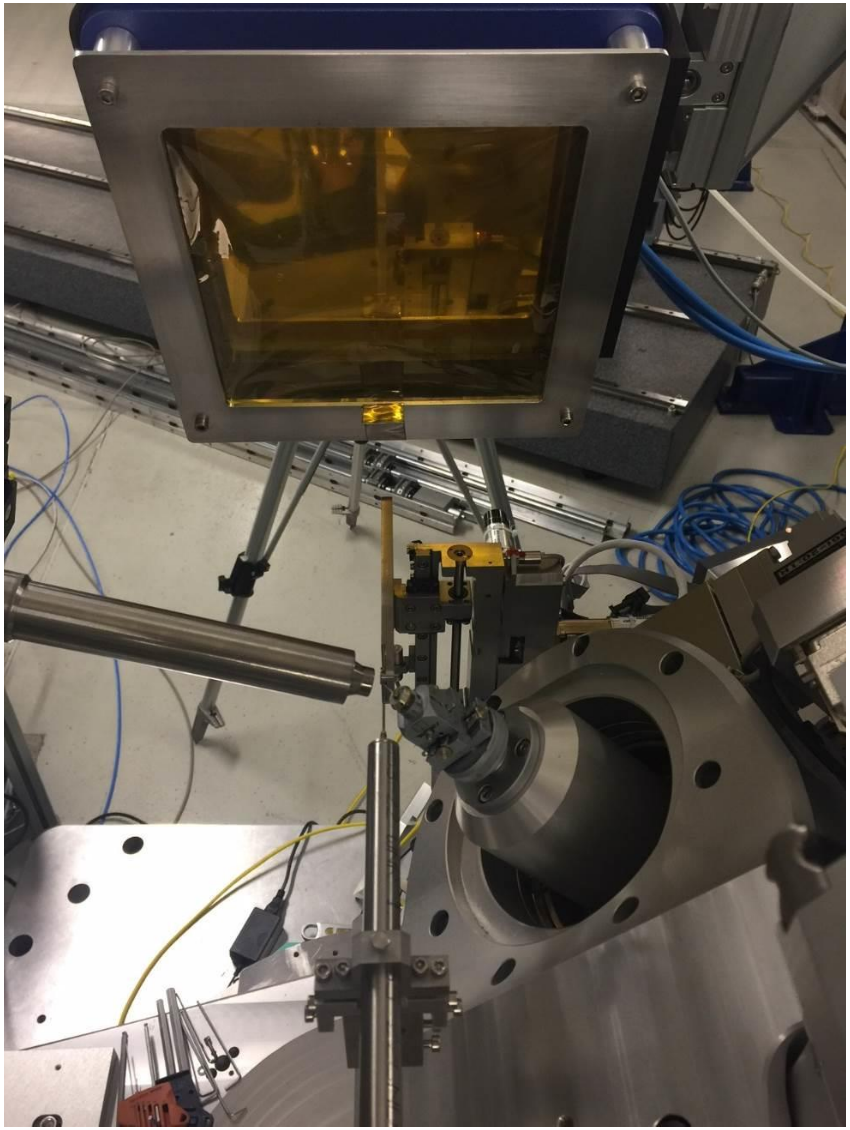
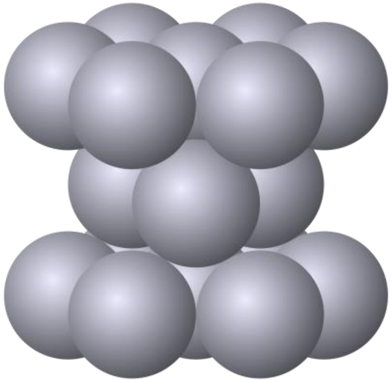


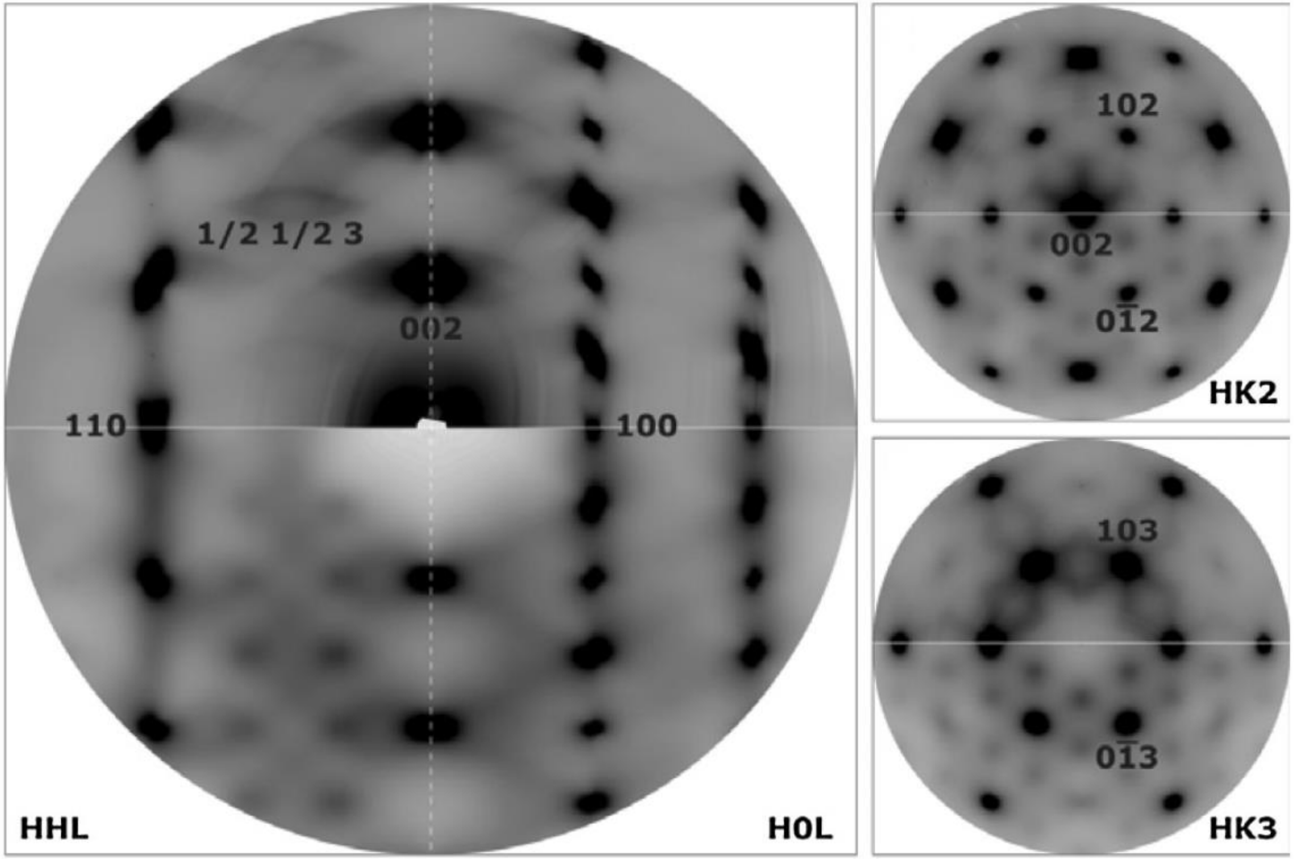
user operation from September 2016

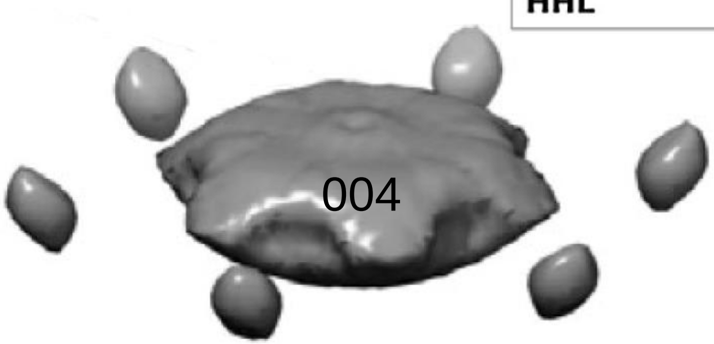
Zinc metal

[A. Bosak et al., PRL 103, 076403 (2009)]

