Ultrafast Dynamics and in-plane Chirality in the CDW phase of 1T-TaS_2

Luca Perfetti *Ecole Polytechnique*

Outline

In Plane Chirality in TaS_2

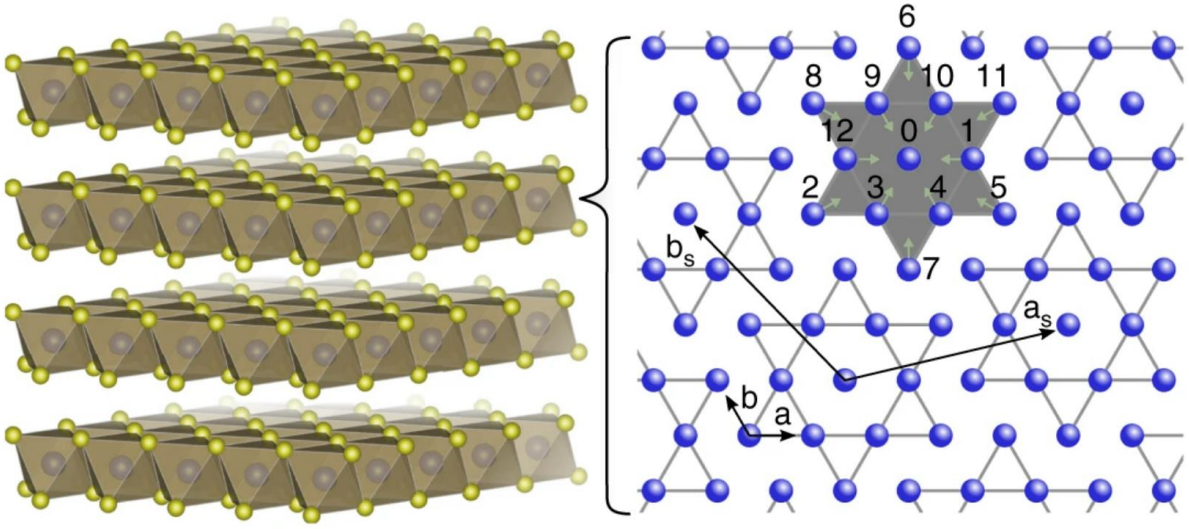
Chirality control

Mott vs Peierls

Photoinduced localization of electrons

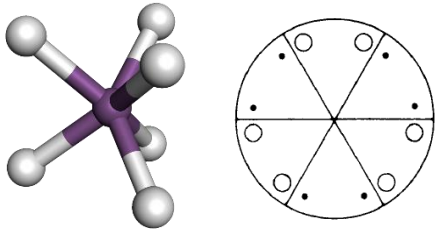
Structure of 1T - TaS_2

Trigonal antiprismatic structure



Large CDW Distortion in the form of David's stars

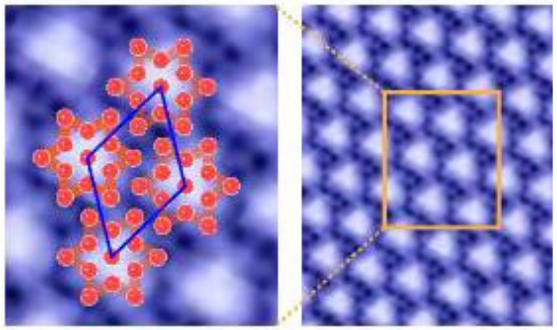
In Plane Chirality



Presence of 3 mirror plane in the high symmetry phase

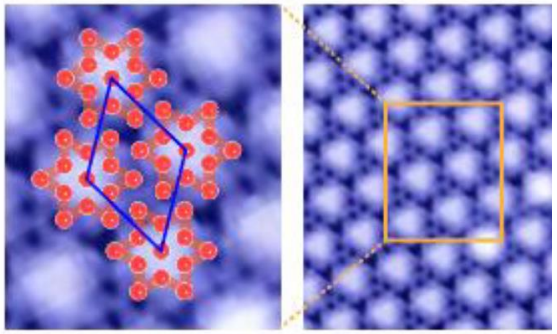
In Plane Chirality

Rotation of Superlattice unit cell by +/- 13.9° with respect to the mirror plane



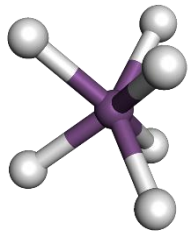
α

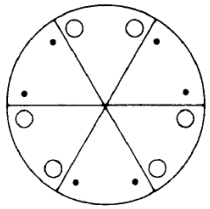
STM topography

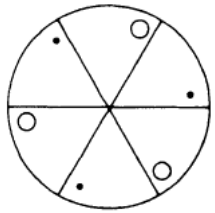


β

Reduction of point group symmetry





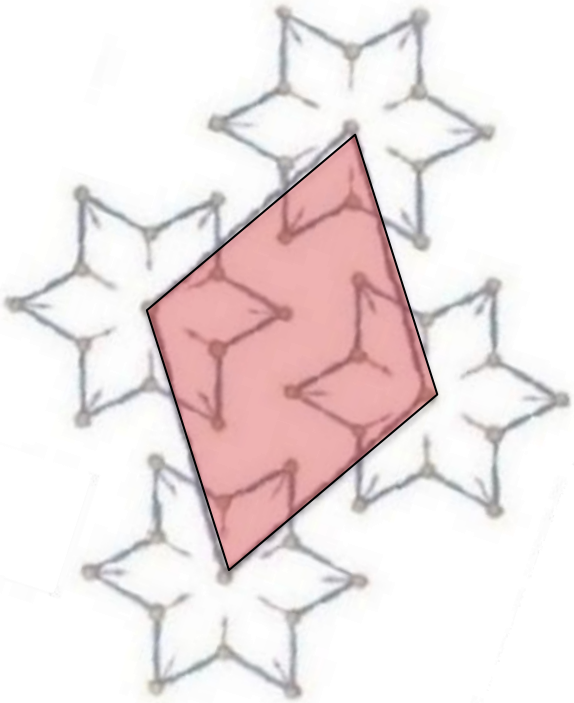


Presence of 3 mirror plane in the high symmetry phase

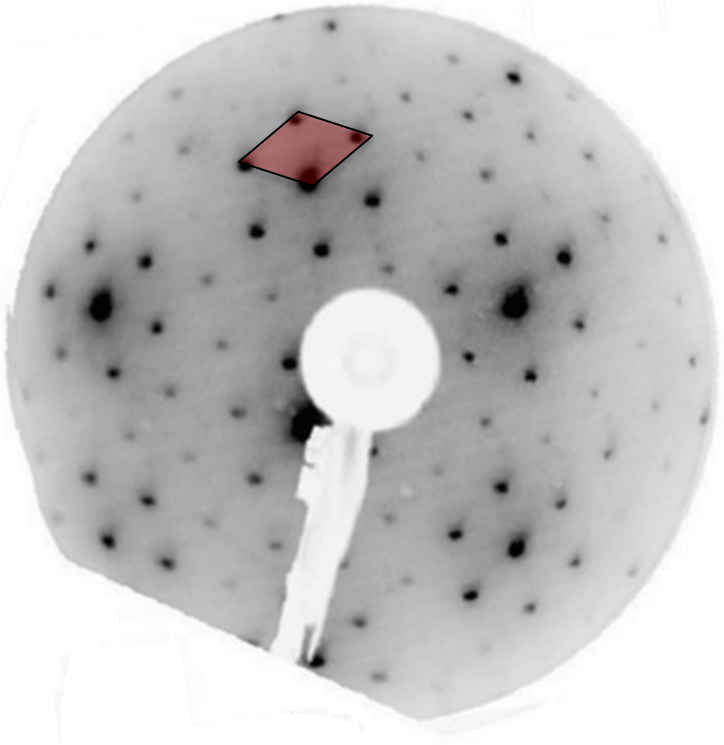
H. F. Yang et al., ***Phys. Rev. Lett.*** 129, 156401 *(2014)*

