Electronic band structure and van der Waals coupling of $ReSe_2$ revealed by high-resolution ARPES

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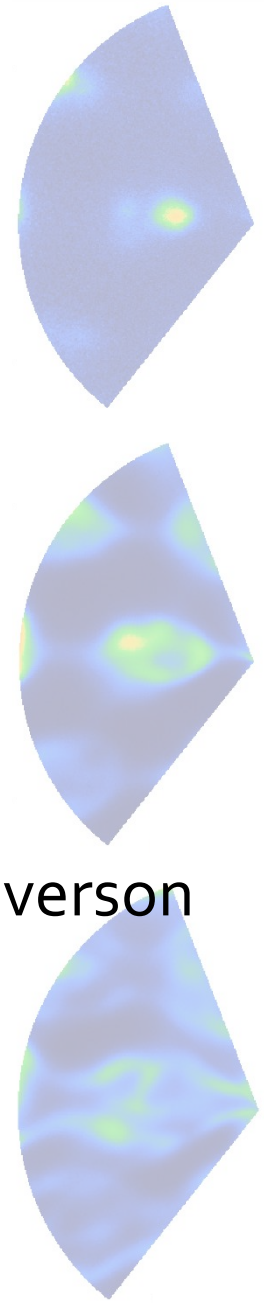
SOLEIL SYNCHROTRON

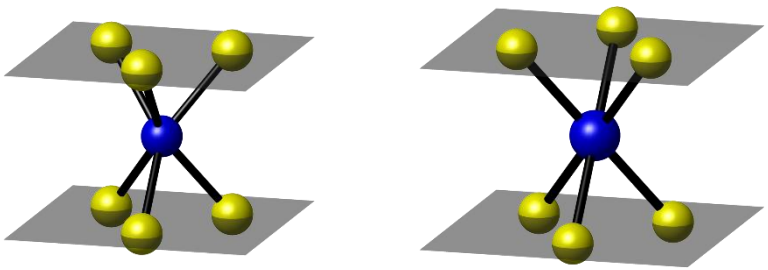


RPGR 2017, Singapore, 19 – 22/09/2017

A.K. Geim and I.V. Grigorieva, Nature **499,** 419 (2013)

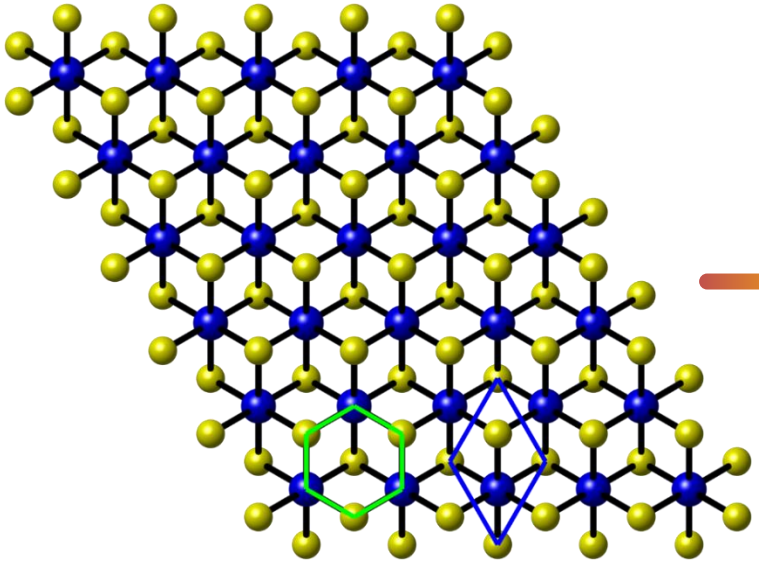
<table>
<tr><td>Graphene family</td><td>Graphene</td><td colspan="2">hBN
'white graphene'</td><td>BCN</td><td>Fluorographene</td><td>Graphene oxide</td></tr>
<tr><td rowspan="2">2D chalcogenIdes</td><td colspan="2" rowspan="2">MoS_2, WS_2, $MoSe_2$, WSe_2</td><td colspan="2" rowspan="2">Semiconducting dichalcogenides:
$MoTe_2$, WTe_2,
ZrS_2, $ZrSe_2$ and so on</td><td colspan="2">Metallic dichalcogenides:
$NbSe_2$, NbS_2, TaS_2, TiS_2, $NiSe_2$ and so on</td></tr>
<tr><td colspan="2">Layered semiconductors:
GaSe, GaTe, InSe, Bi_2Se_3 and so on</td></tr>
<tr><td rowspan="2">2D oxides</td><td>Micas, BSCCO</td><td>MoO_3, WO_3</td><td rowspan="2" colspan="2">Perovskite-type:
$LaNb_2O_7$, $(Ca,Sr)_2Nb_3O_{10}$,
$Bi_4Ti_3O_{12}$, $Ca_2Ta_2TiO_{10}$ and so on</td><td colspan="2">Hydroxides:
$Ni(OH)_2$, $Eu(OH)_2$ and so on</td></tr>
<tr><td>Layered Cu oxides</td><td>TiO_2, MnO_2, V_2O_5,
TaO_3, RuO_2 and so on</td><td colspan="2">Others</td></tr>
</table>