Zinc metal

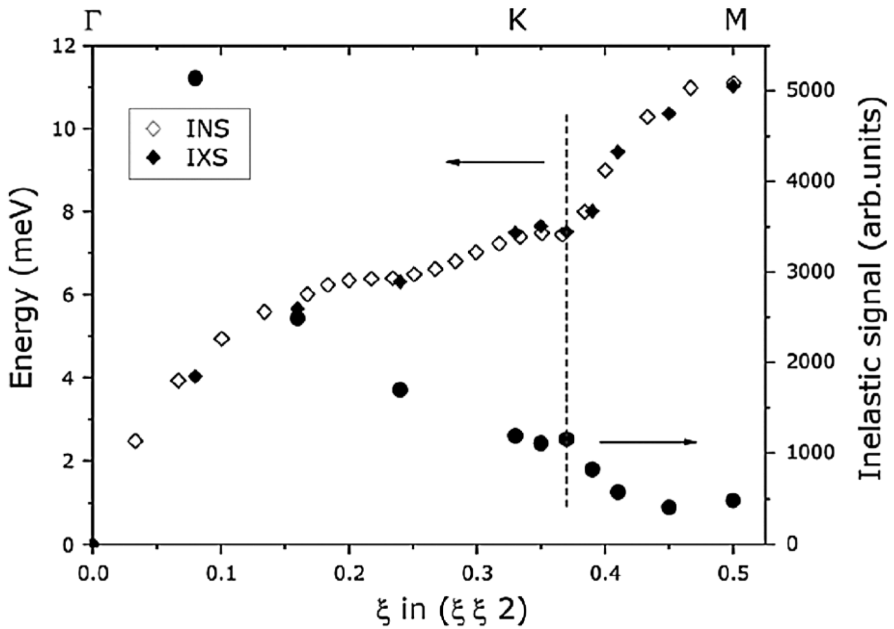


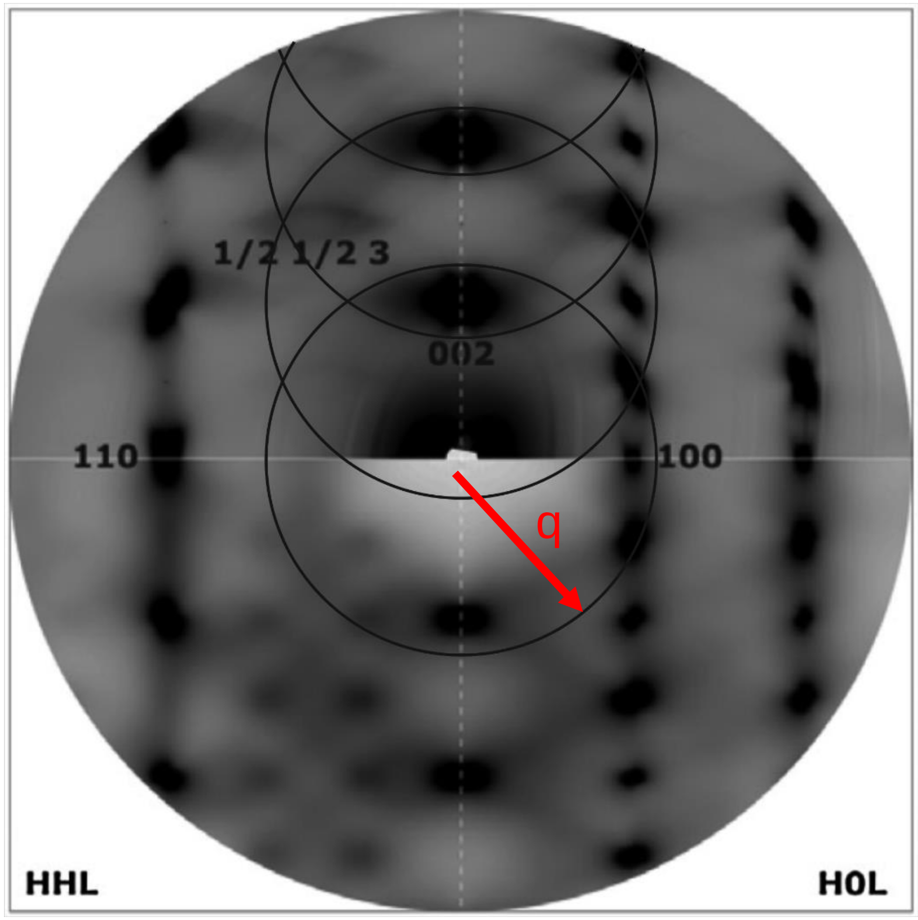




[PRL 103, 076403 (2009), Bosak et al.]

Zinc metal



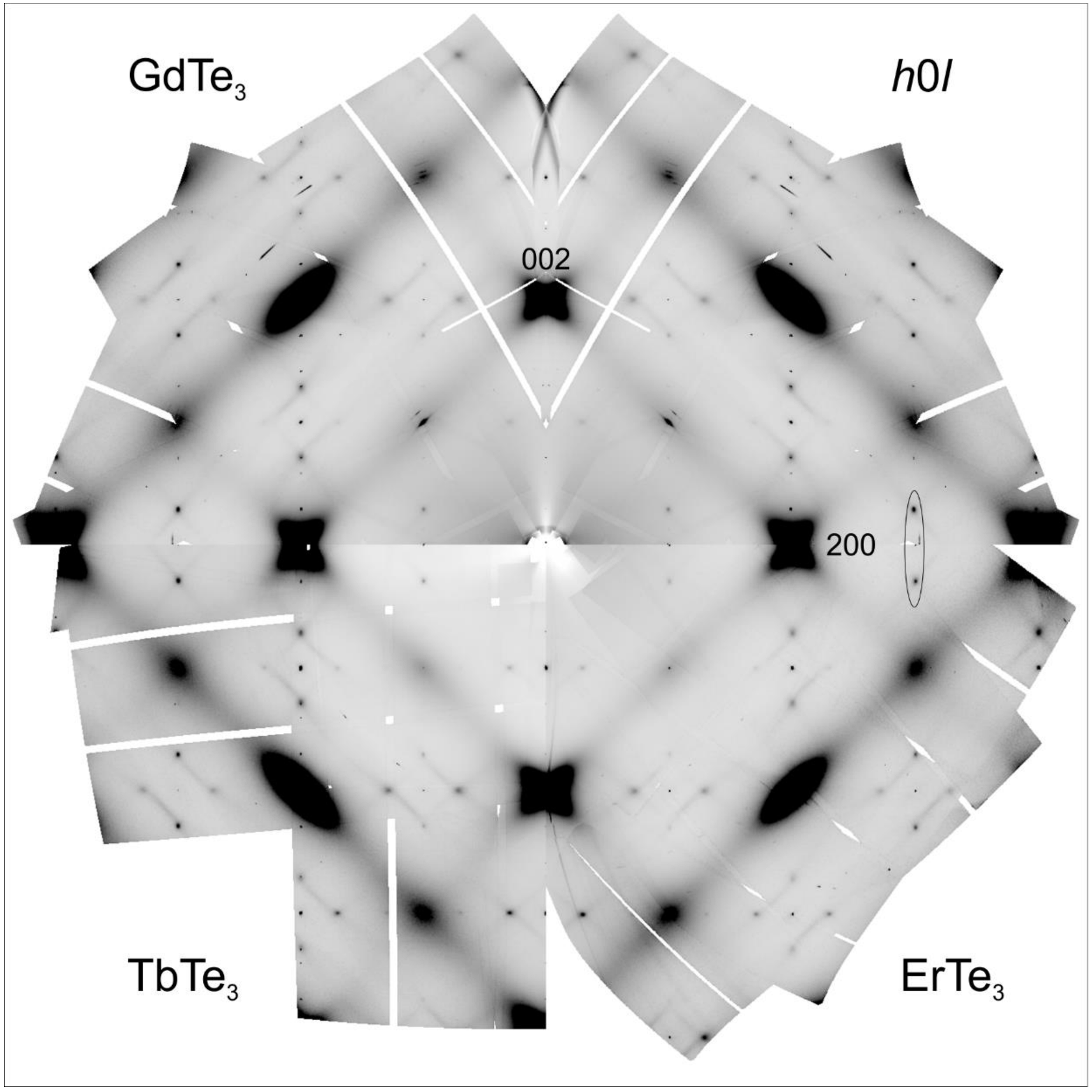


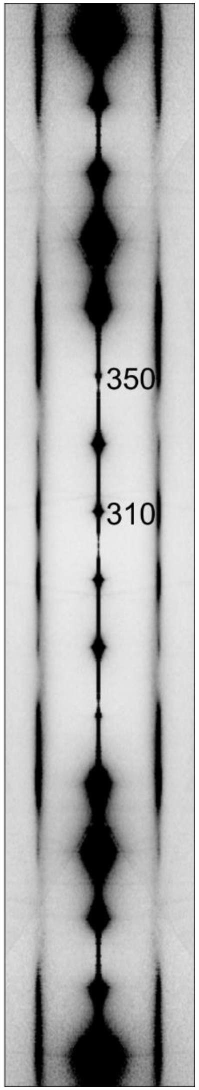
Free electron model:
$k_F = q/2 = 1.57$ Å^{-1}
=> 2 electrons / Zn atom

RTe_3

[with P. Quemerais, P. Monceau, E. Lorenzo, P. Rodier, L. Ortega, A. Sinchenko, E. Bellec]

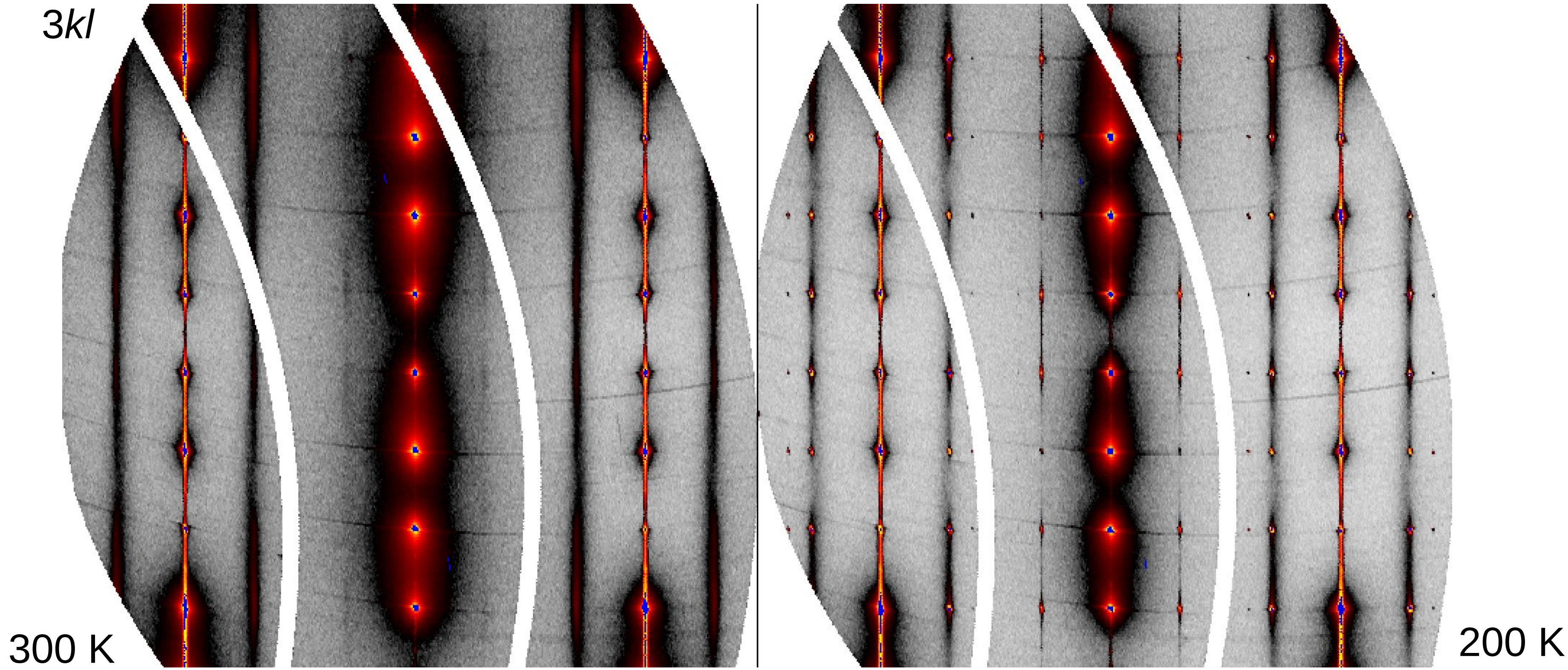
Diffuse scattering in RTe_3





$ErTe_3$, $TbTe_3$, $GdTe_3$ all look the same above T_{CDW}

Diffuse scattering in $ErTe_3$



- $ErTe_3$, $TbTe_3$, $GdTe_3$ all look the same below T_{CDW1}
- Deviation from sinus modulation
- Suspicious contribution from planar defects