Electron diffraction and In Plane Chirality

α

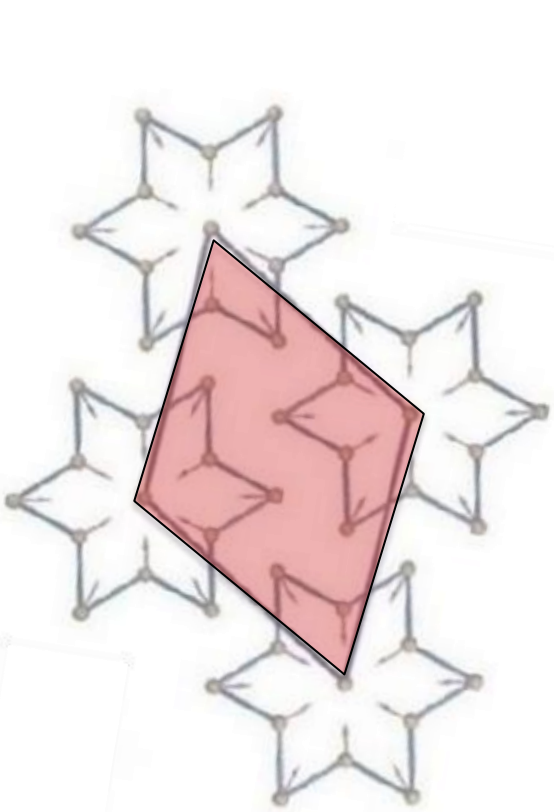


13.9° clockwise



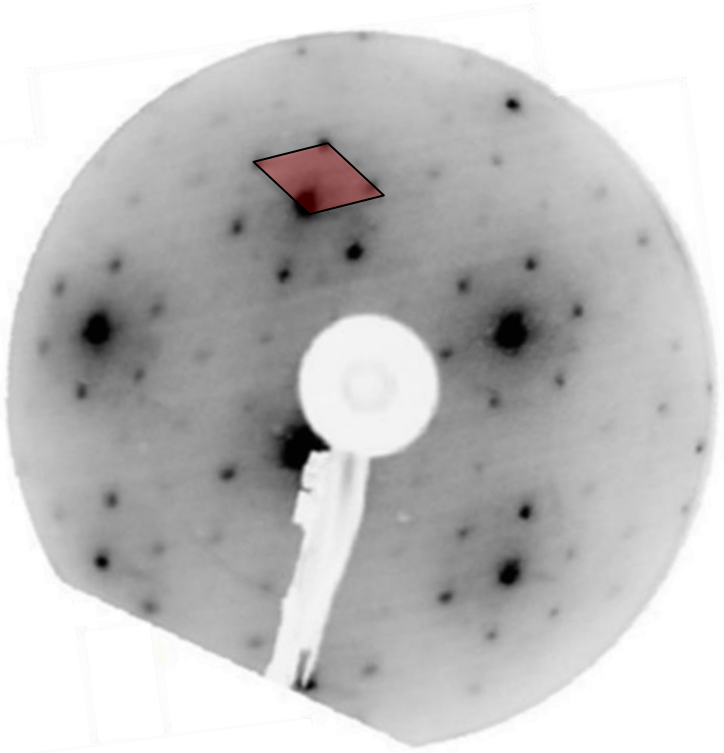
13.9° counterclockwise

Electron diffraction and In Plane Chirality



13.9° counterclockwise

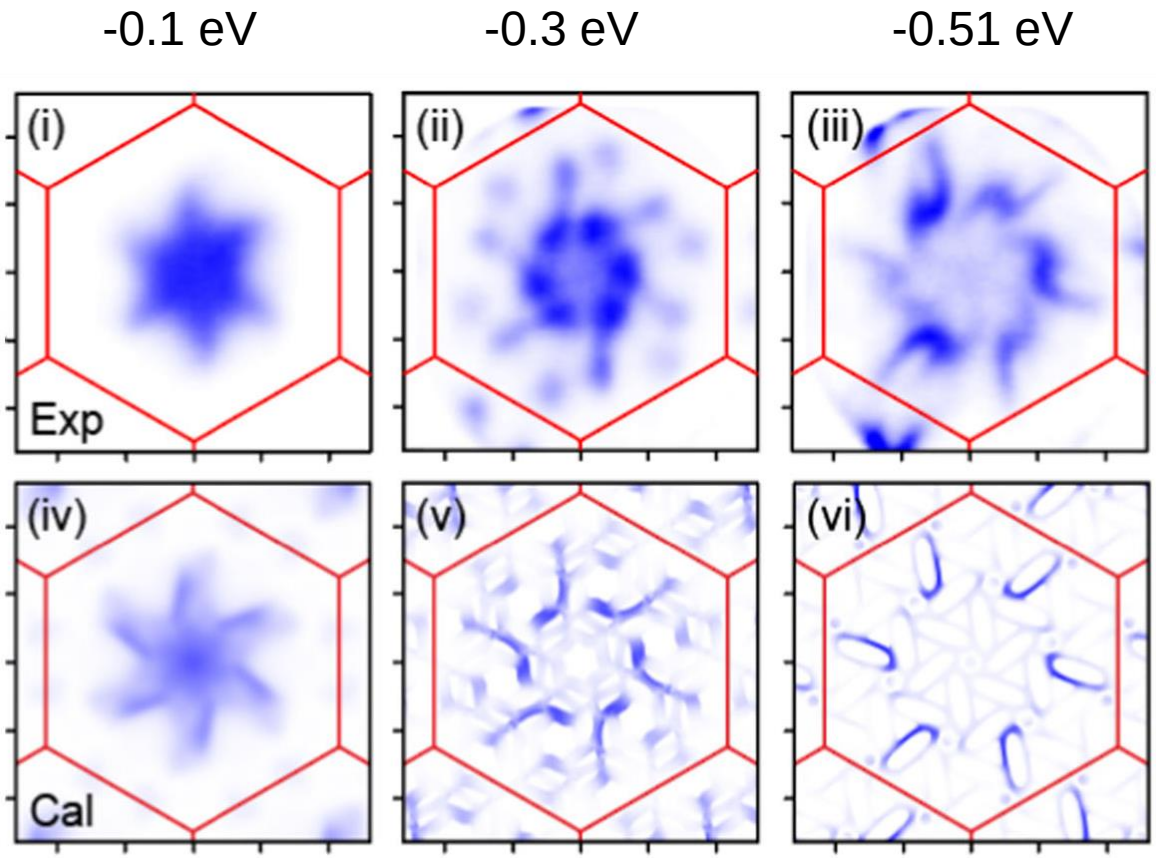
β



13.9° clockwise

ARPES and CDW chirality

Constant energy cuts



H. F. Yang et al., ***Phys. Rev. Lett.*** *129, 156401 (2022)*

Raman and in Plane Chirality

Raman dichroic contrast of E_g mode

H. F. Yang et al., ***Phys. Rev. Lett.*** *129, 156401 (2022)*

$$\mathbf{R}_{^1E_g} = Ce^{i\gamma}\begin{pmatrix} 1 & Ae^{i\alpha} \\ Ae^{i\alpha} & -1 \end{pmatrix}$$

$$\mathbf{e}_{\sigma^+} = \frac{1}{\sqrt{2}}(1, i)$$ Incoming

$$\mathbf{e}_{\sigma^-} = \frac{1}{\sqrt{2}}(1, -i)$$ Scatterred

$$I_{\sigma^+\sigma^-} \propto C^2(1 + A^2 - 2A\sin\alpha)$$
$$I_{\sigma^-\sigma^+} \propto C^2(1 + A^2 + 2A\sin\alpha)$$

Raman and in Plane Chirality

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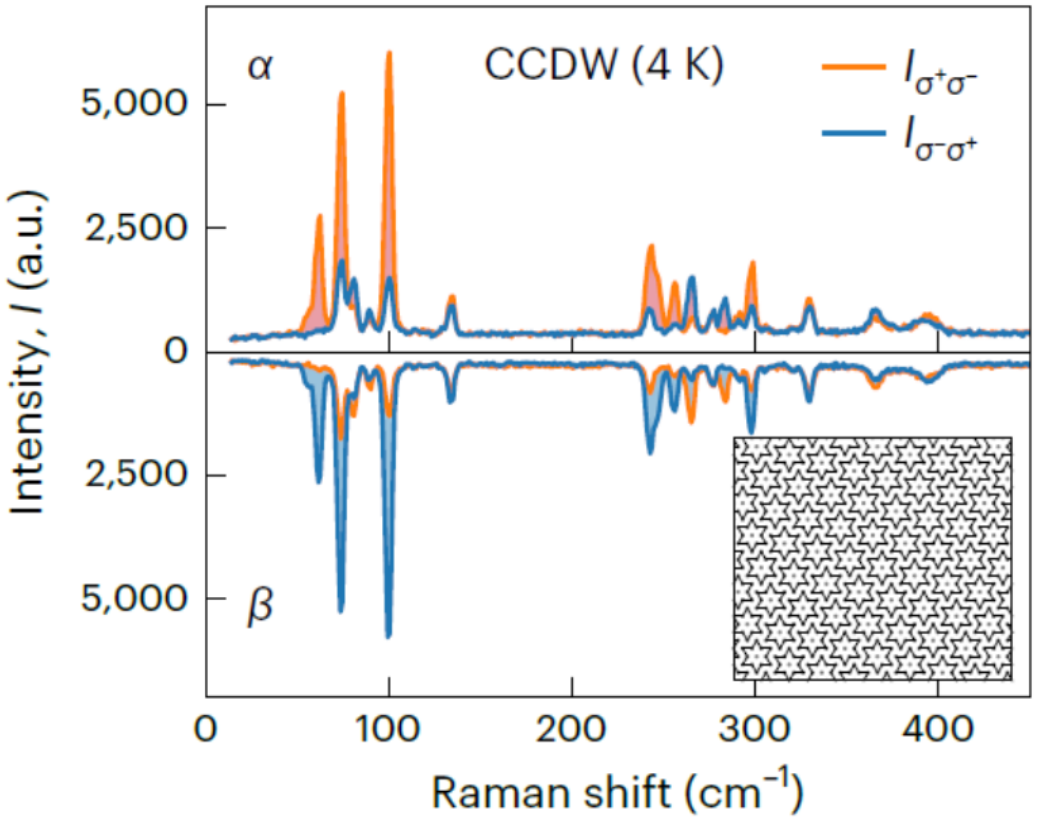
Raman and in Plane Chirality

Raman dichroic contrast of E_g mode

G. Liu et al., ***Nature Nanonotech.*** *18, 854 (2023)*



Outline

In Plane Chirality in TaS_2

Chirality control

Mott vs Peierls

Photoinduced localization of electrons

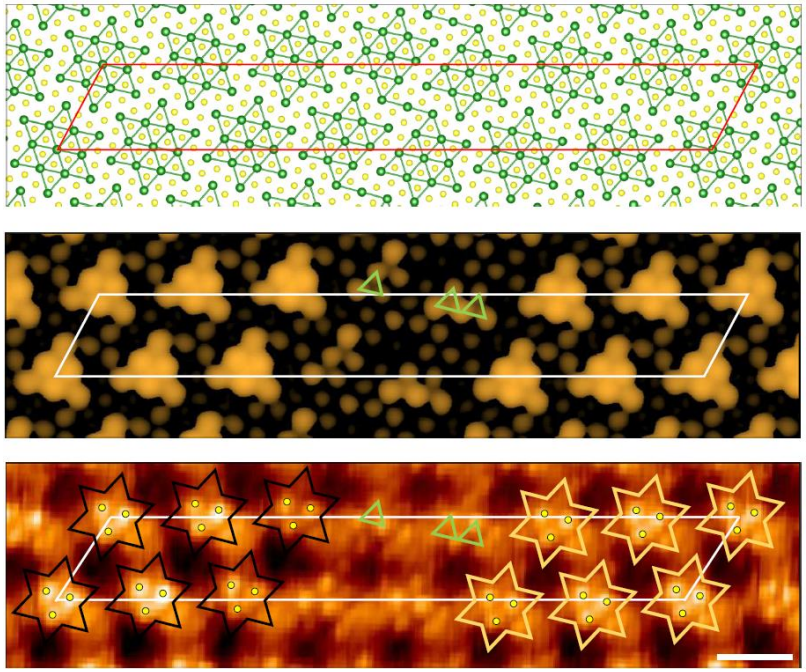
Metallic Domain Walls

Internal energy 10-30 meV/nm

Atoms

STM Simulation

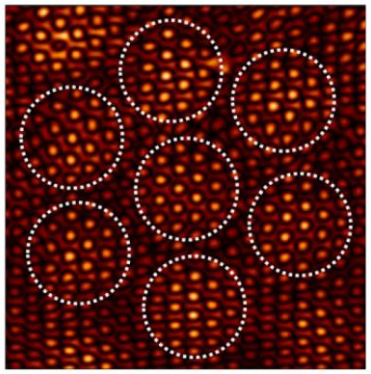
STM Measure



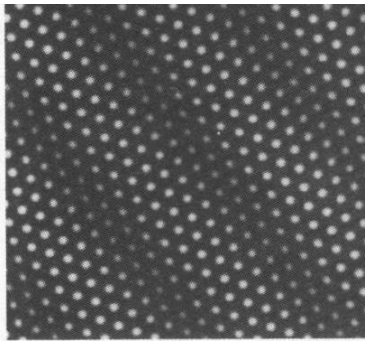
B. Burk et al., ***Science*** *257, 362 (1992)*