H **T**

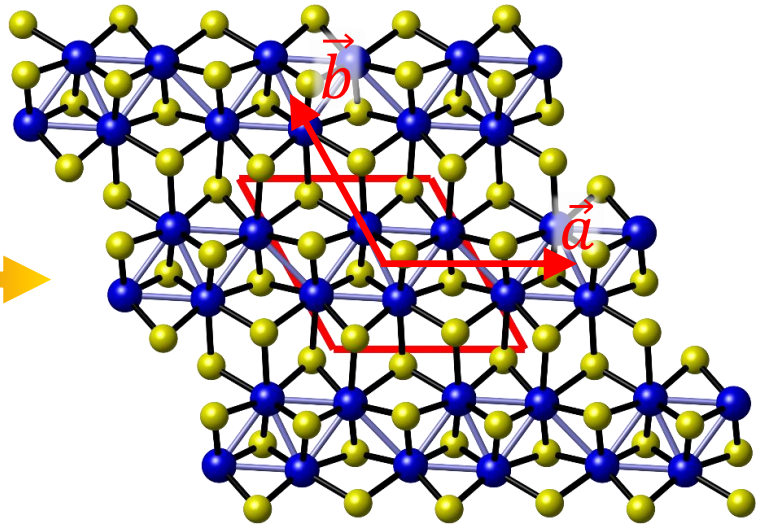


Real and reciprocal lattices of $ReSe_2$

1T – top view



(Not quite) **1T'** – top view



Real and reciprocal lattices of $ReSe_2$

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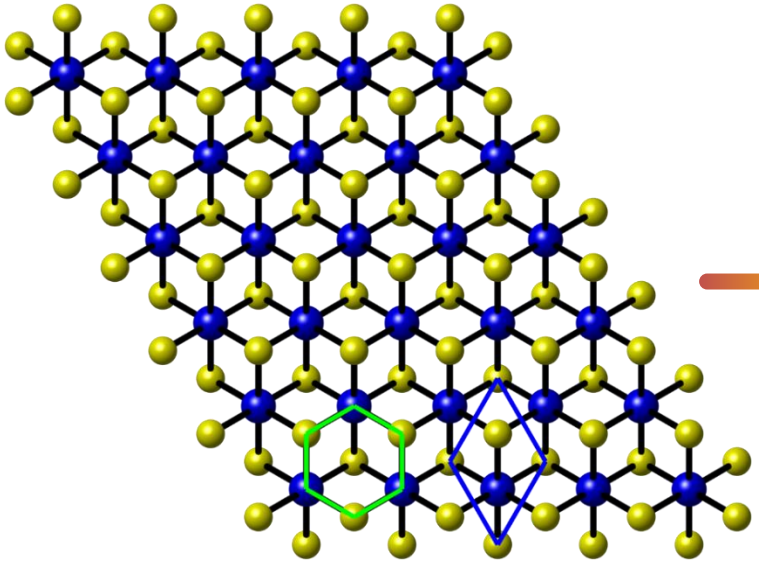
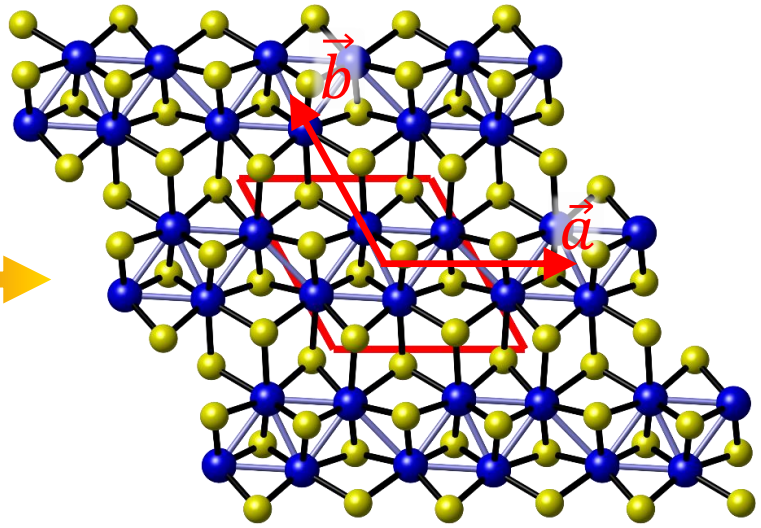
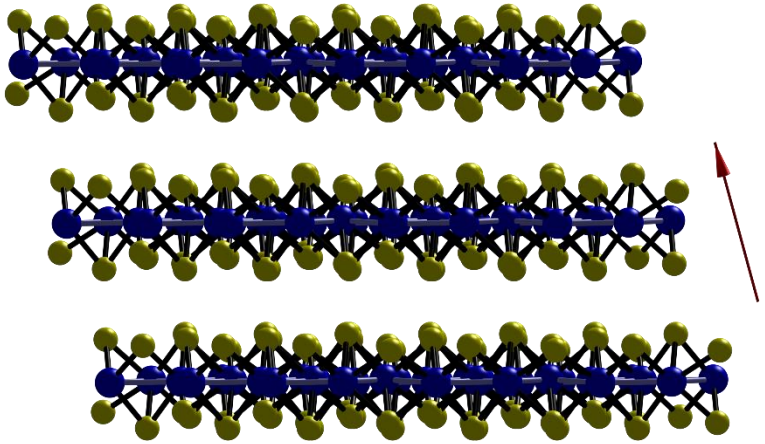