RTe_3 – no nesting behind CDW

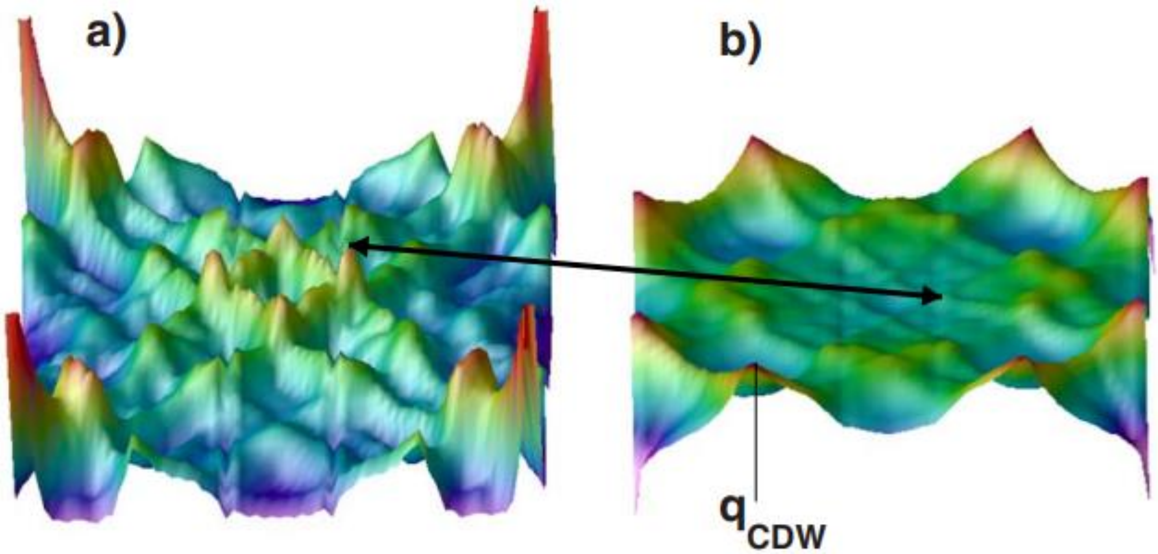
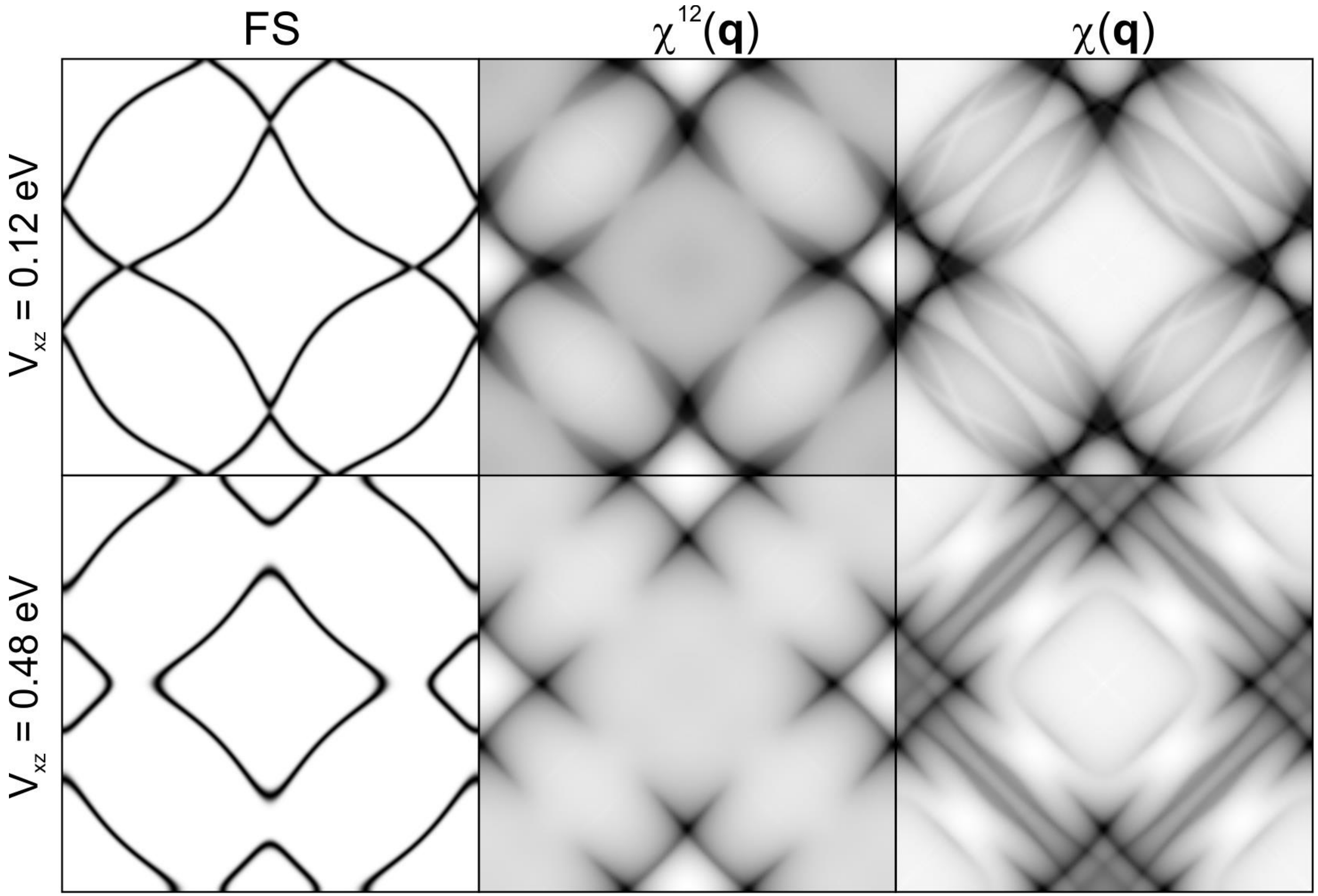


FIG. 6. (Color online) A diagram showing the imaginary (left) and real (right) parts of the susceptibility as a function of q_x, q_y, with $q_z=0$. The arrow connects the strongest peak in the imaginary part, located at $\mathbf{q}_{\text{nest}}$, to its corresponding position in the real part. In the real part, the nesting peak is absent and $\mathbf{q}_{\text{CDW}}$ dominates the spectrum, indicating the importance of states away from E_F.

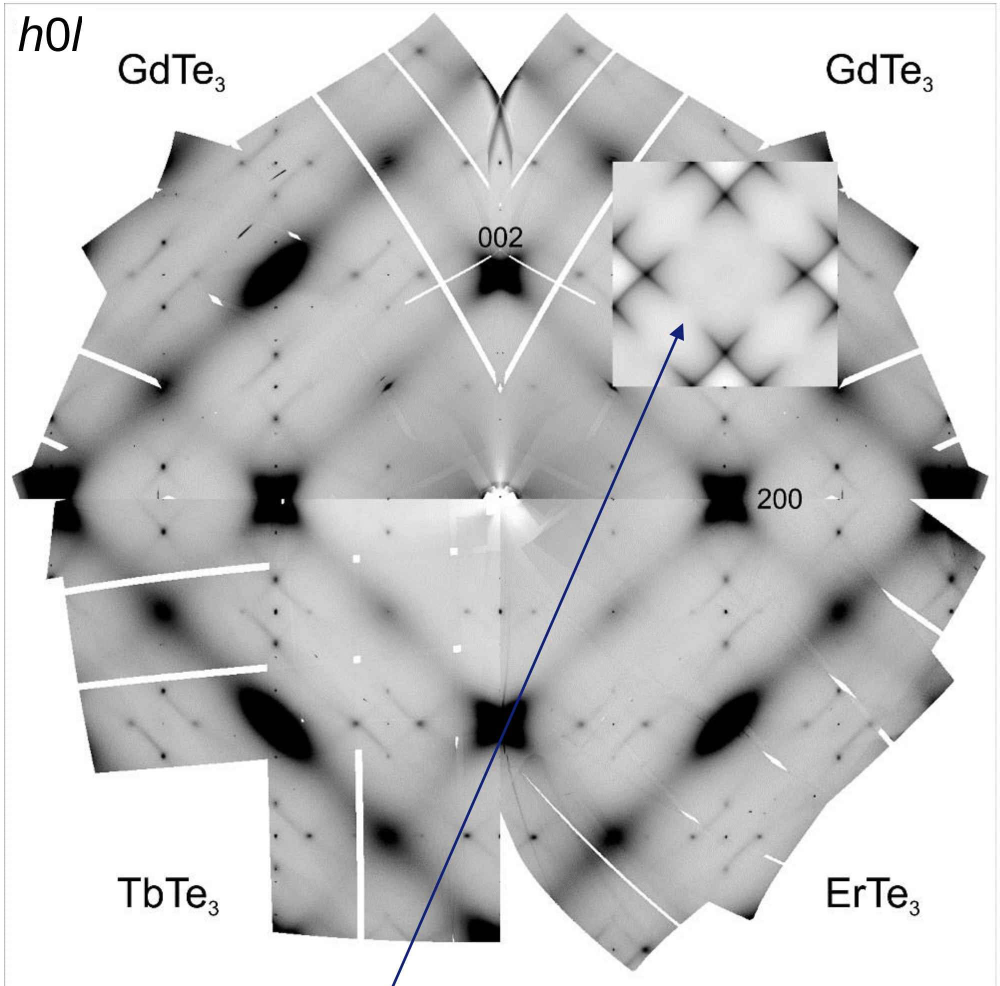
[M.D. Johannes and I.I. Mazin, PRB 77, 165135 (2008)]