J W. Park et al., ***Nature Comm.*** *10, 4038 (2019)*

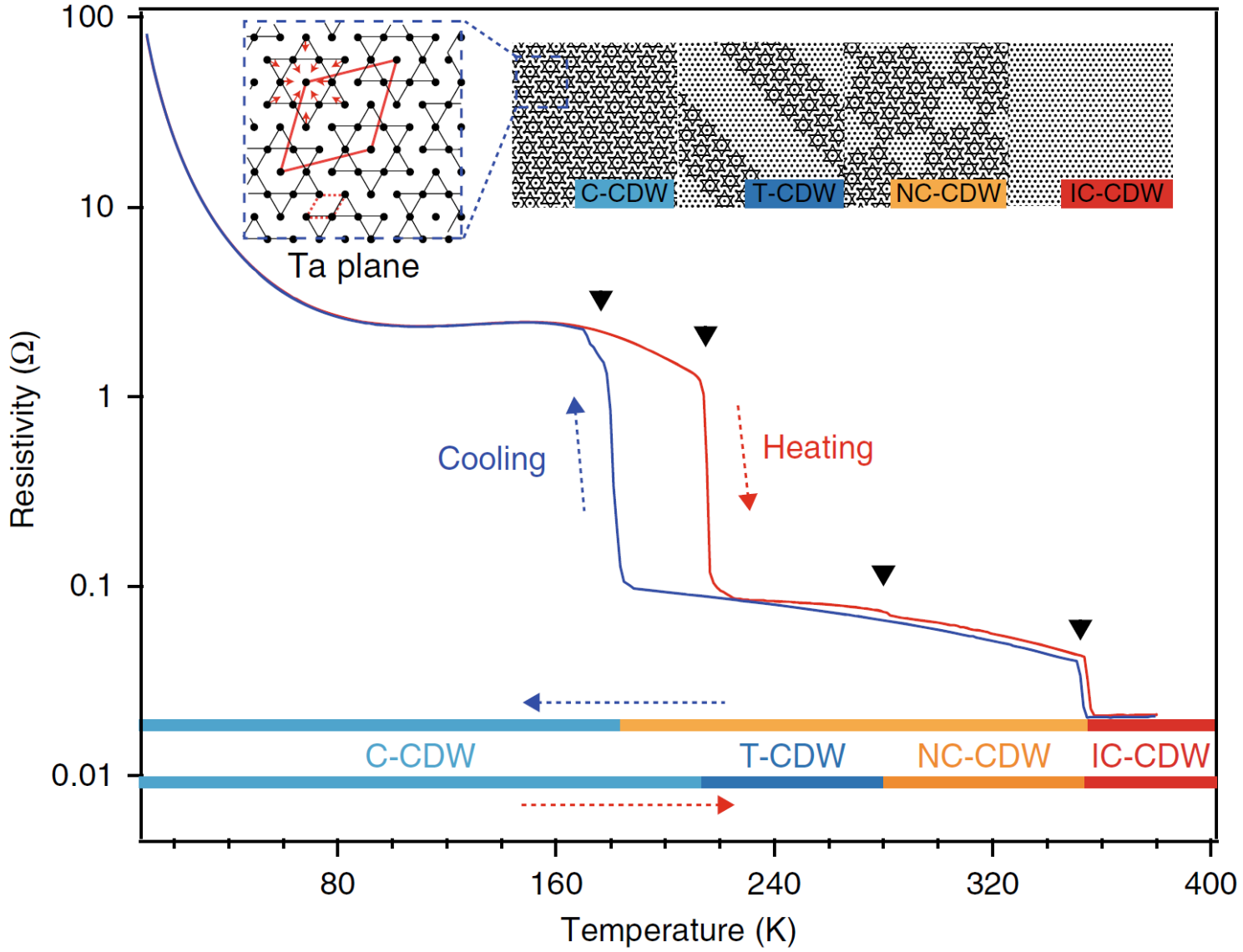
NC-CDW



T-CDW

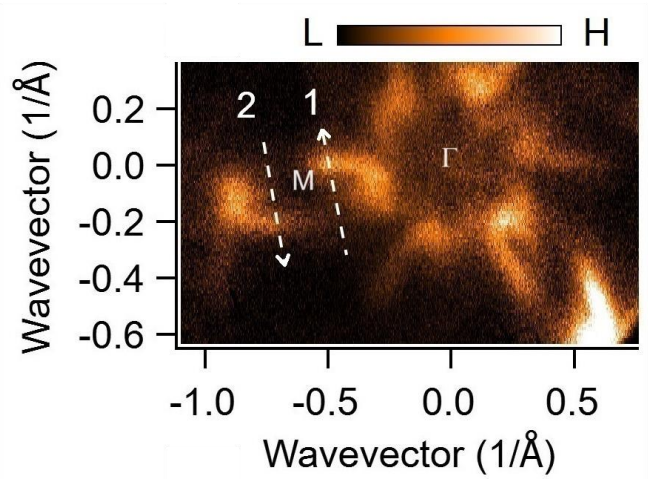


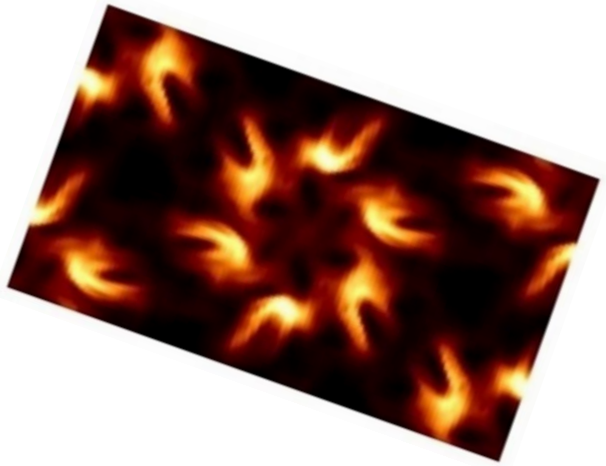
Phase diagram



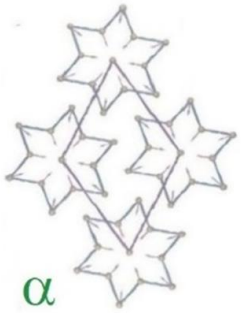
ARPES and CDW chirality

C-CDW phase

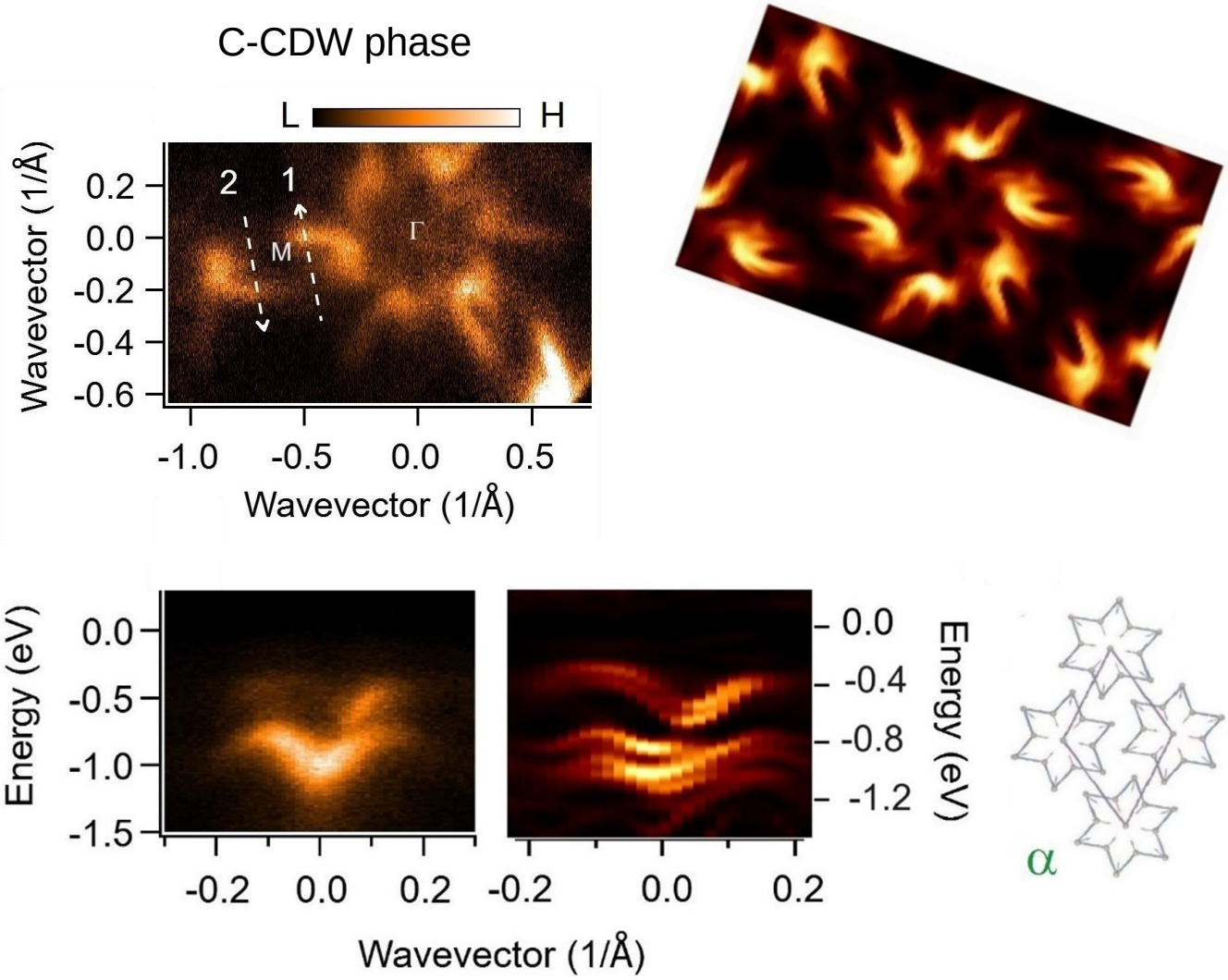




DFT
simulation

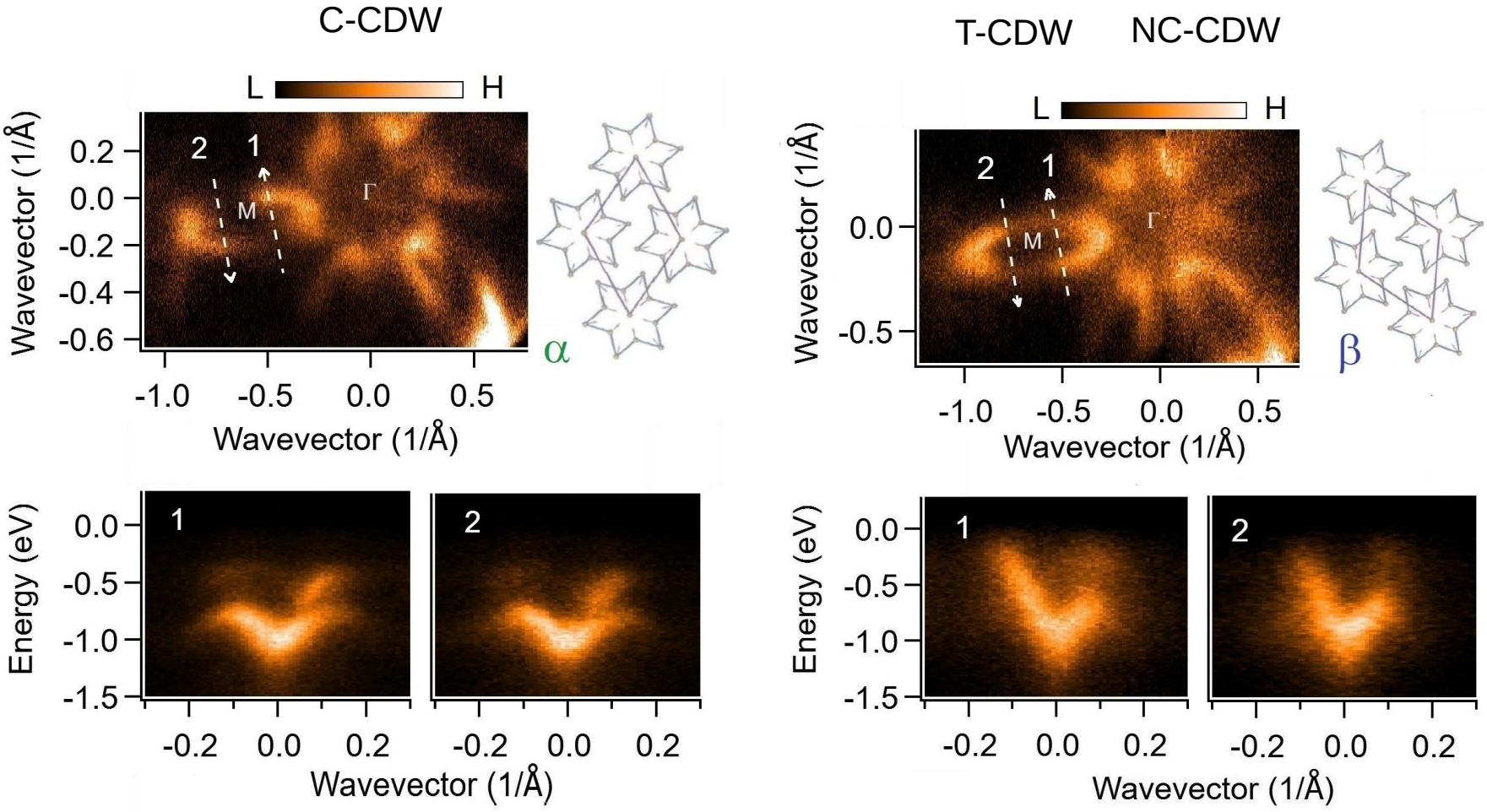


ARPES and CDW chirality