(Not quite) **1T'** – top view



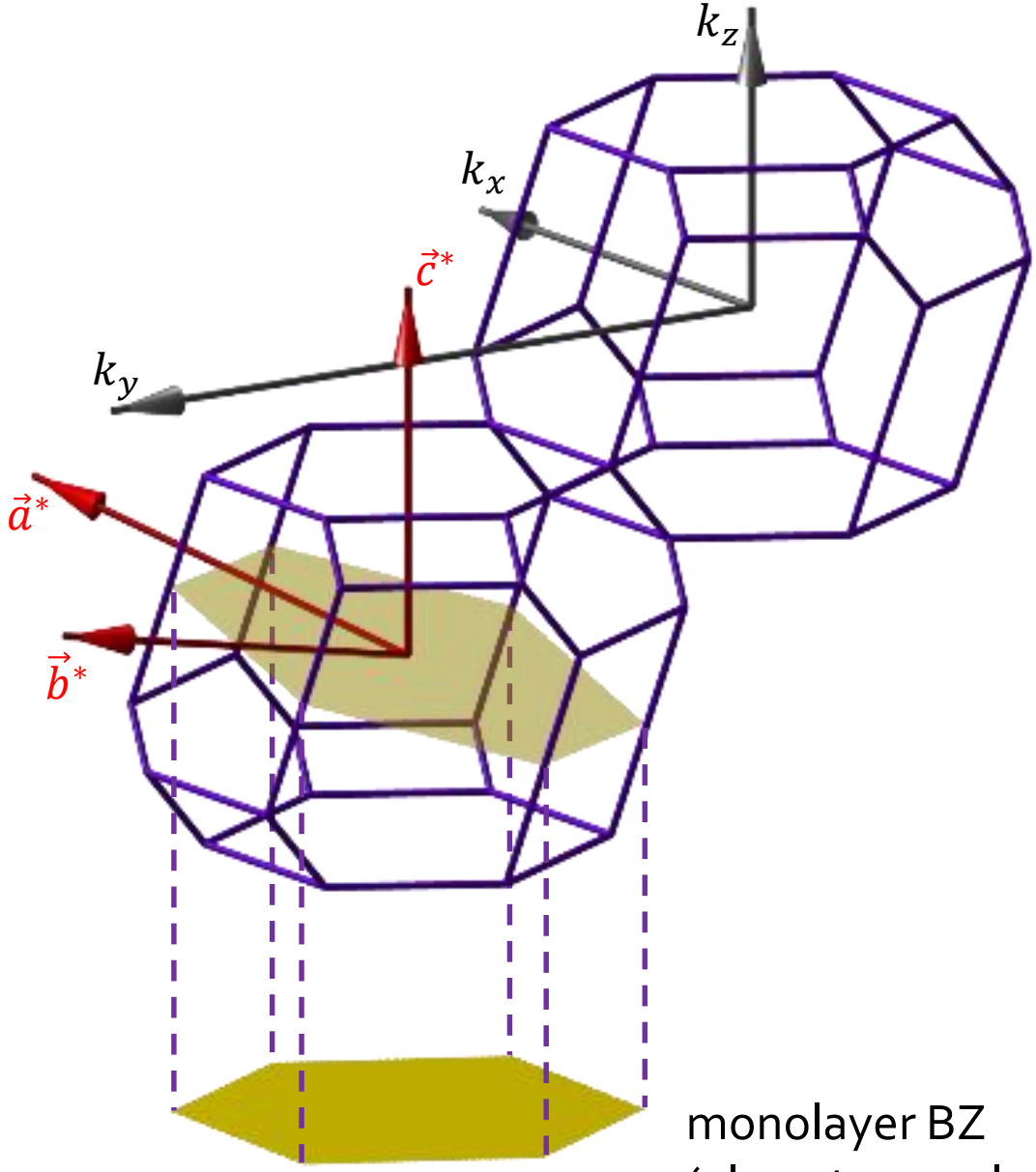
- Low symmetry (group $P\bar{1}$)
- Characteristic chains of Re "lozenges"
- The *c*-axis not perpendicular to the layers
- However, inversion symmetry present even in monolayers [in contrast to semiconducting MoS_2 which has a mirror plane]



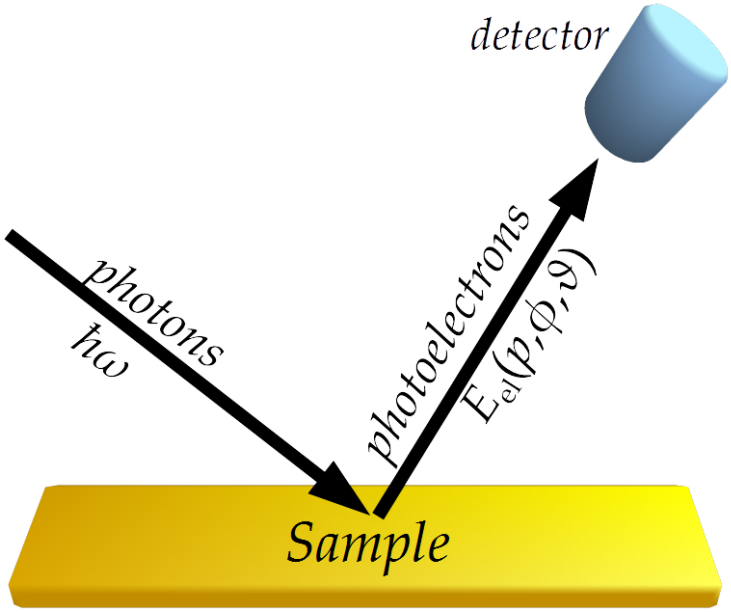
Questions:

- Where is the valence band maximum?
- Is the interlayer coupling significant?
- How significant is the distortion-induced anisotropy?

Real and reciprocal lattices of $ReSe_2$



monolayer BZ
(almost a regular hexagon)