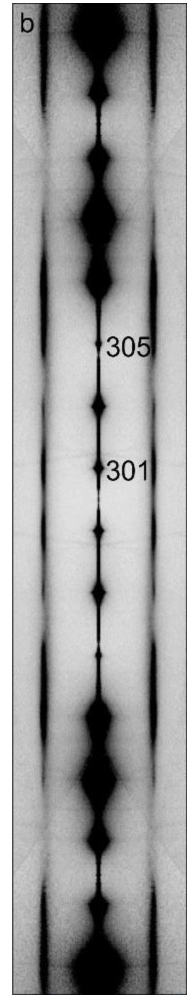
RTe_3 - nesting behind CDW



$$\chi^{ij}(\boldsymbol{q}) = \sum_k \frac{n_F[E^i(\boldsymbol{k})] - n_F[E^j(\boldsymbol{k}+\boldsymbol{q})]}{E^i(\boldsymbol{k}) - E^j(\boldsymbol{k}+\boldsymbol{q})}$$

RTe_3 - nesting behind CDW



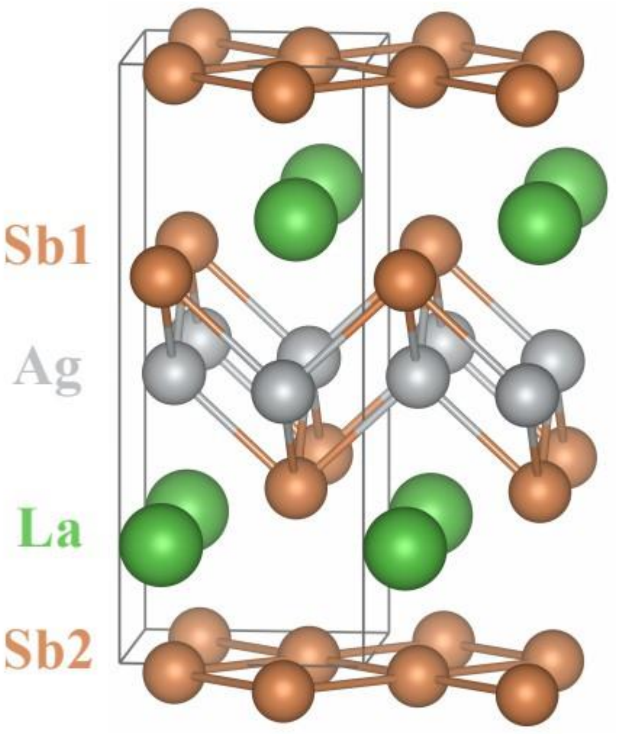


interband susceptibility

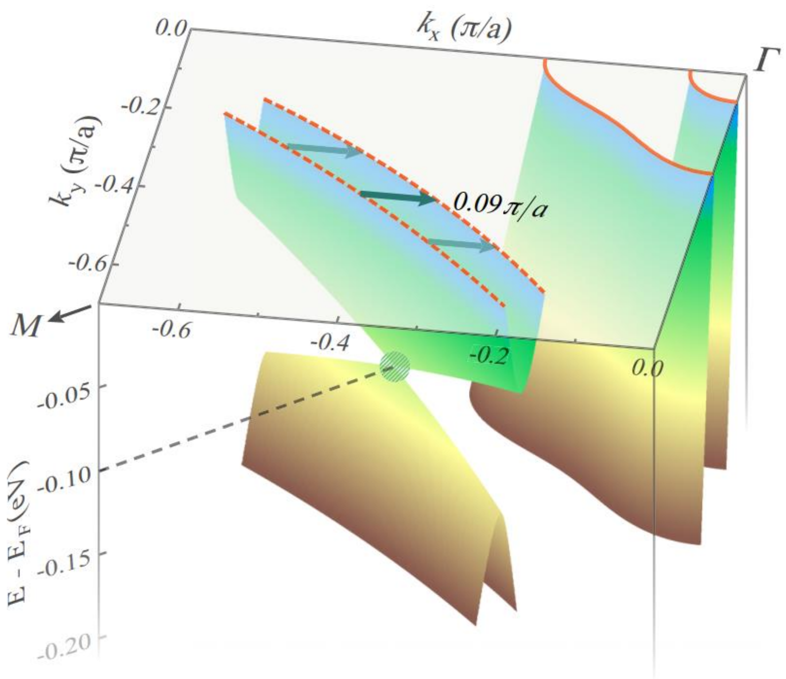
$LaAgSb_2$

[A. Bosak et al., Phys. Rev. Res. **3**, 033020 (2021)]

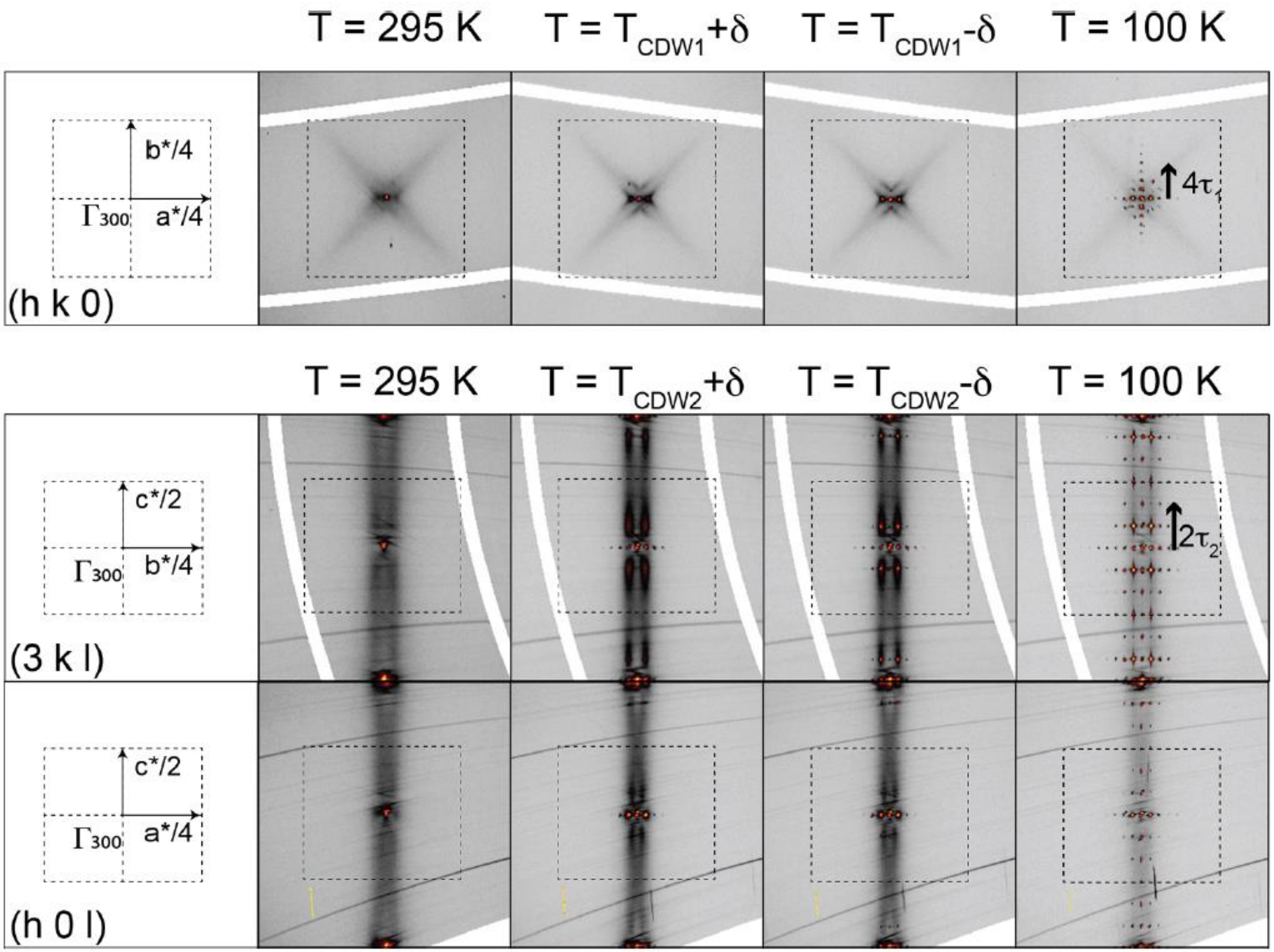
$LaAgSb_2$



[X. Shi, P. Richard, K. Wang, M. Liu, C.E. Matt, N. Xu, R.S. Dhaka, Z. Ristic, T. Qian, Y.-F. Yang, C. Petrovic, M. Shi, and H. Ding, Observation of Dirac-like band dispersion in $LaAgSb_2$, Phys. Rev. B **93**, 081105 (2016)]