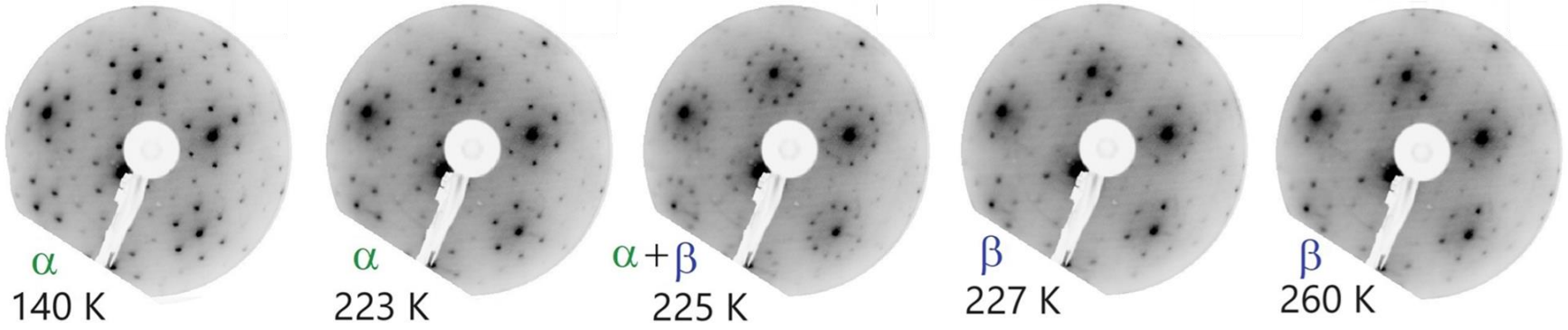
ARPES and chirality switching

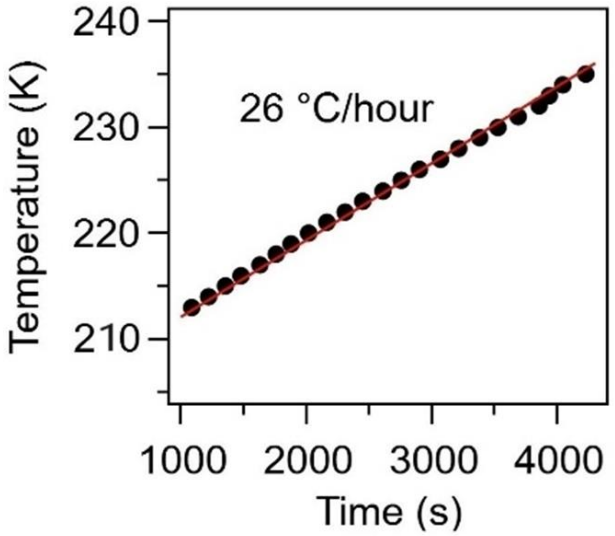
Quasistatic heating

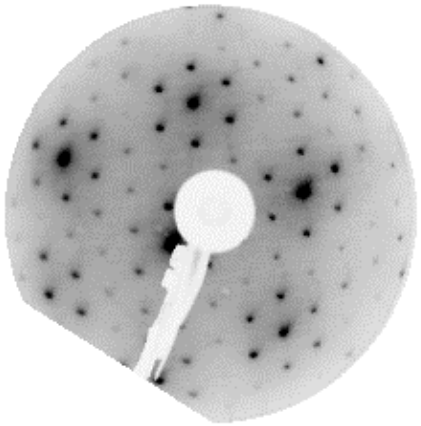


LEED and chirality switching

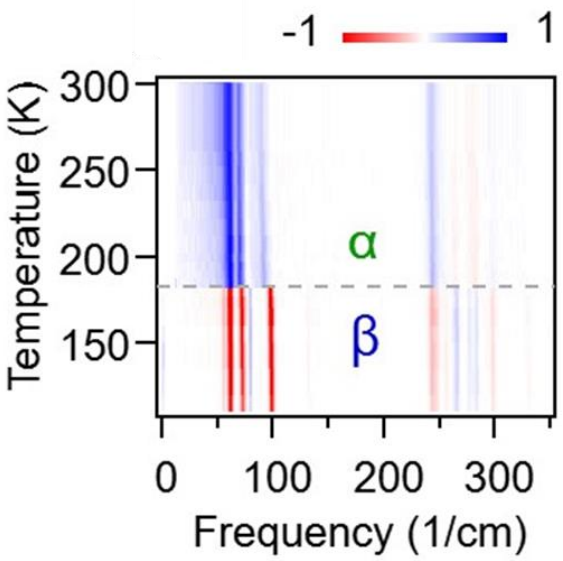
Quasistatic heating



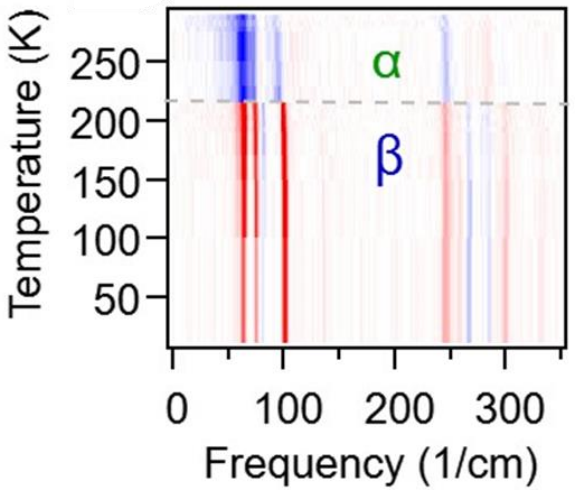


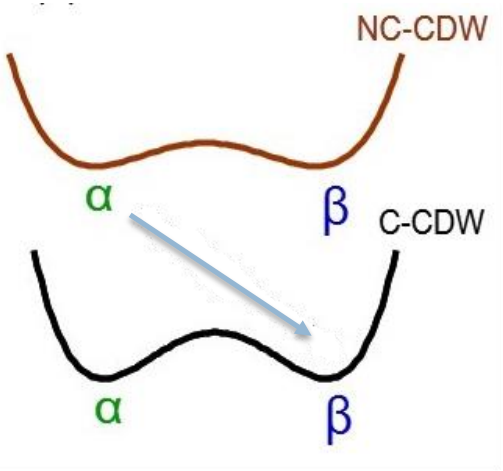


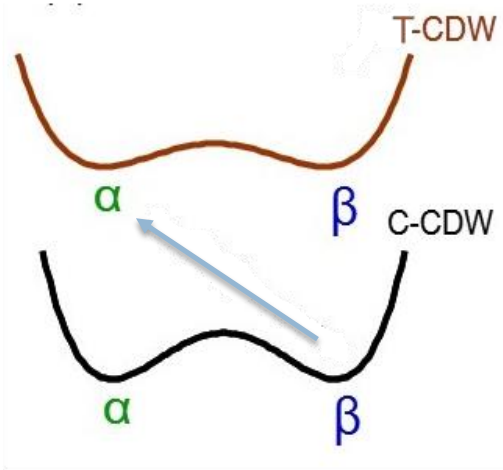
Raman and chirality switching