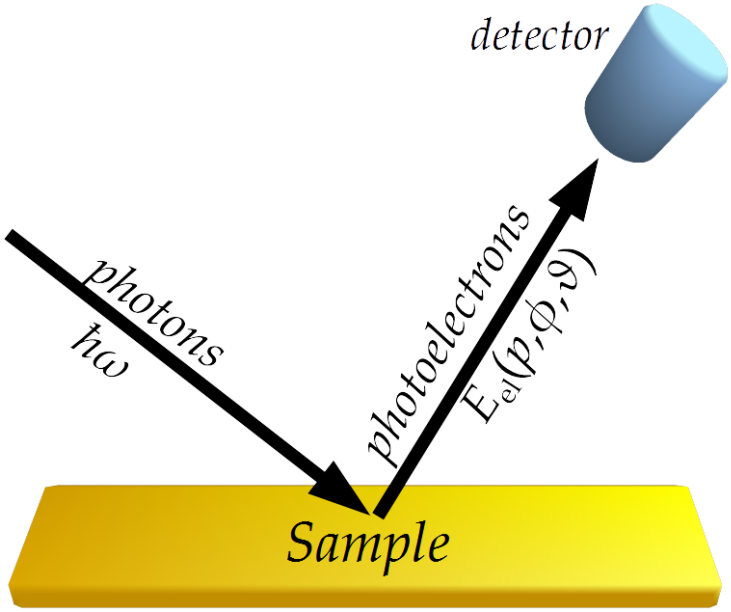


1) $\hbar\omega + (E_0 + \varepsilon_{\boldsymbol{k}}) = E_{\mathrm{el}} + V_0$

2) $\hbar(\boldsymbol{k_x} + \boldsymbol{k_y}) = \boldsymbol{p}_{\parallel}$

valence band bottom

inner potential



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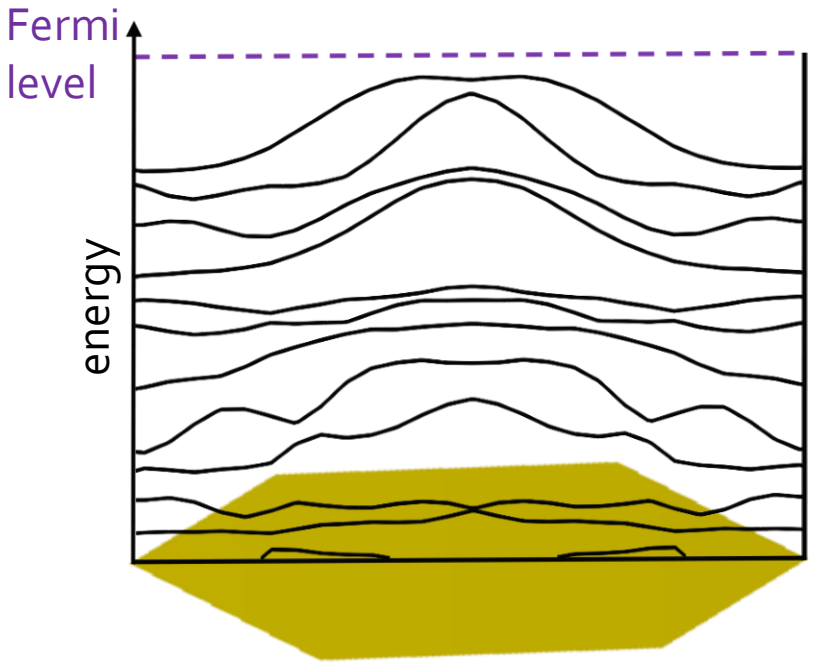

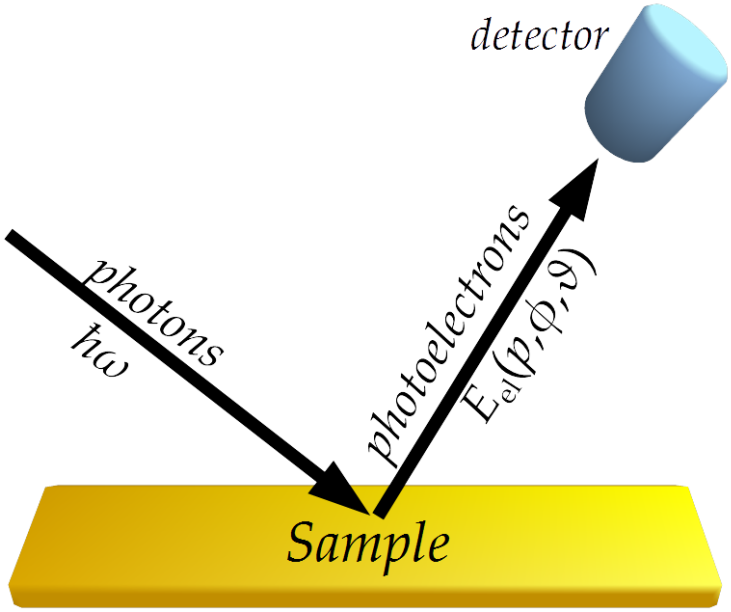

1) $\hbar\omega + (E_0 + \varepsilon_{\boldsymbol{k}}) = E_{\mathrm{el}} + V_0$

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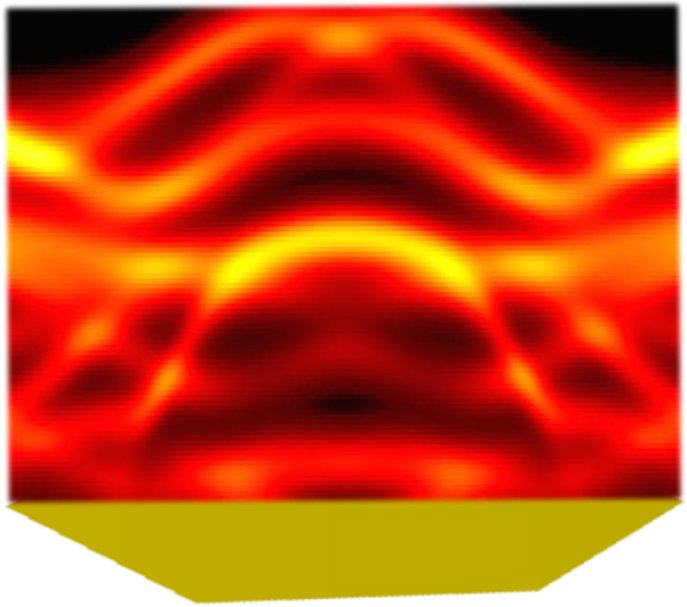
(simulated)