Diffuse scattering in $LaAgSb_2$

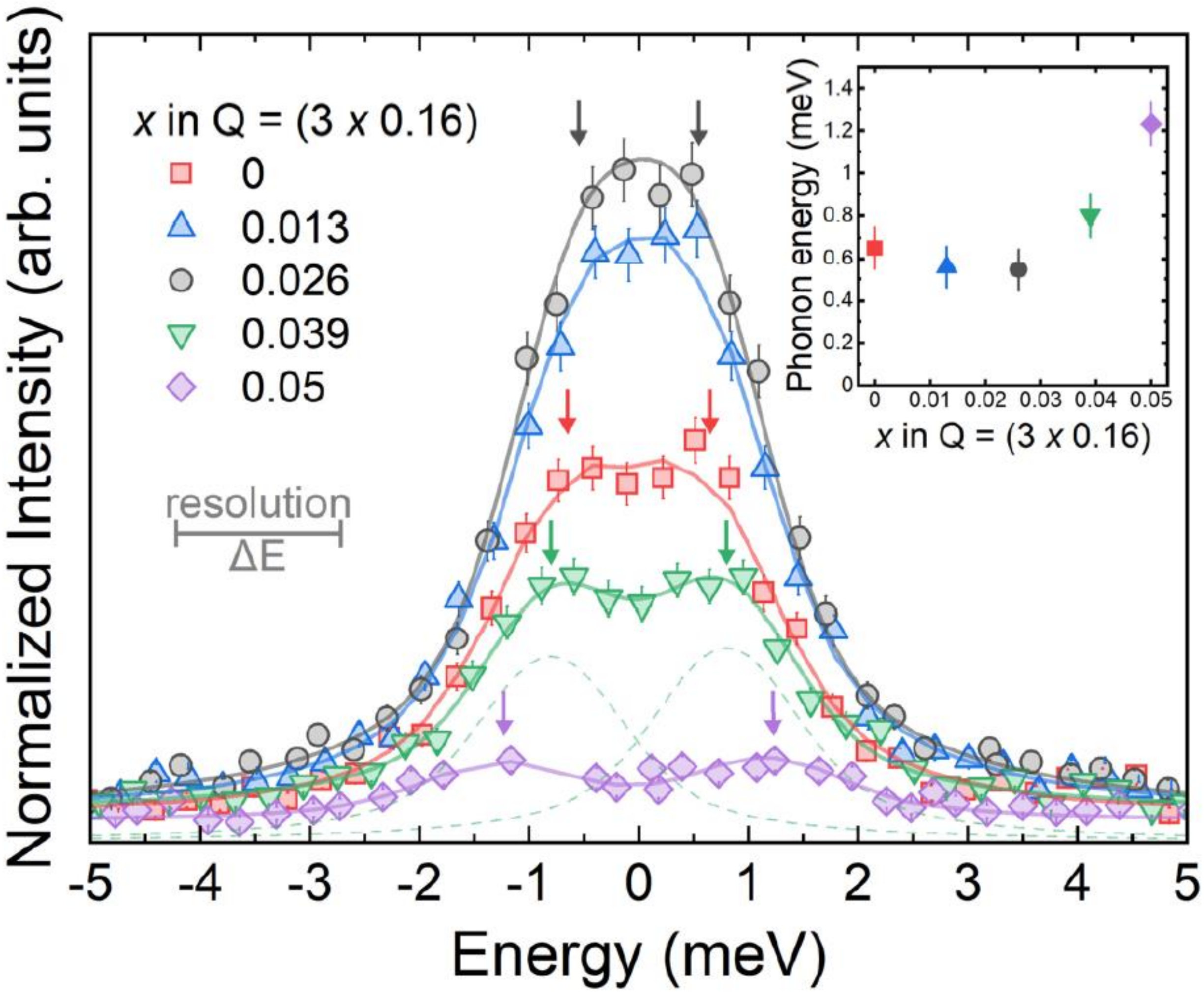


to CDW satellites up to 7th order

diffuse tubes with κ_x ~ 30 nm

τ_1 ~ 0.026 a* τ_1 ~ 0.026 a* + τ_2' = 1/6 c*

Inelastic scattering in $LaAgSb_2$



Diffuse features are inelastic

True Kohn anomaly

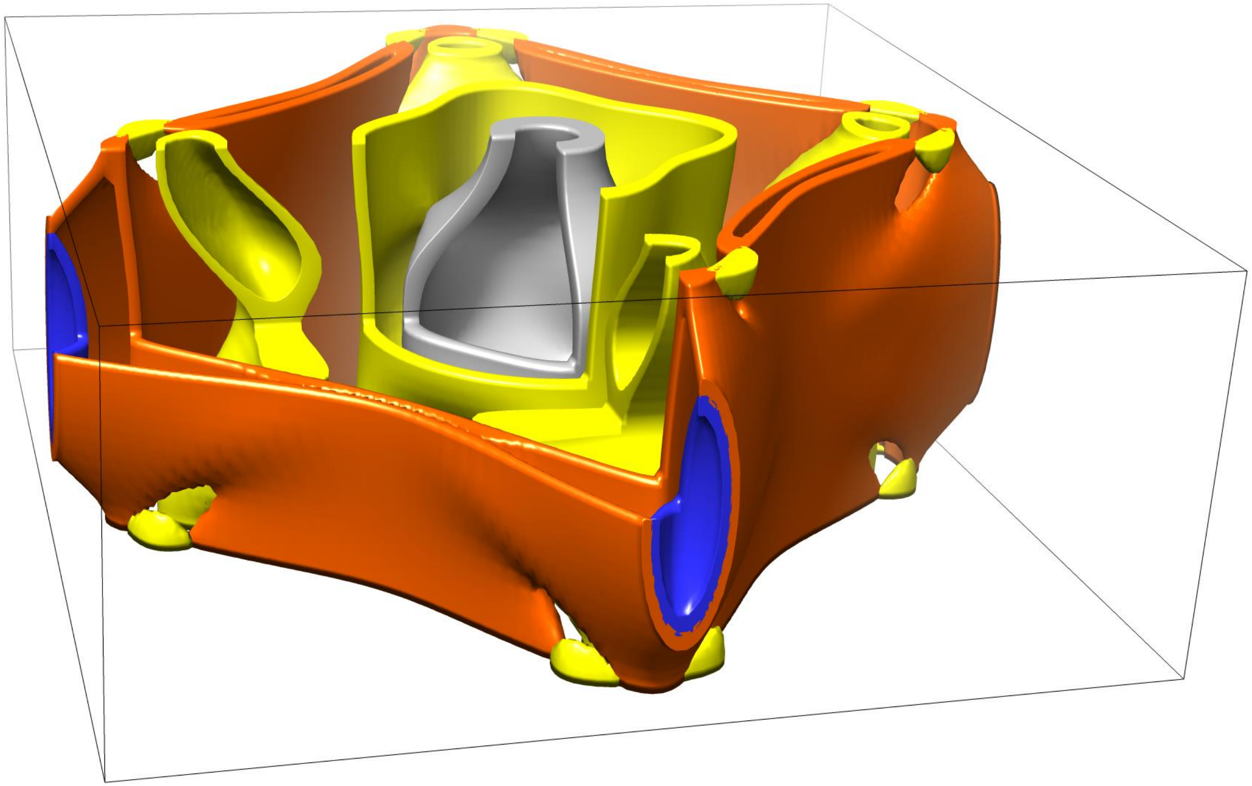
Soft phonon mechanism

What is behind?