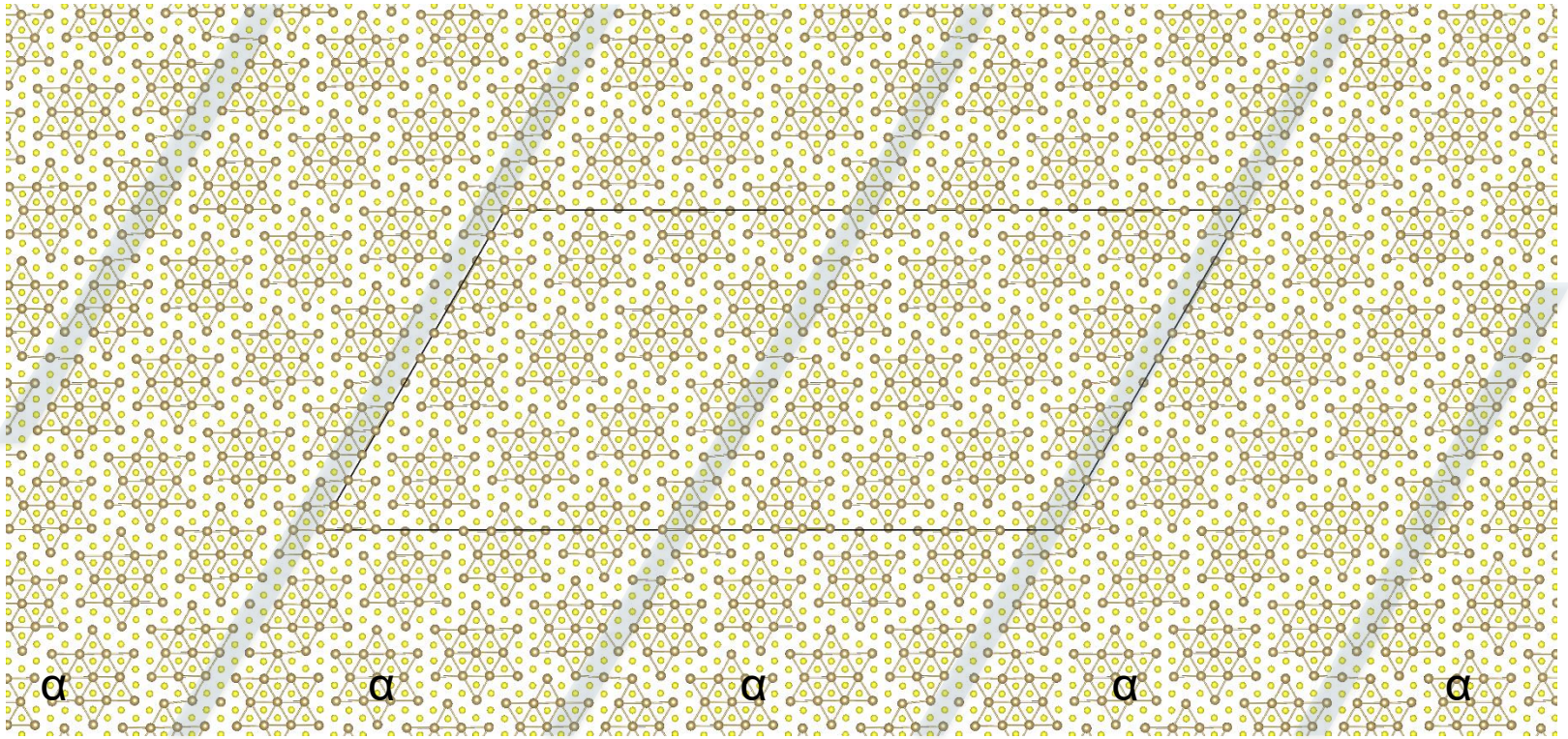
Dichroic contrast



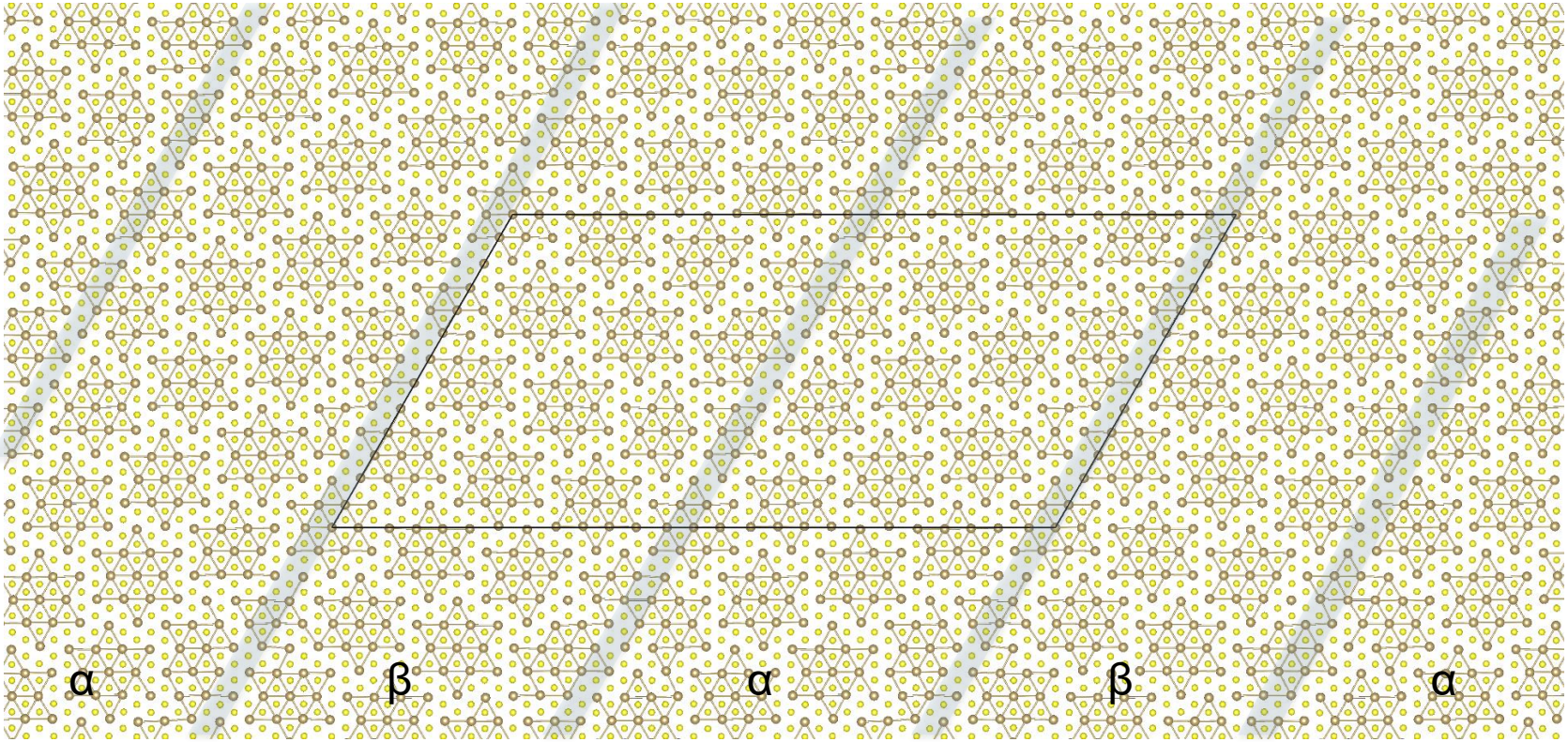




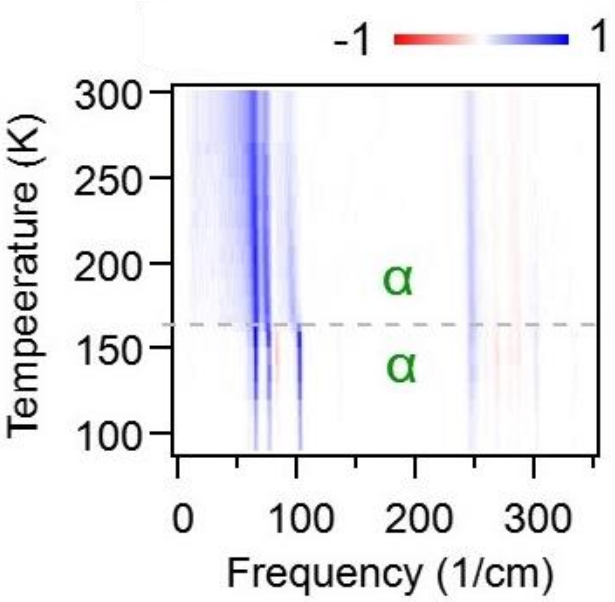
α – α domains



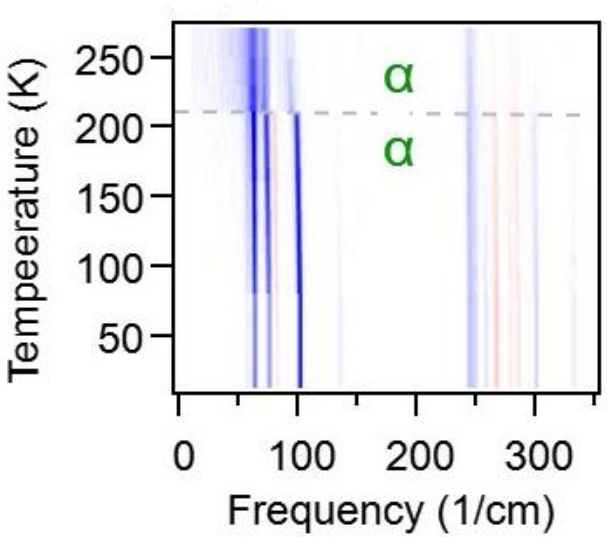
α – β domains

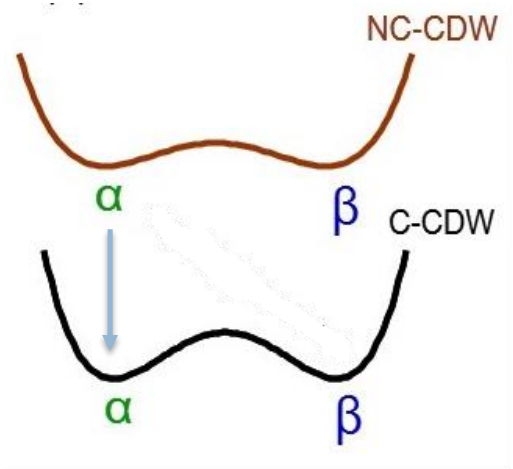


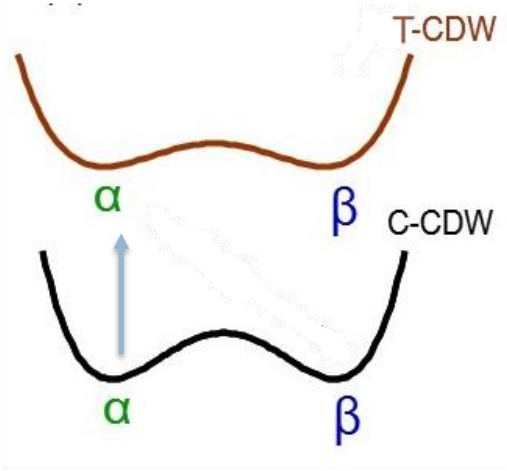
Raman and chirality pinning



10 K thermal gradient

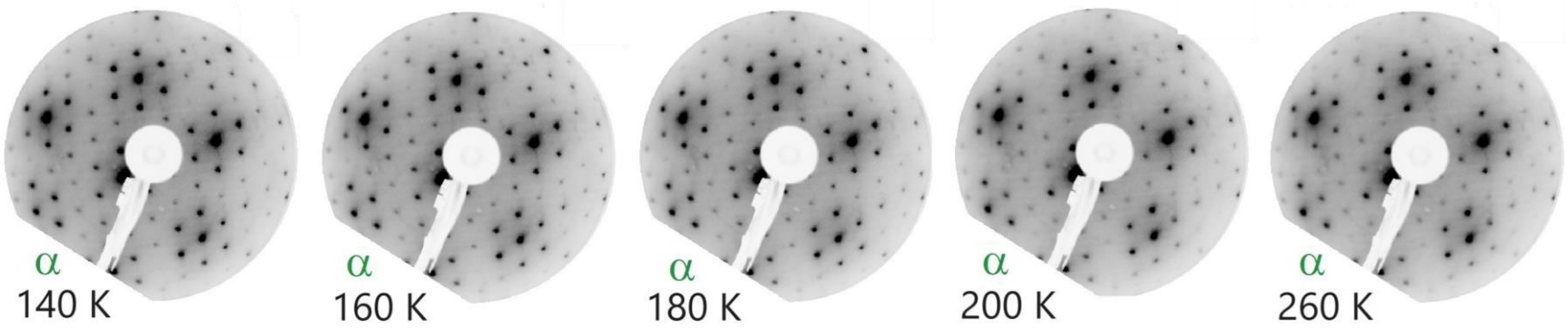


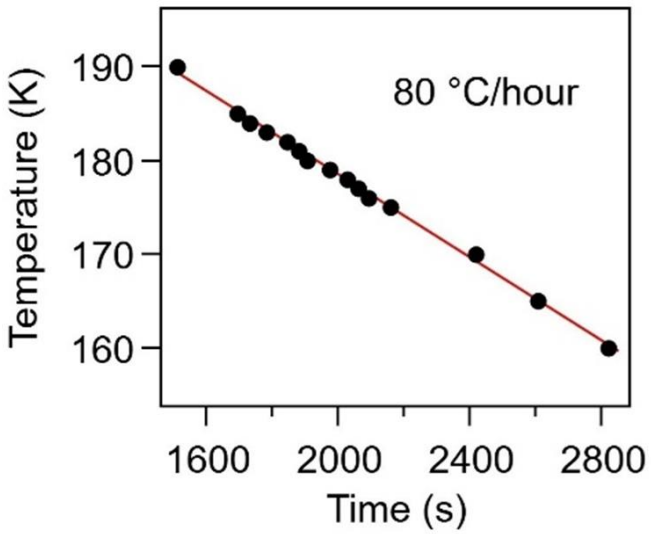