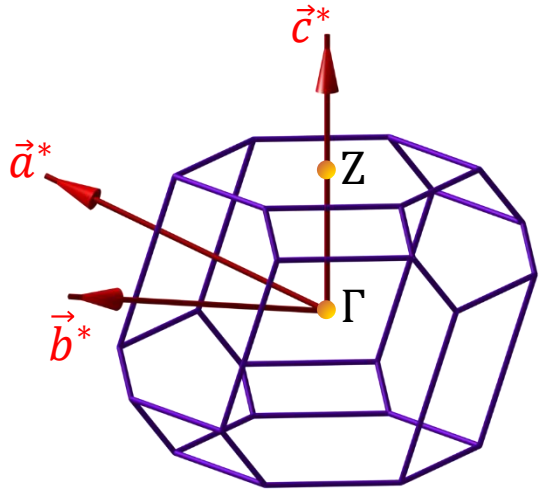


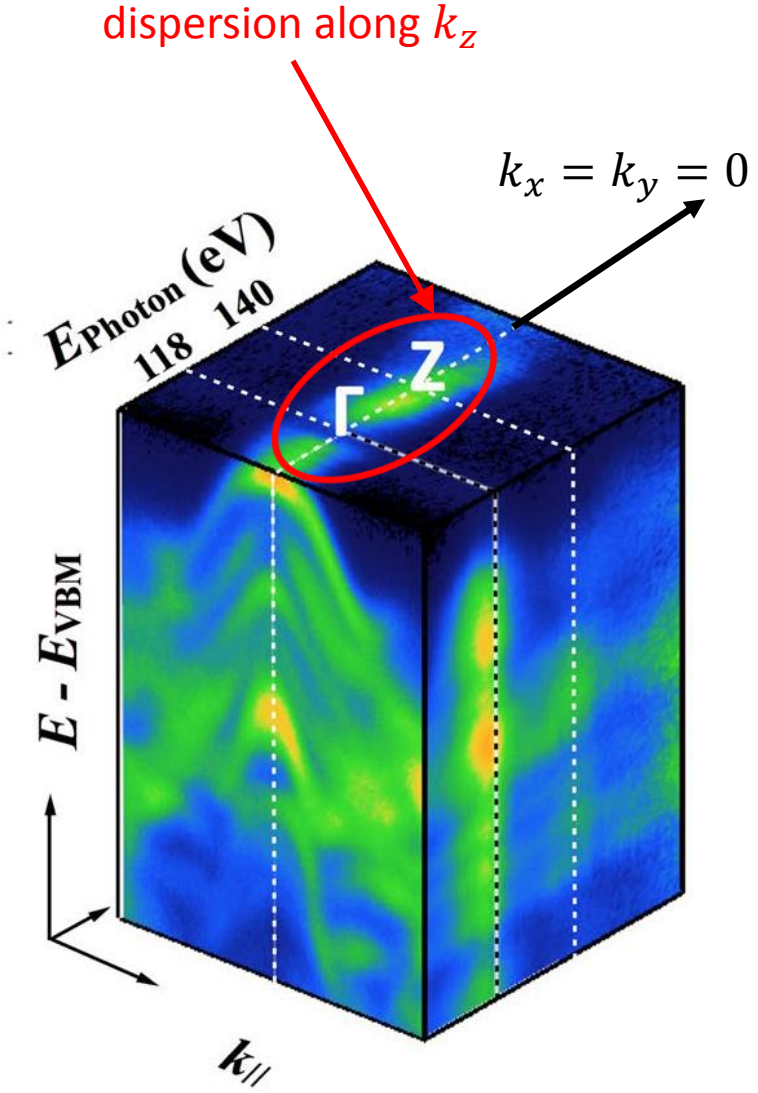
I. Handling wave vector perpendicular to the layers

- Dispersion along k_z implies significant interlayer coupling
- Knowledge of $\vec{c}^*$ allows determination of the inner potential and assignment of the Γ and Z points

1) $\hbar\omega + (E_0 + \varepsilon_{\boldsymbol{k}}) = E_{\mathrm{el}} + V_0$

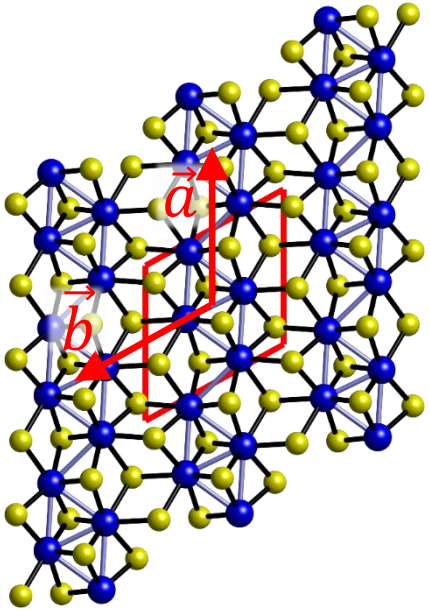
~~2) $\hbar(\boldsymbol{k_x} + \boldsymbol{k_y}) = \boldsymbol{p}_{\parallel}$~~





II. Studying $k_z = 0$ plane

- No periodicity in the (k_x, k_y) plane
- VBM away from the Γ point?



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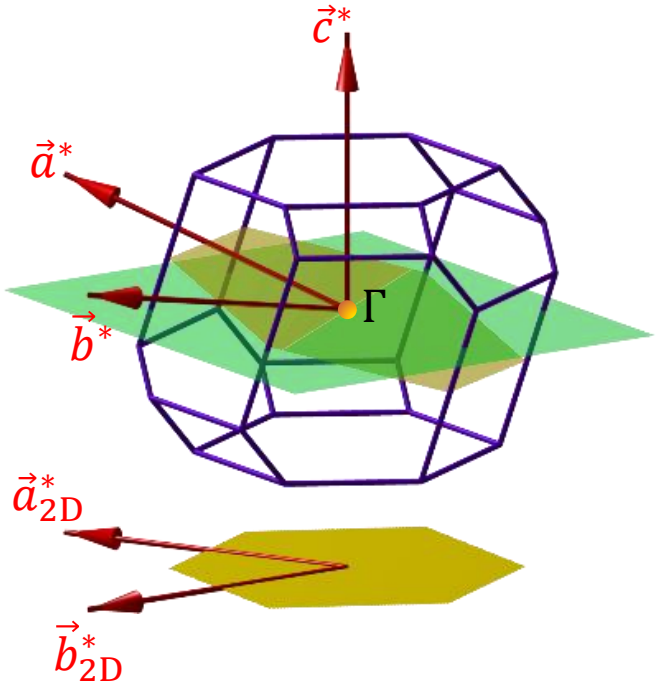
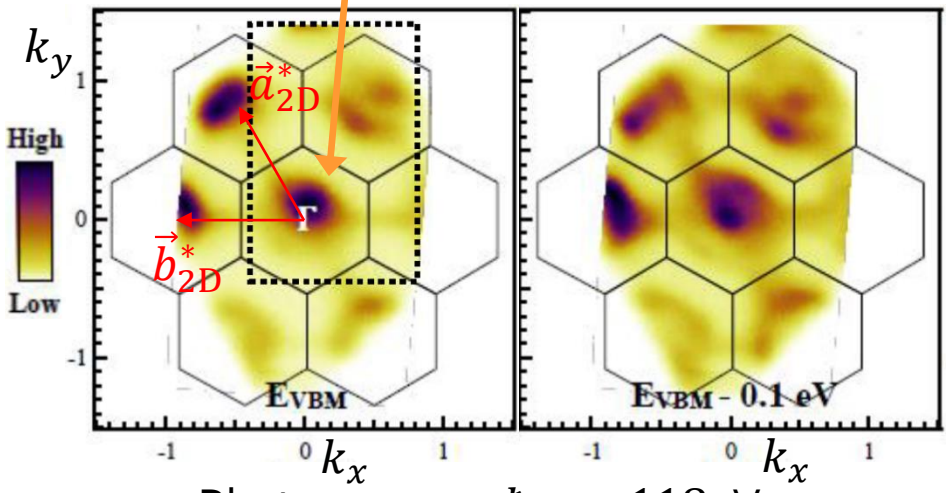