$\tau_1 \sim 0.026\ a^* + \tau_2' = 1/6\ c^*$

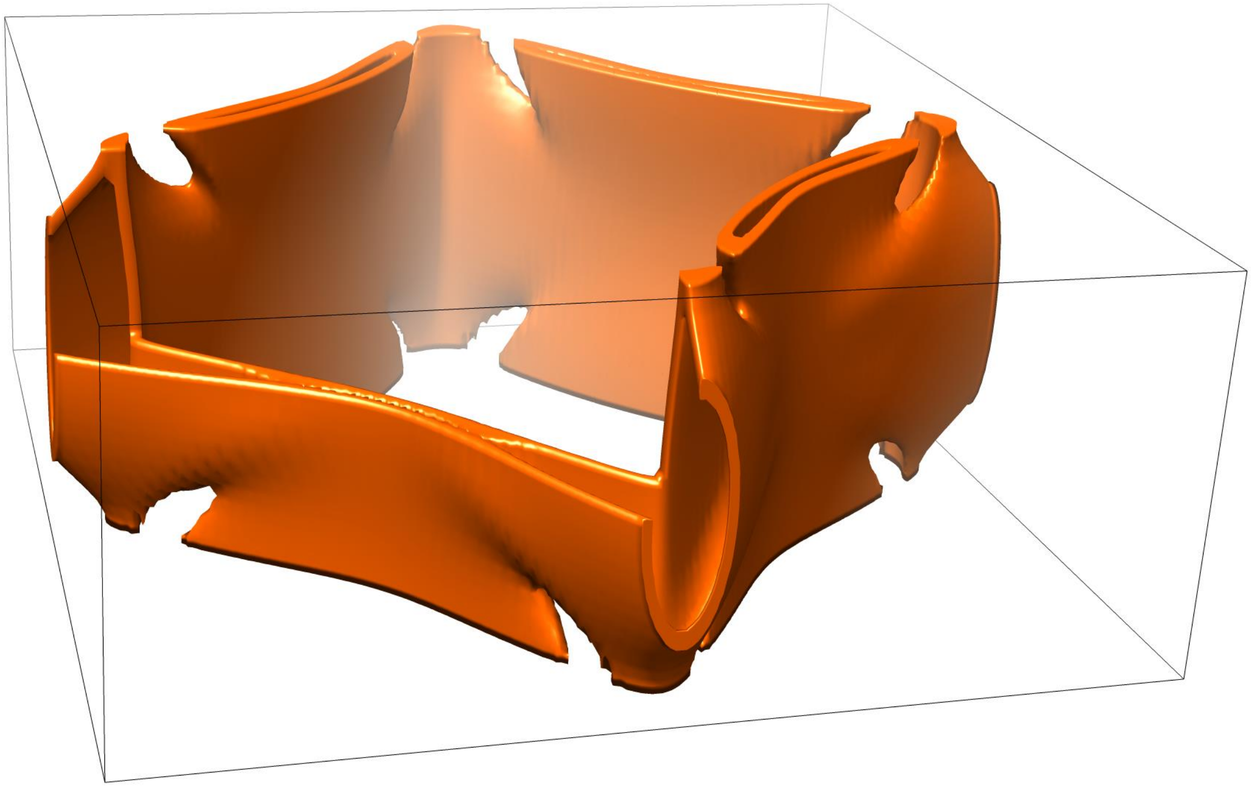
Choosing good band

4 bands

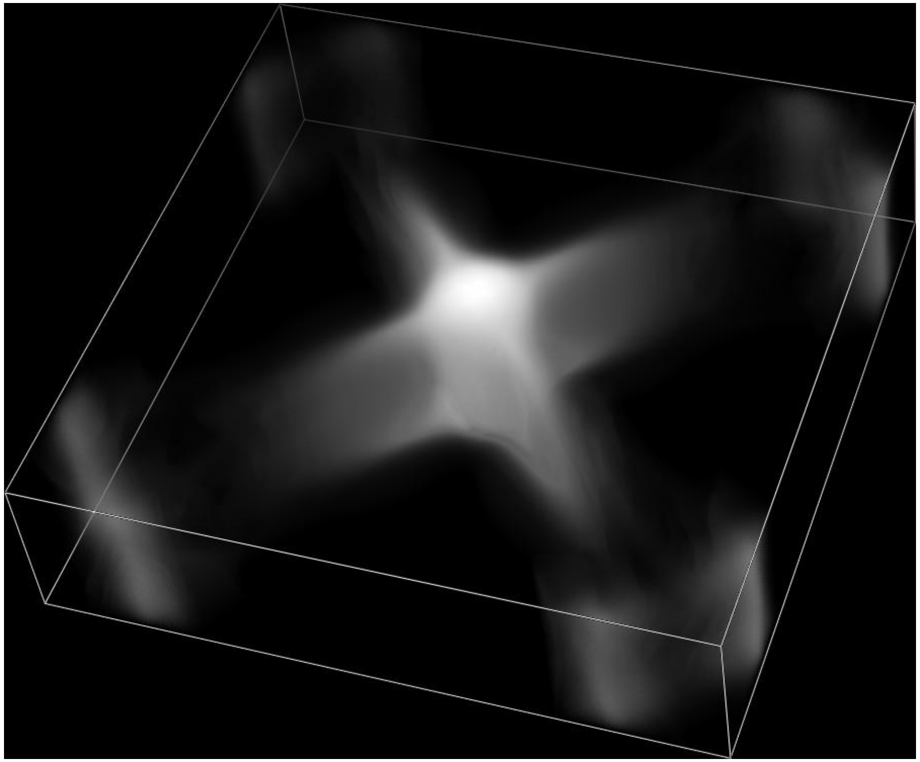


Choosing good band

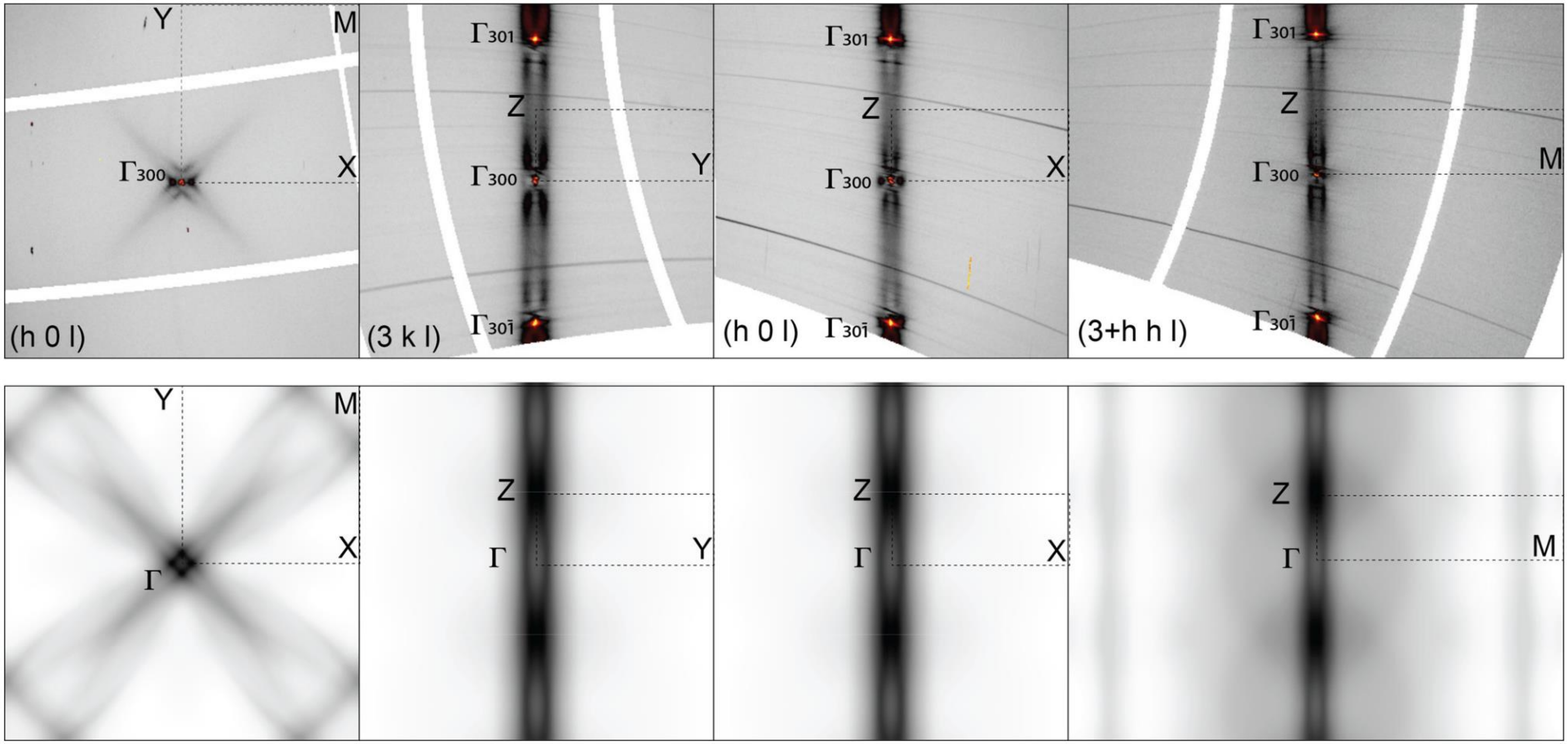
1 "good" band

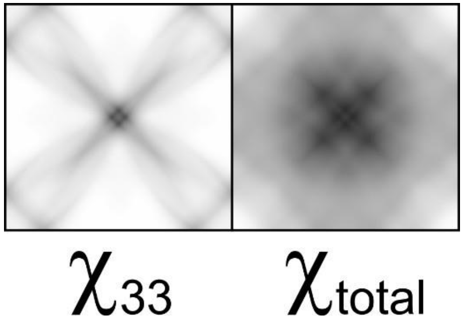


Susceptibility



$$\chi^{ij}(\boldsymbol{q}) = \sum_k \frac{n_F[E^i(\boldsymbol{k})] - n_F[E^j(\boldsymbol{k}+\boldsymbol{q})]}{E^i(\boldsymbol{k}) - E^j(\boldsymbol{k}+\boldsymbol{q})}$$





All band contributions are equal, but some band contributions are more equal than others

Pseudo-Dirac dispersion

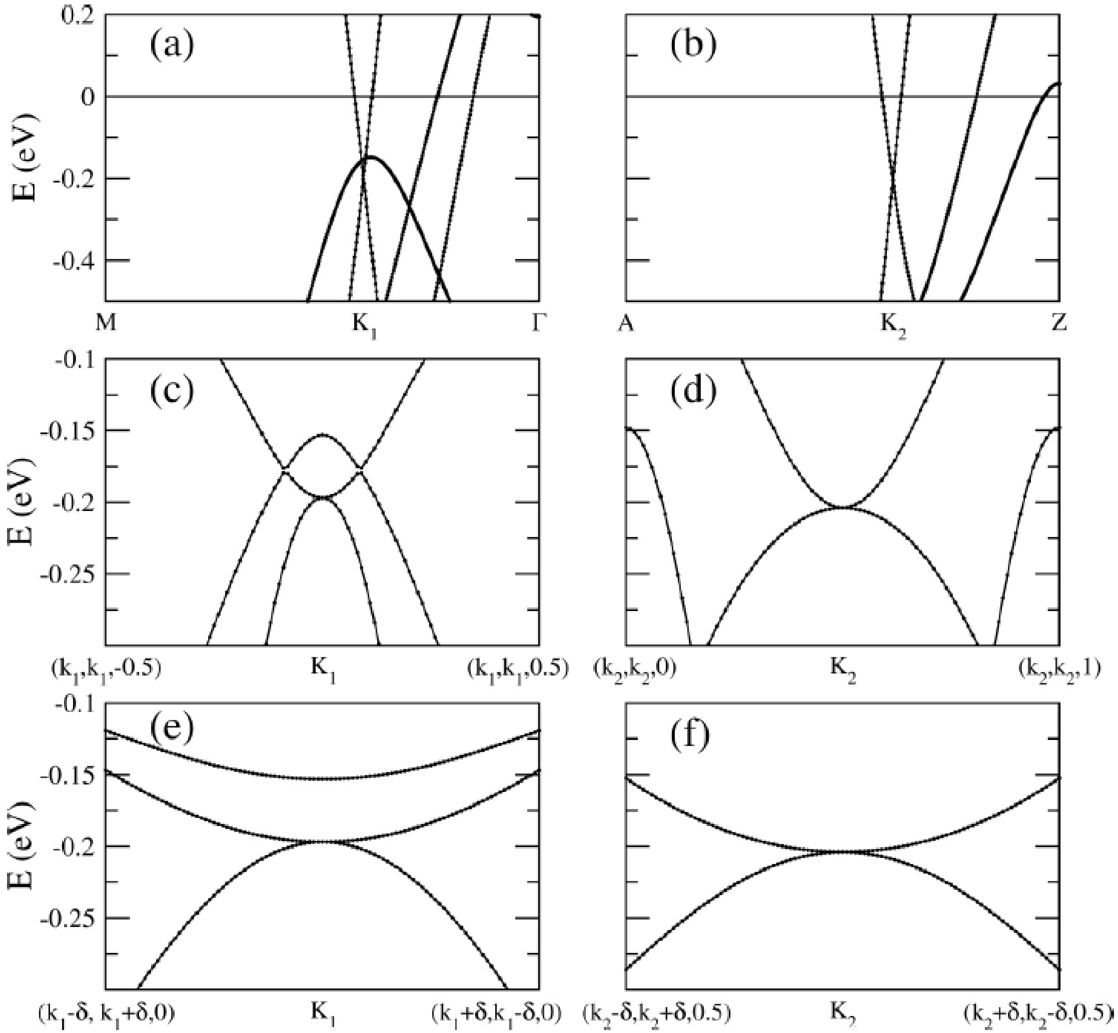


FIG. 8. Electronic band structure of $LaAgSb_2$ in the vicinity of the Dirac-type points. Band crossings with linear dispersive bands appear along the high-symmetry lines M-Γ and A-Z at points (a) $K_1 = (k_1, k_1, 0)$ with $k_1 = 0.1920$ and (b) $K_2 = (k_2, k_2, 0.5)$ with $k_2 = 0.2028$, respectively. (c) Band dispersion along parallel to the z axis across $K1$ (c) and $K2$ (d), and along an orthogonal direction in the xy plane ($\delta = 0.05$).