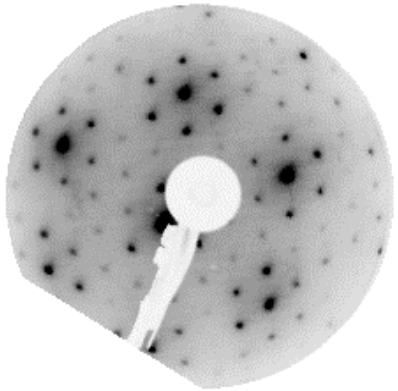


LEED and chirality pinning

Rapid quench





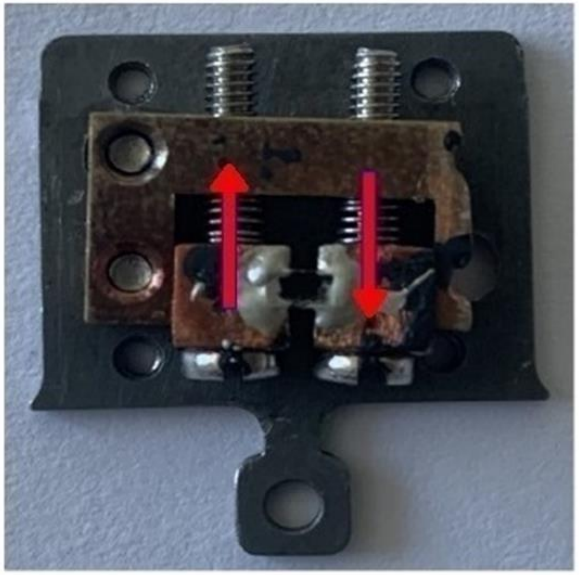


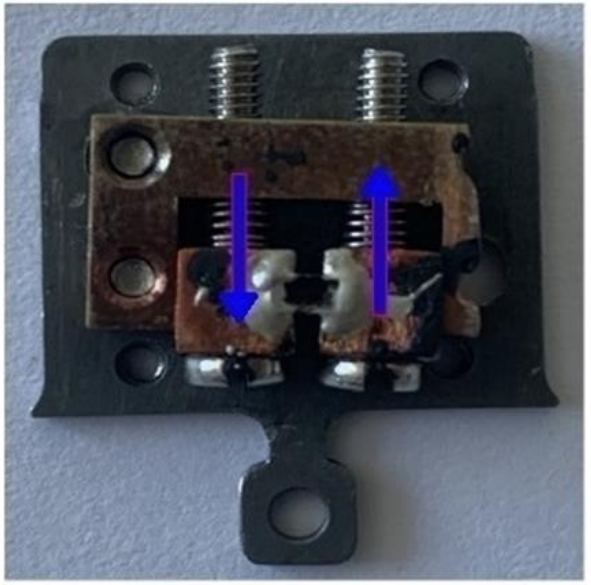
Switching control

No T - gradients		
Switching	**YES**	**NO**
ARPES	3	1
LEED	5	0
RAMAN	6	1
Total	**14**	**2**

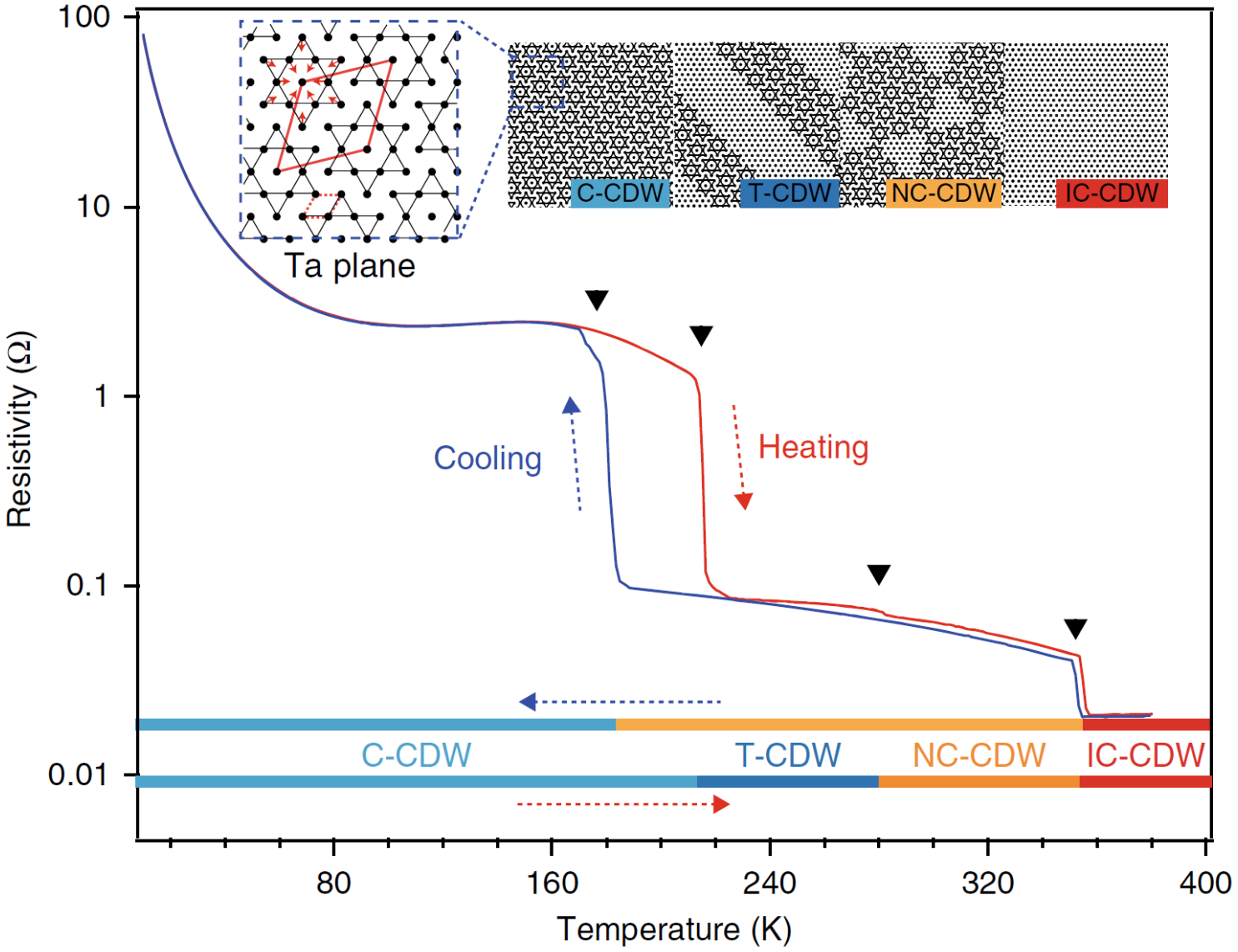
With T - gradients		
Switching	**YES**	**NO**
ARPES	1	1
LEED	0	3
RAMAN	0	4
Total	**1**	**8**