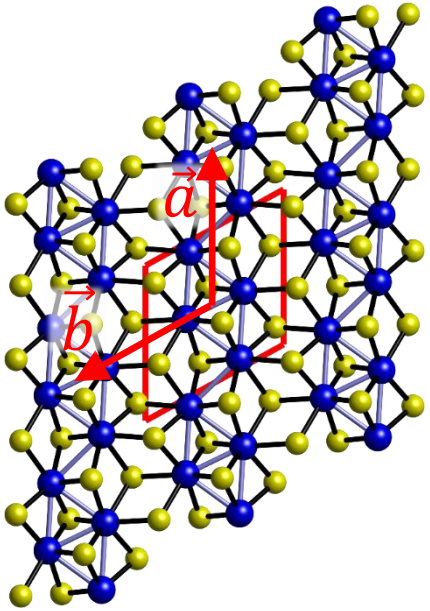
Valence band maximum away from Γ



Photon energy $\hbar\omega = 118$eV

III. Studying in-plane anisotropy

- Chain-like ARPES features perpendicular to the Re chains
- Dispersion flatter between chains than along chains – weaker coupling



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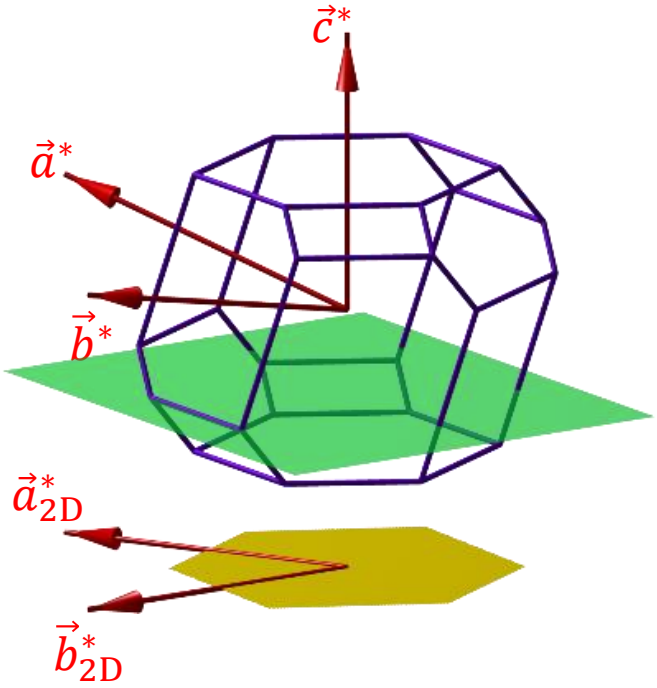
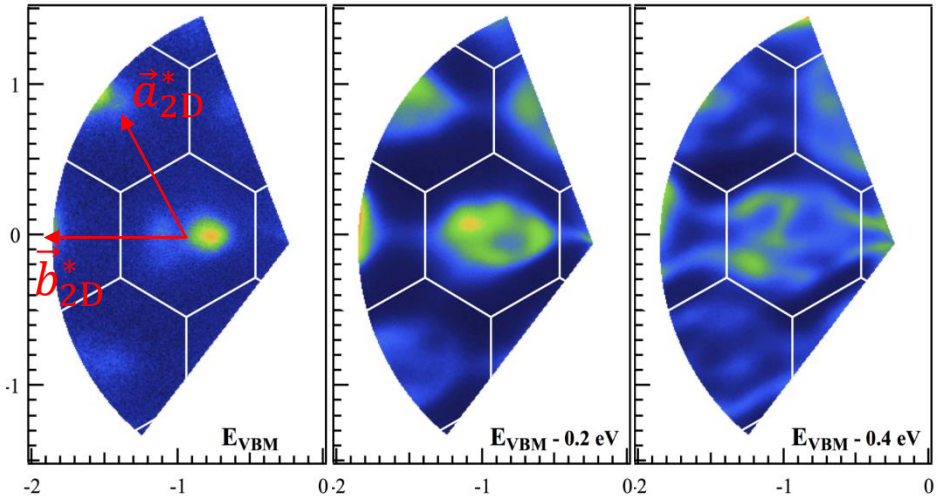
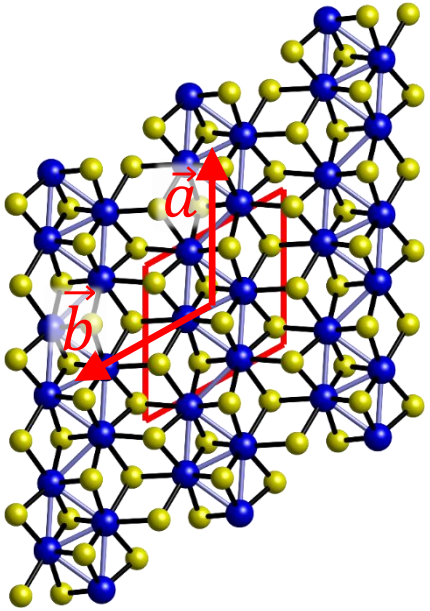




Photon energy $\hbar\omega = 100$eV

III. Studying in-plane anisotropy

- Chain-like ARPES features perpendicular to the Re Chains
- Dispersion flatter between chains than along chains – weaker coupling