$NbSe_2$

[with P. Rodiere, M. Leroux]

$NbSe_2$ – no nesting behind CDW

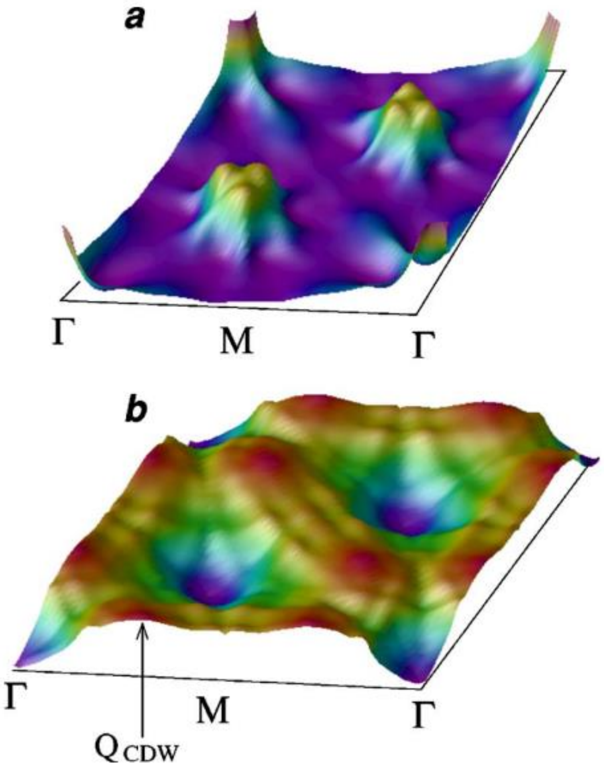


FIG. 5. (Color online) The noninteracting susceptibility of $NbSe_2$. (a) The imaginary part exhibits FS nesting driven peaks at $\mathbf{Q}=(\frac{1}{3},\frac{1}{3},0)$. The plane at the bottom is a guide for the eye and corresponds to the lowest value of $\mathrm{Im}\chi_0$. (b) The real part has very weak peaks at $\mathbf{Q}_{CDW}=(\frac{1}{3},0,0)$ that come from energy intervals away from E_F (see text). The plane corresponds to the lowest value of $\mathrm{Re}\chi_0$, which is also the density of states at the Fermi level.

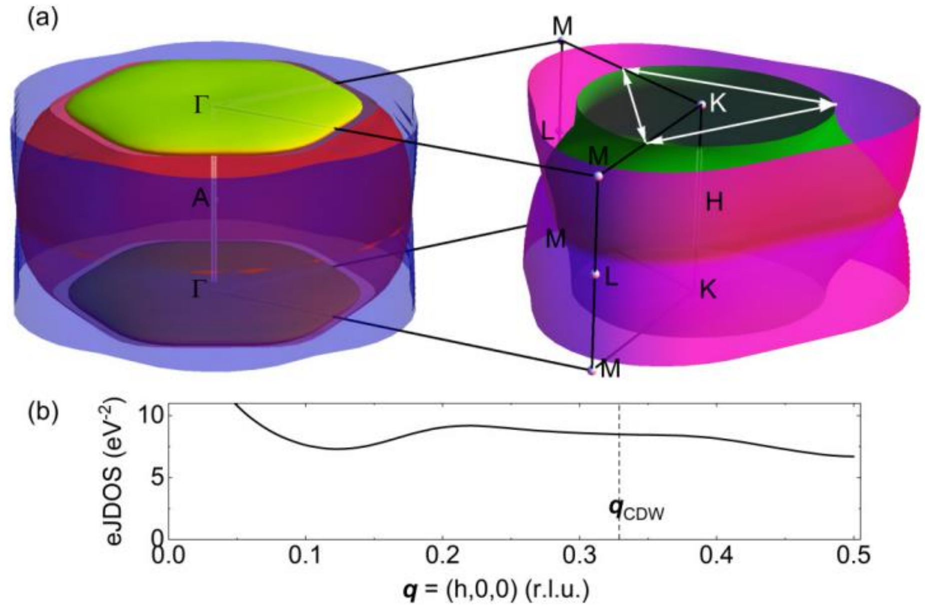
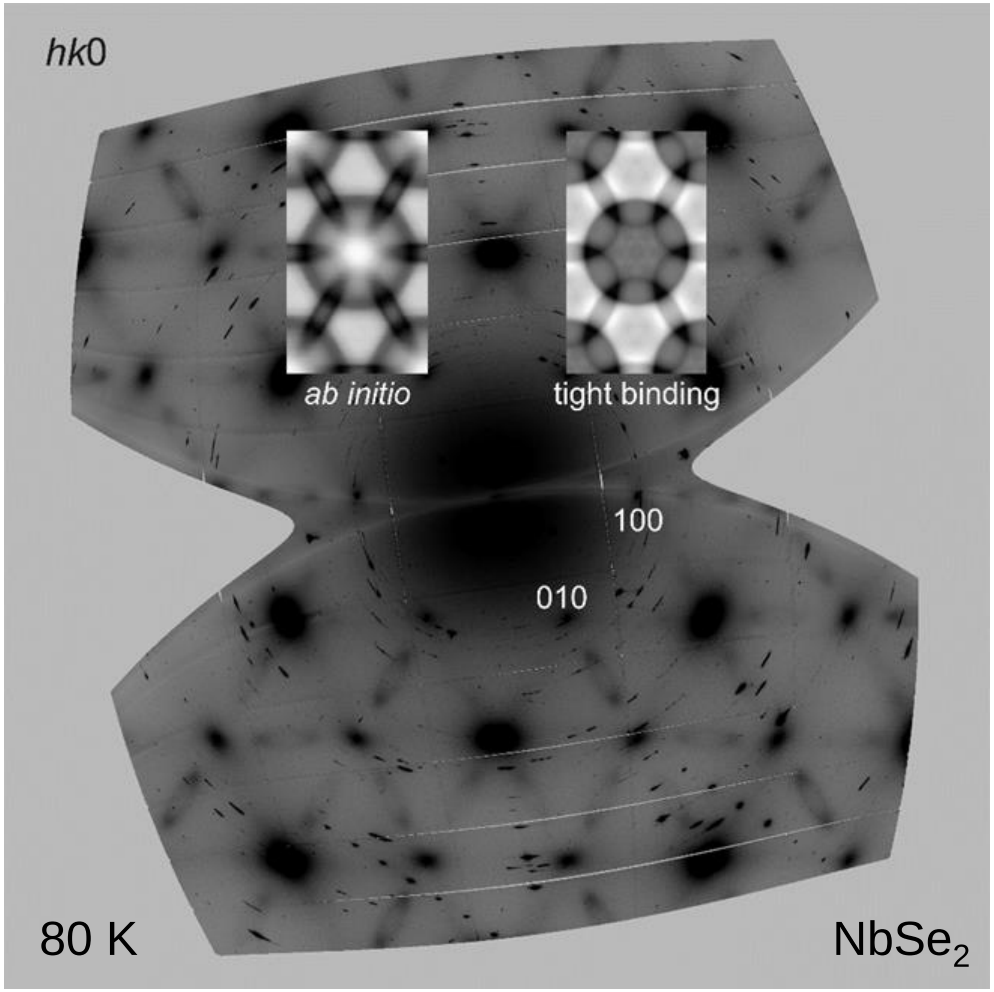


FIG. 4. (a) Calculated 3D FS. Capital letters denote high-symmetry points of the Brillouin zone. White arrows connect parts of the inner K pocket, where nesting was proposed [14] and CDW hotspots were reported [15]. (b) Calculated electronic joint density of states (eJDOS) corresponding to the FS shown in (a).

[Johannes et al., PRB 73, 205102 (2006)]

[Weber et al., PRB 97, 235122 (2018)]