External control



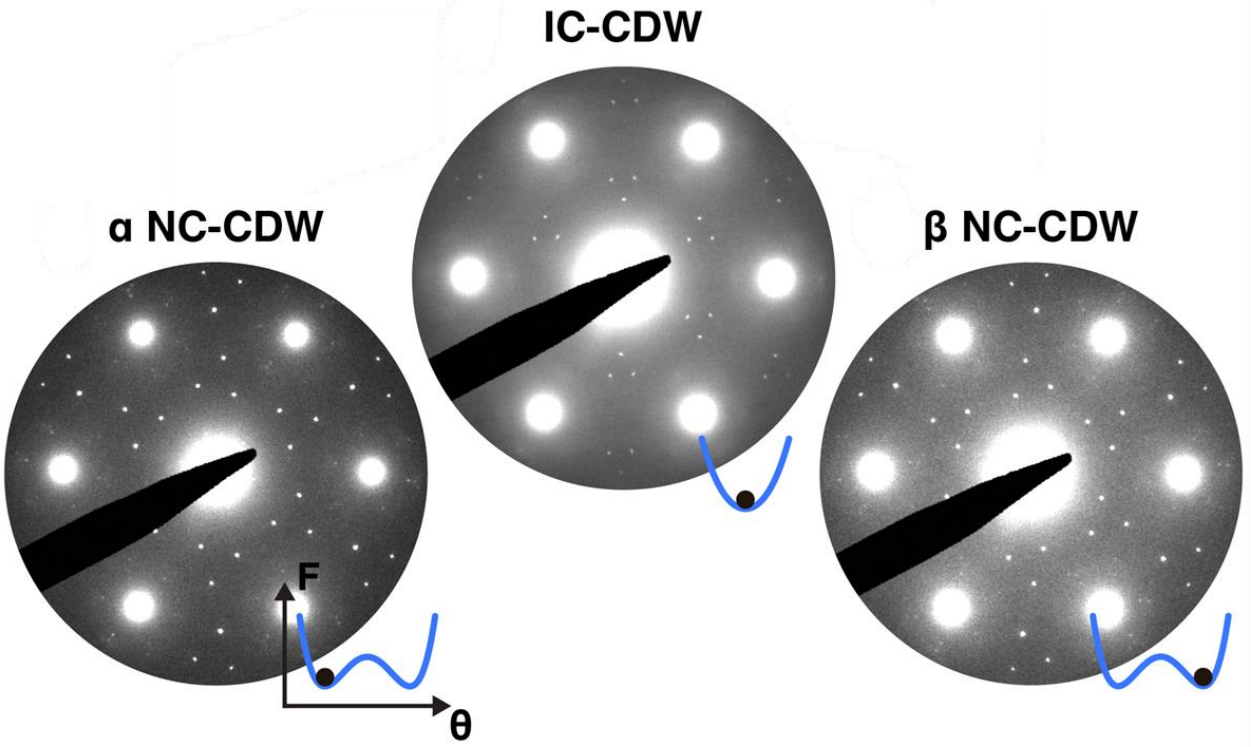


Phase transition

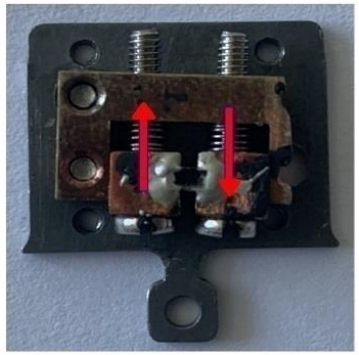


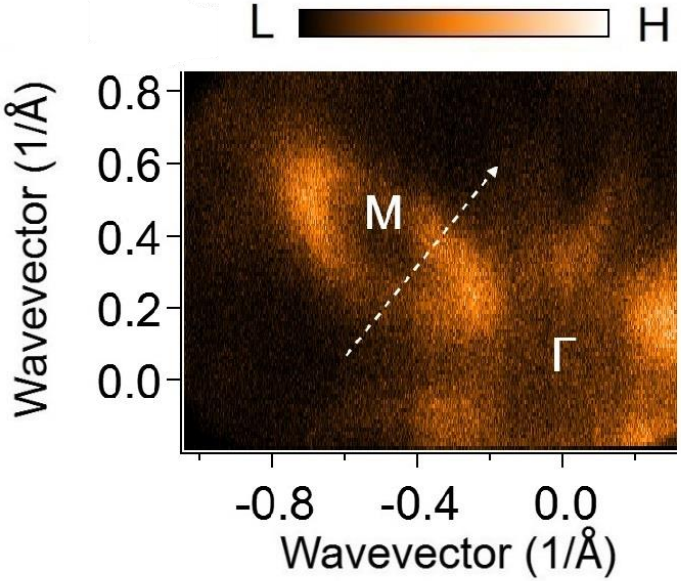
Switching and IC phase

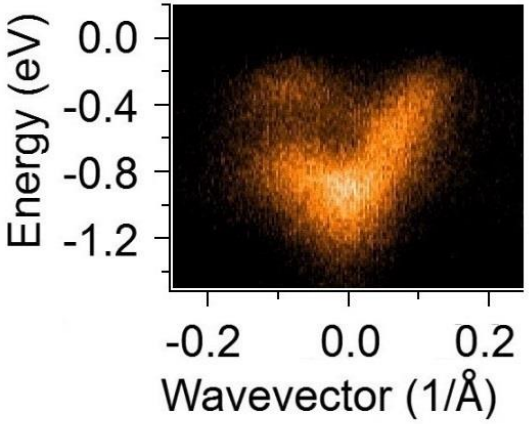
Cooling under external strain

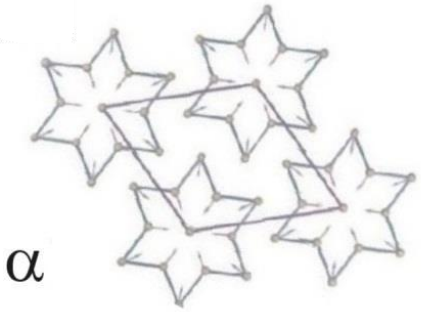


Control by torque and ARPES

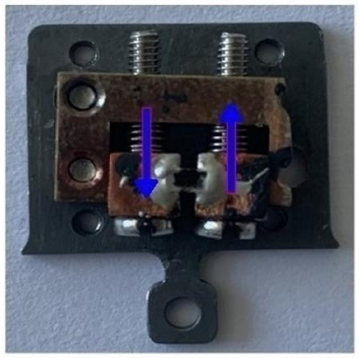


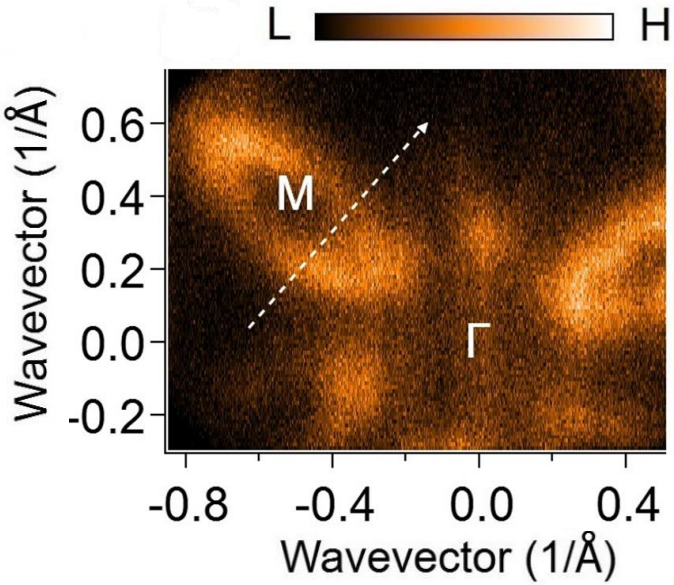


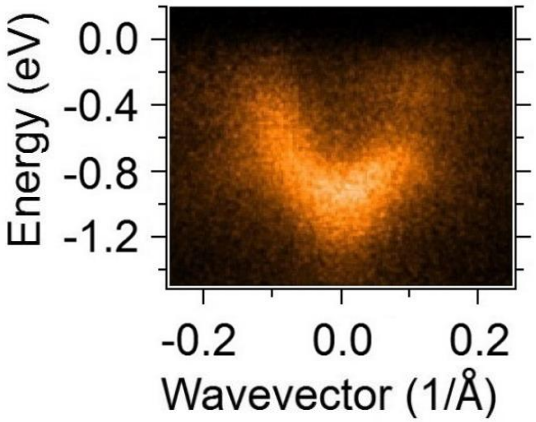


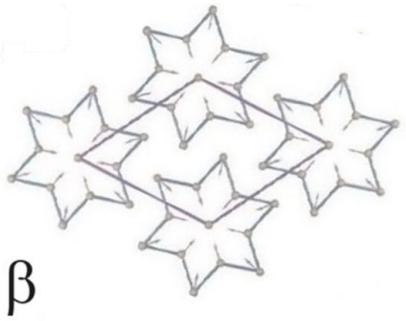


Control by torque and ARPES

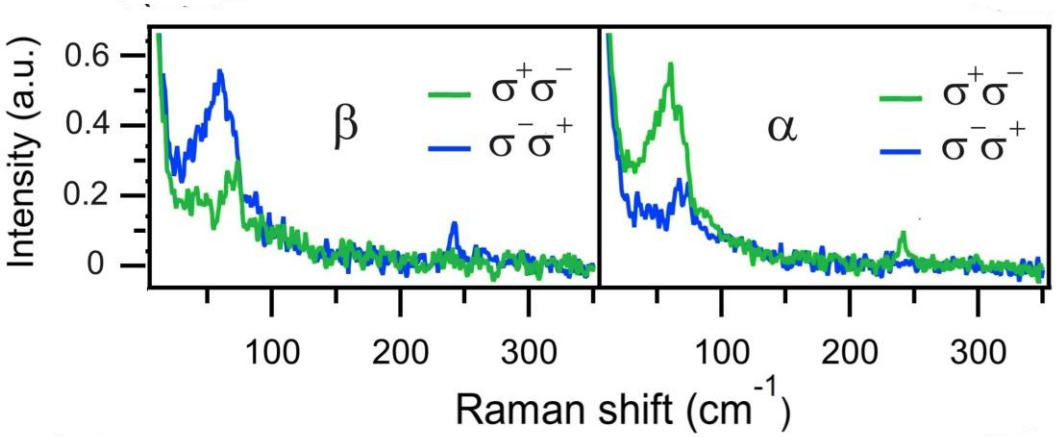


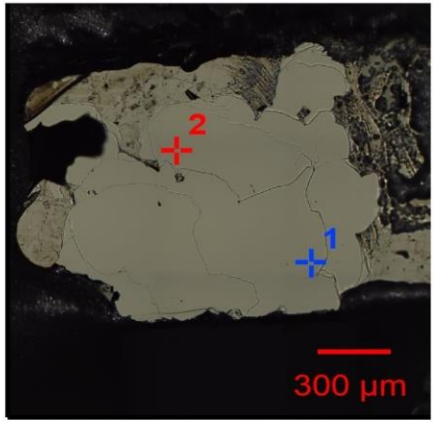


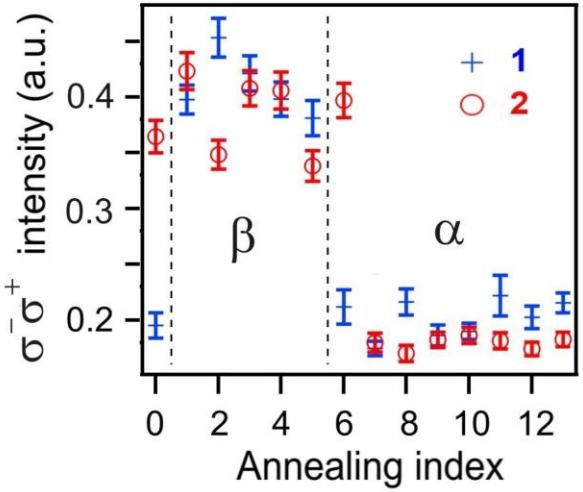




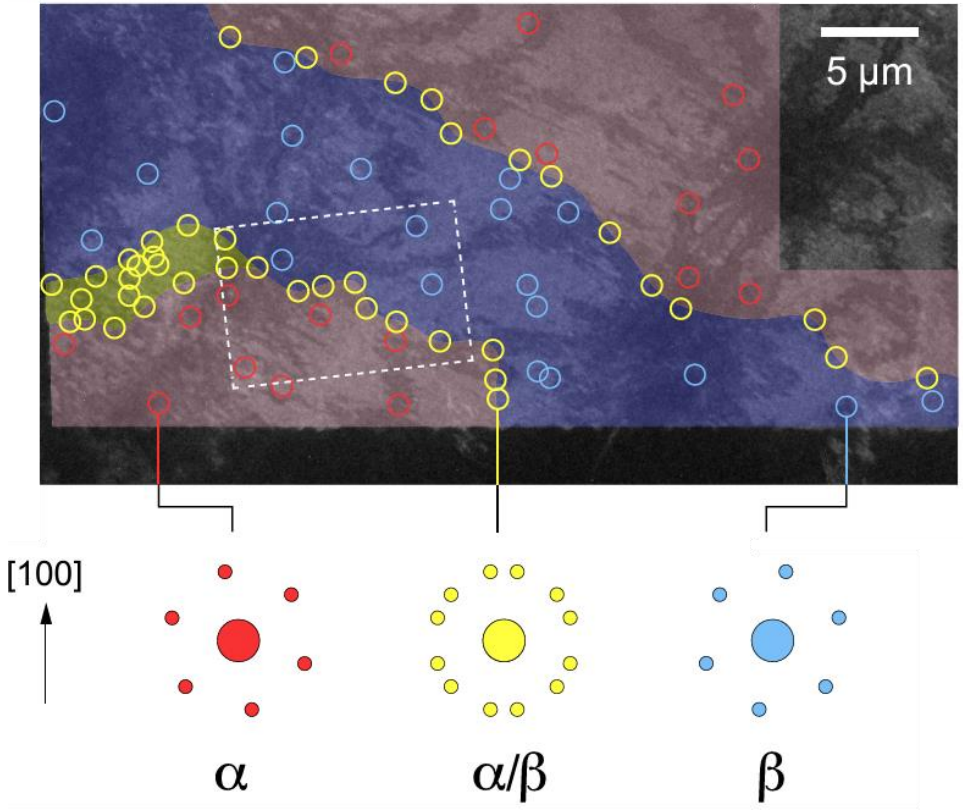
Control by torque and Raman

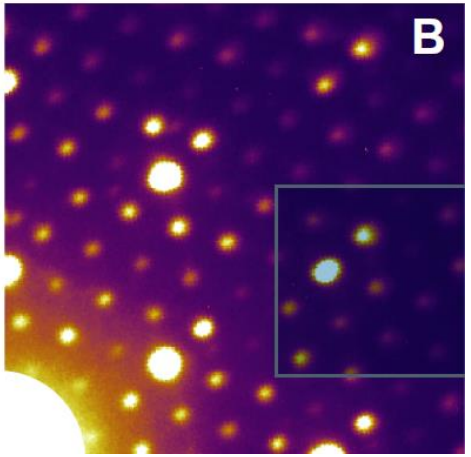