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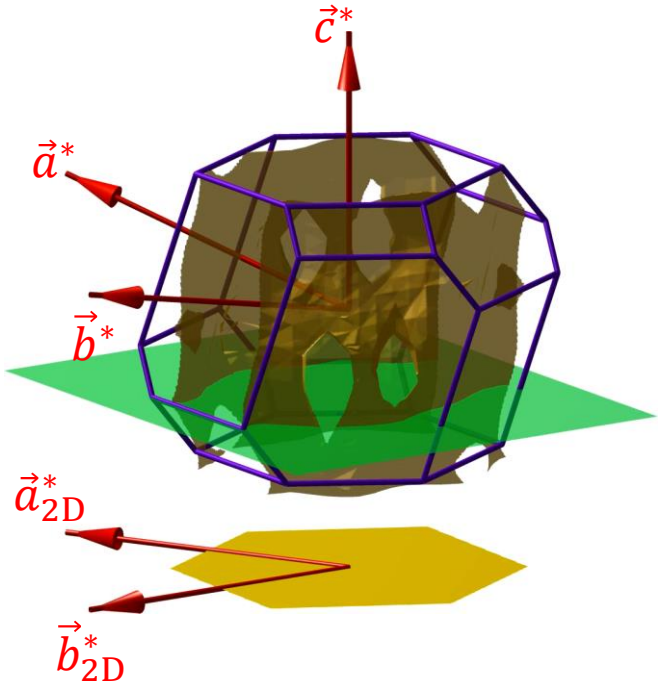

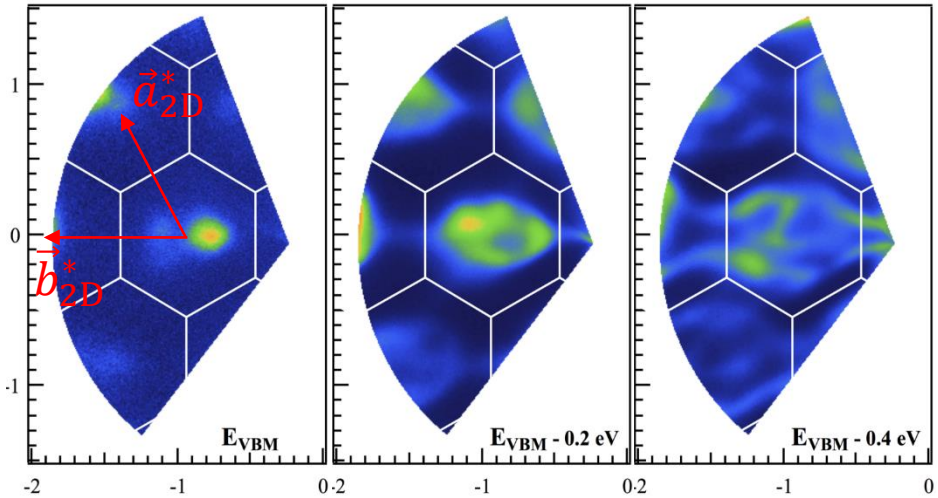

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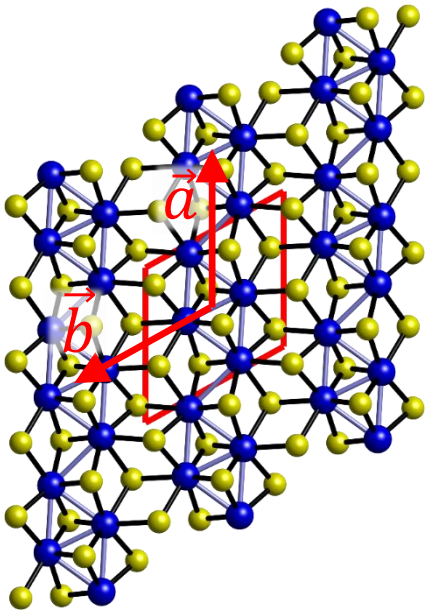
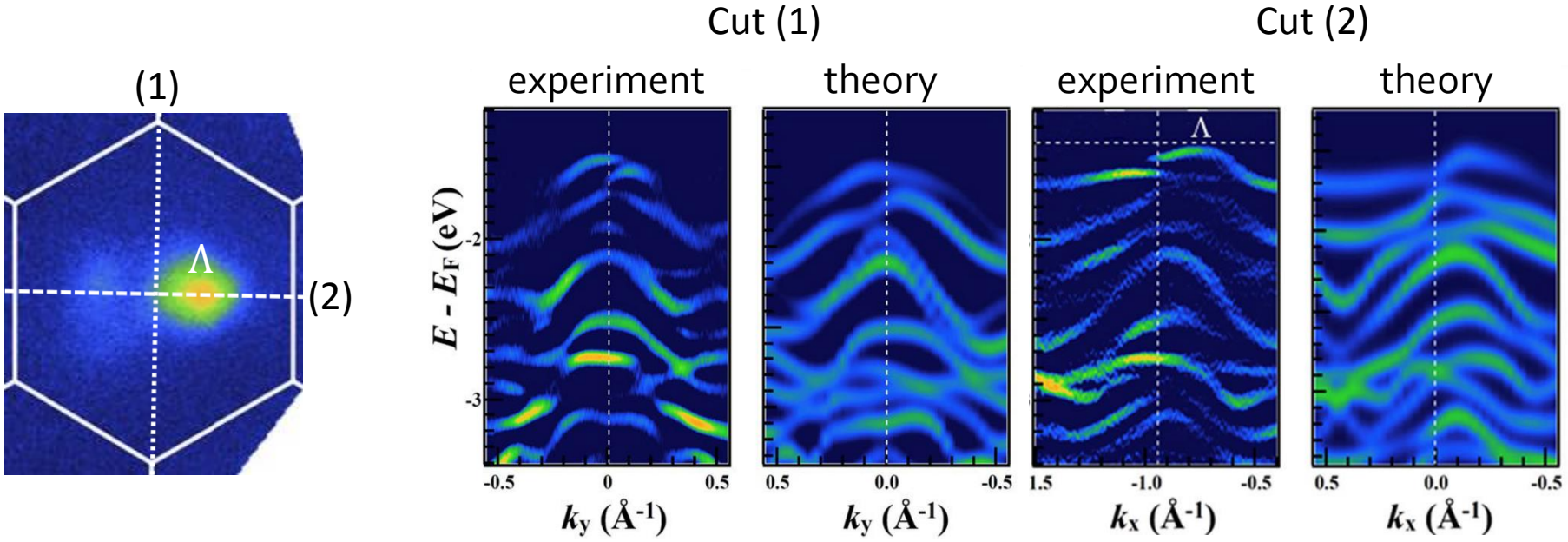
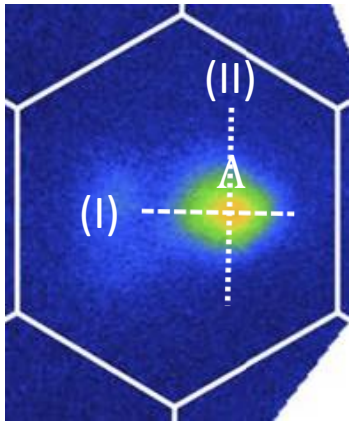
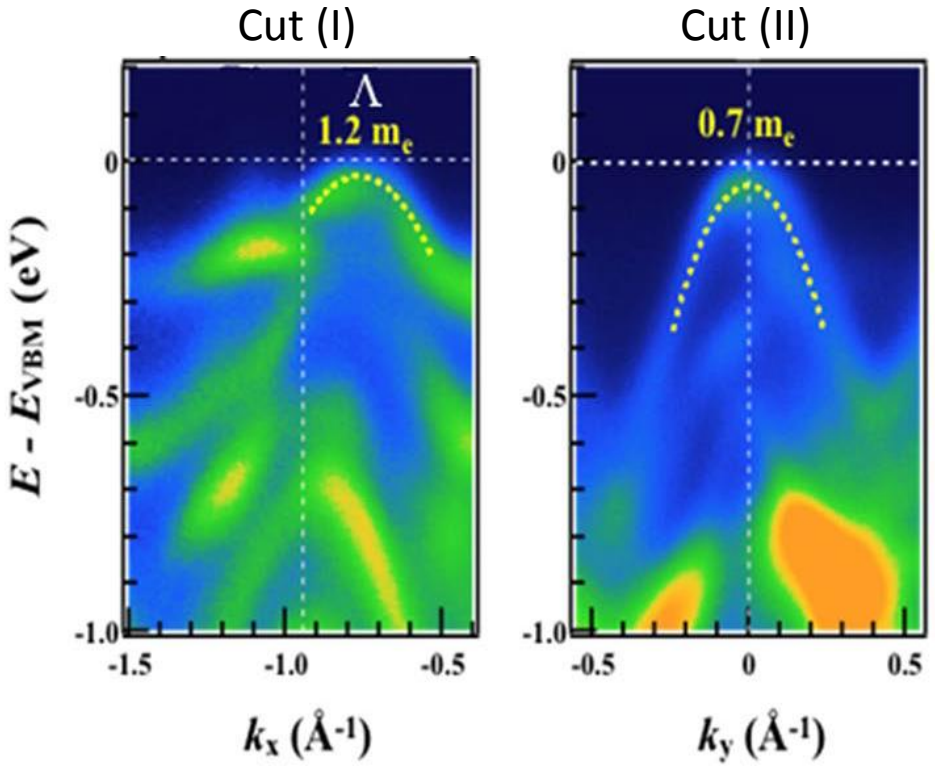