$NbSe_2$ – nesting behind CDW

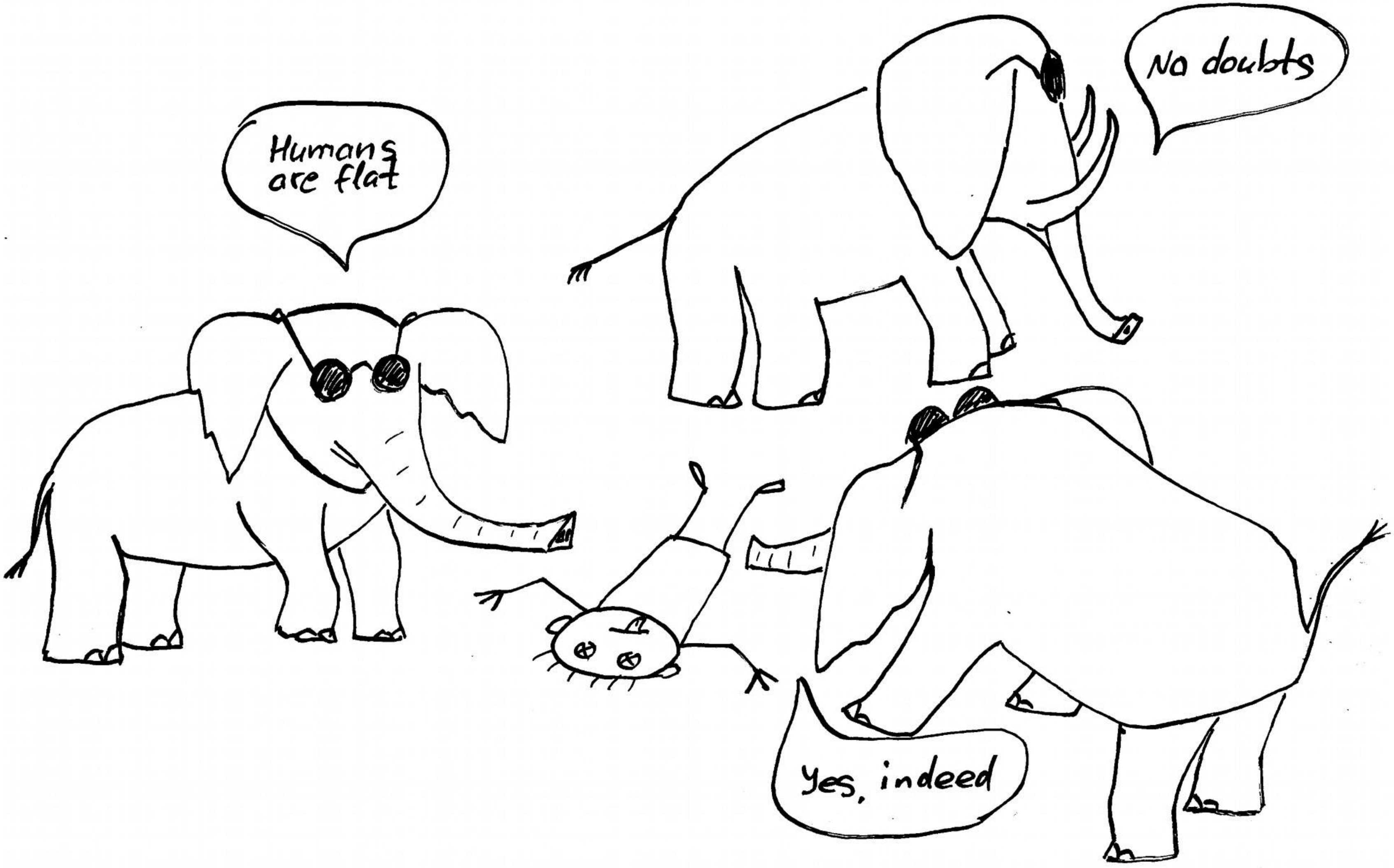


OK, no clear features at q_{CDW} in total χ

High degree of similarity for selected interband nesting

Not only q_{CDW} is reproduced, but 2D/3D shape of Kohn anomaly

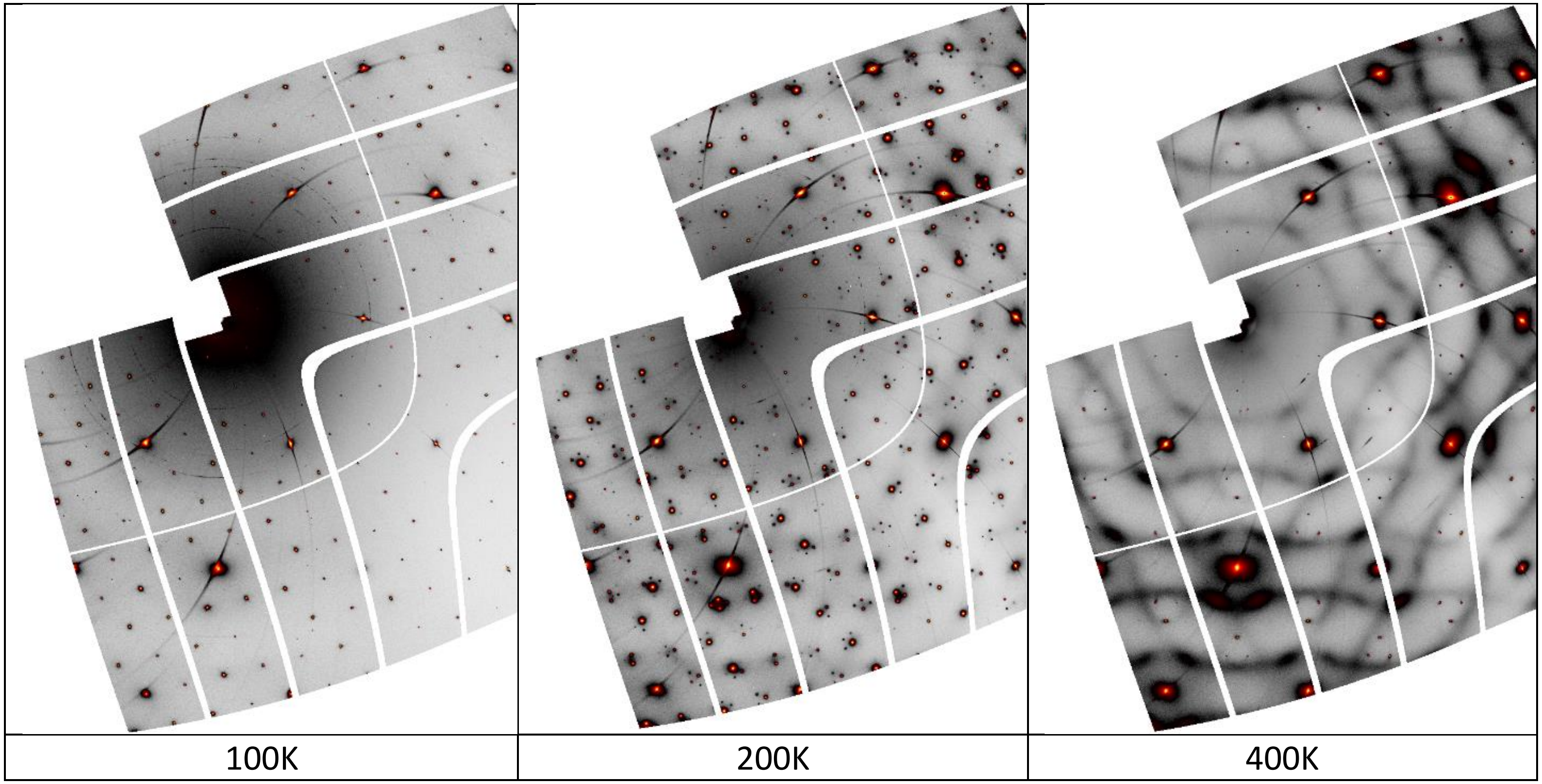
Biased views



TaS_2

[with J. Geck, A. Korshunov]

TaS_2 – no nesting behind CDW

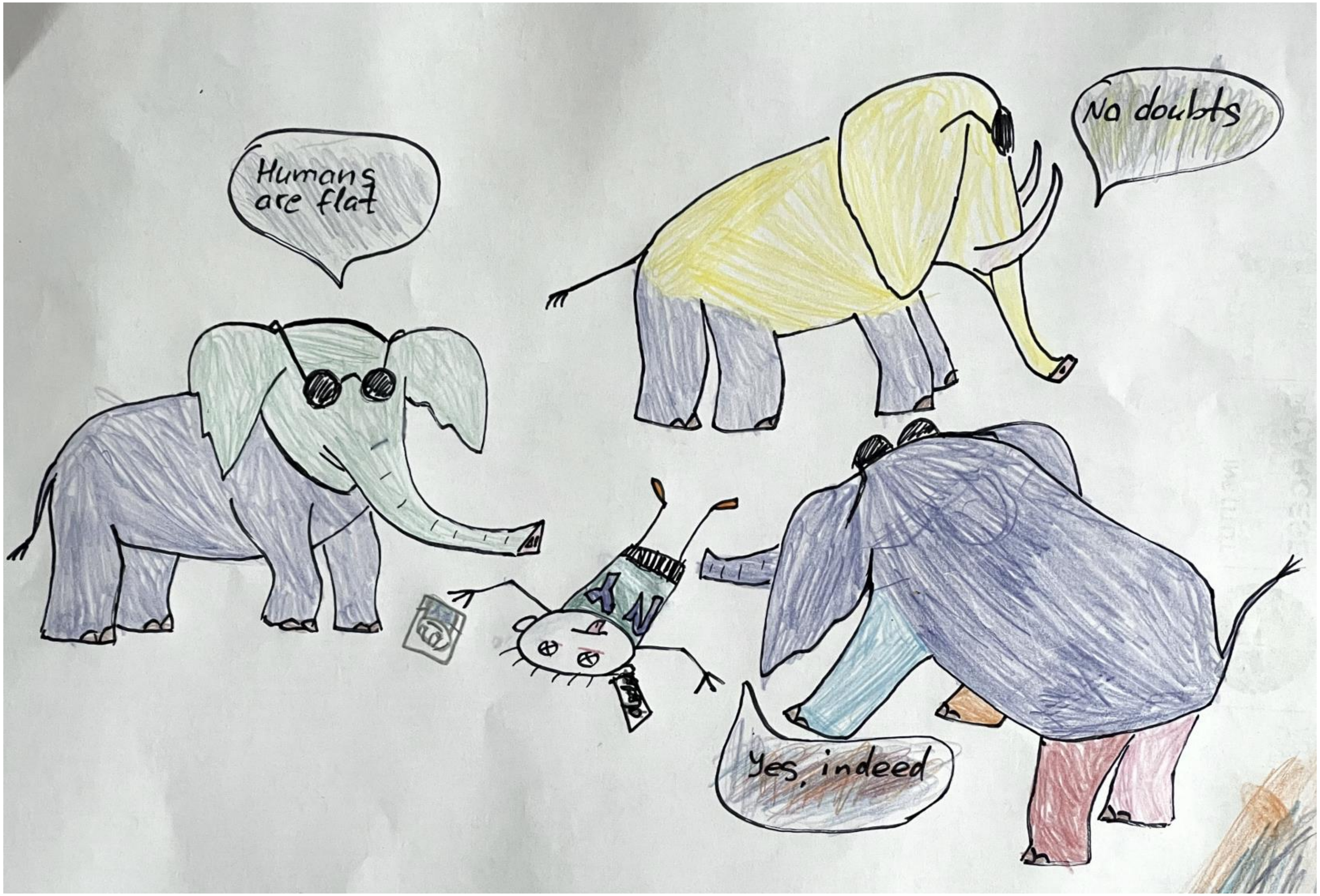


- Nice background of soft phonons responsible for CDW transition
- No nesting can be taken responsible for this softening

Conclusions

- DS helps to locate soft phonon features beyond of simple spots
- DS shape is more discriminating than just q_{CDW}
- Nesting and EPC are NOT mutually excluding
- It helps to combine DS with IXS
- (ID28 ESRF beamline offers tandem use of methods)

proposal submission deadline 12.09.2022



[A. Bosak, V. Bosak, 2022]

Zinc Fermi surface and nesting picture