III. Studying in-plane anisotropy

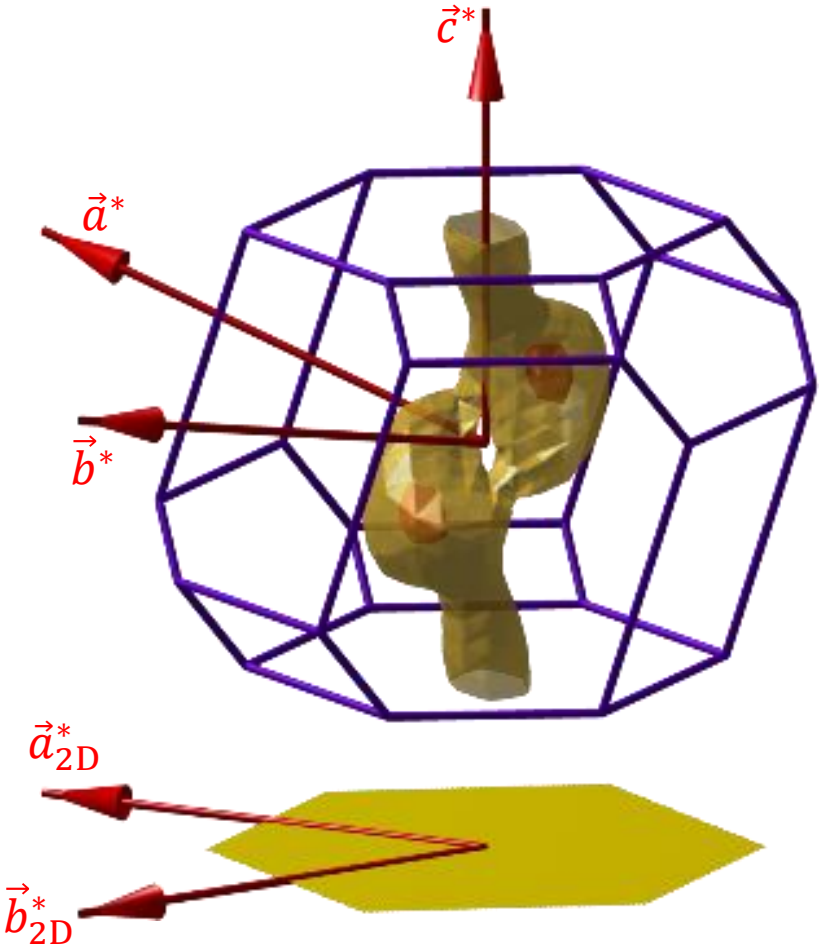
- Chain-like ARPES features perpendicular to the Re chains
- Dispersion flatter between chains than along chains – weaker coupling
- Effective mass perpendicular to the Re chains almost twice that of the value along the chains





IV. Where is the valence band maximum?

- Not at the Γ point
- Not positioned along any of the high-symmetry directions



Summary

- Highly anisotropic valence band (effective mass doubled in direction perpendicular to Re chains as compared to along the chains)
- Significant interlayer coupling – how does the spectrum change when moving to monolayer?
- We find the valence band maximum located away from the Γ point, not in any high-symmetry direction