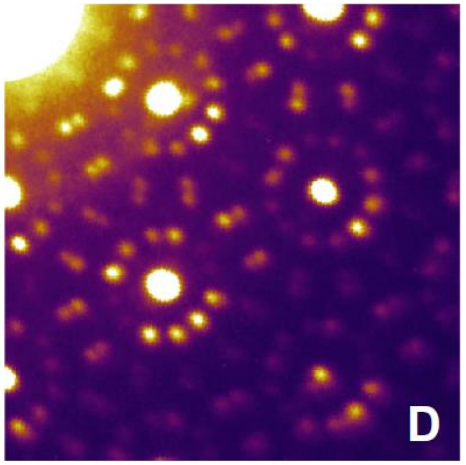




Partial switching via Laser pulse



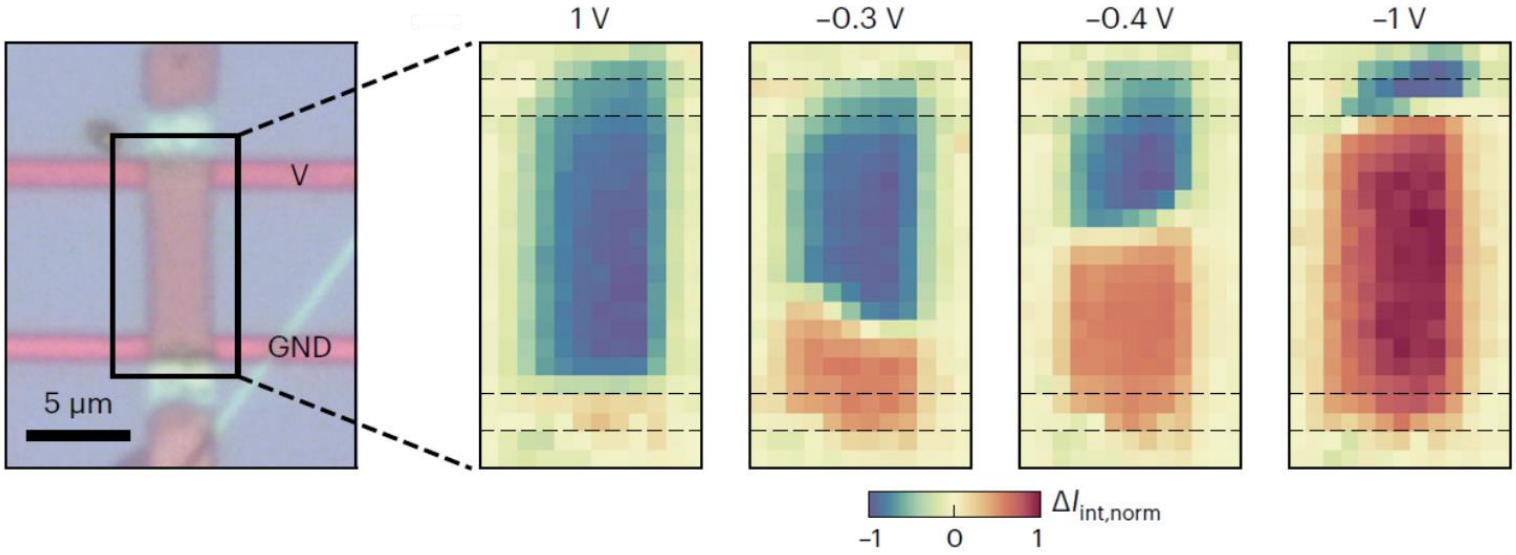




A Zong et al., ***Sci Adv.*** *4, eaau5501 (2005)*

Control by Electric field and Raman

G. Liu et al., ***Nature Naonotech.*** *18, 854 (2023)*



Chirality switching by means of applied electric field

Outline

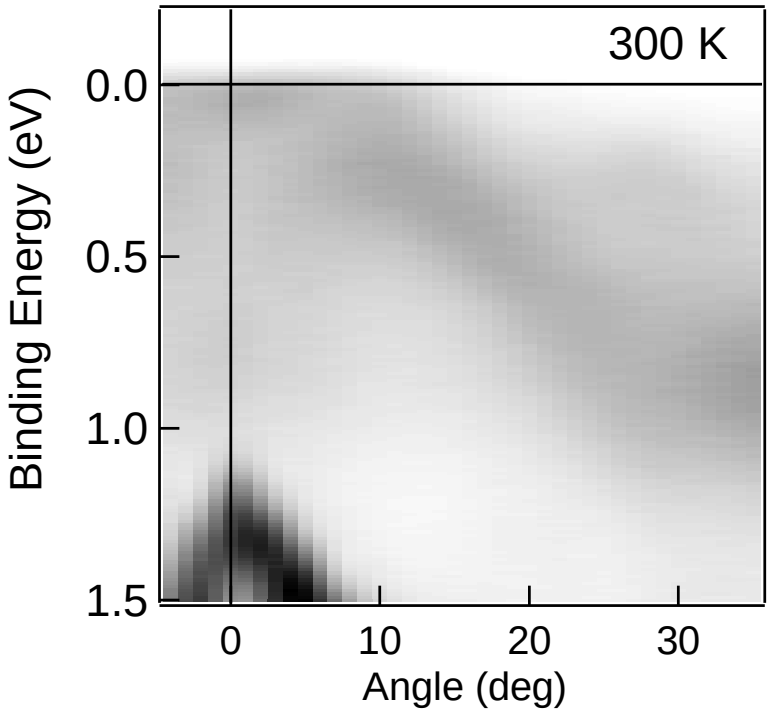
In Plane Chirality in TaS_2

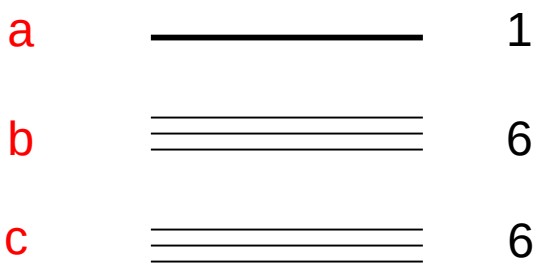
Chirality control

Mott vs Peierls

Photoinduced localization of electrons

Electronic states at the phase transition

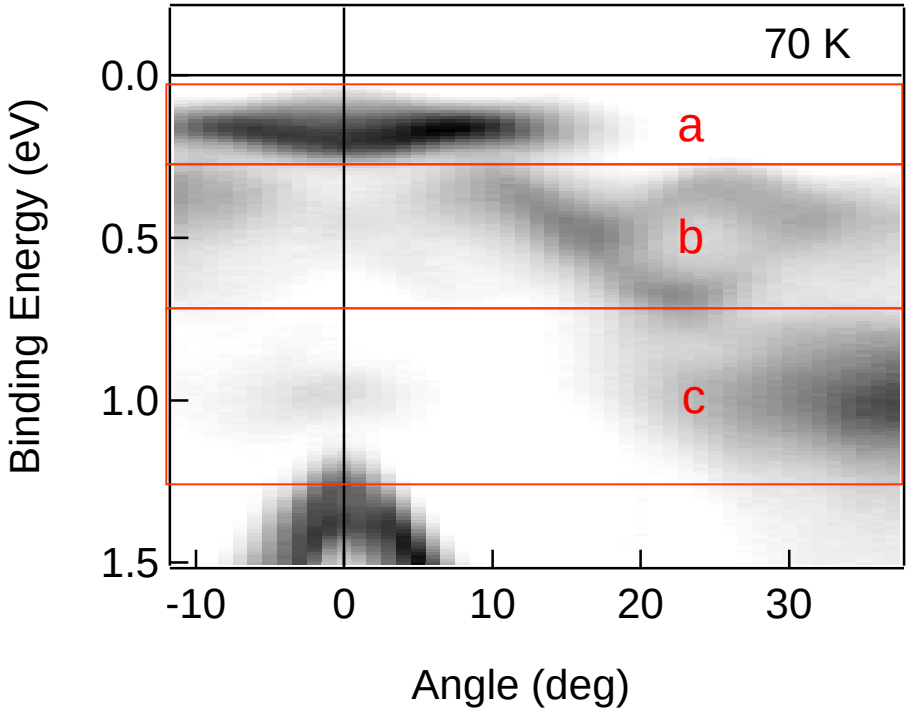




3 many-folds induced by the CDW.

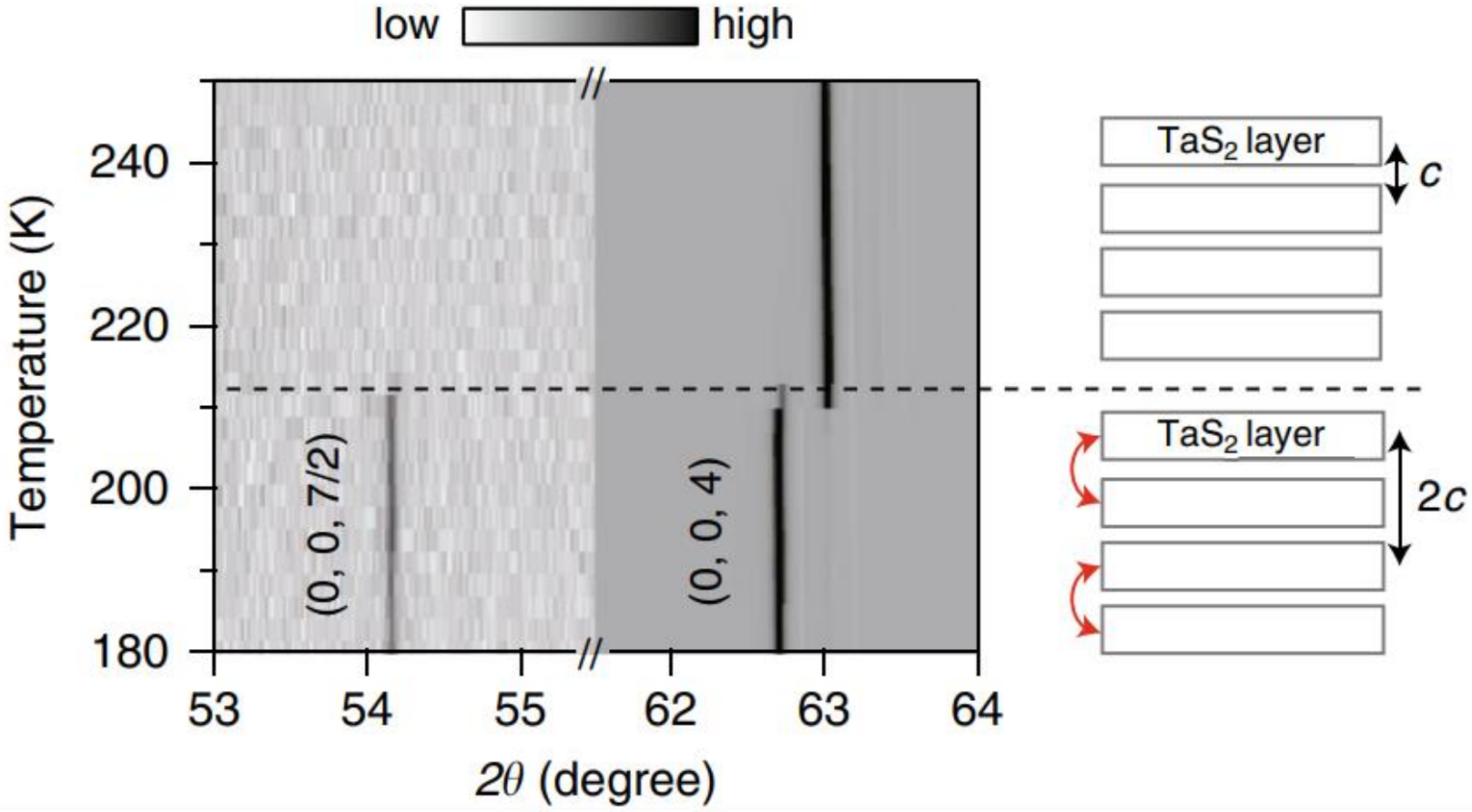
Gapped groundstate

L. Perfetti et al., ***Phys. Rev. B*** *71, 153101 (2005)*



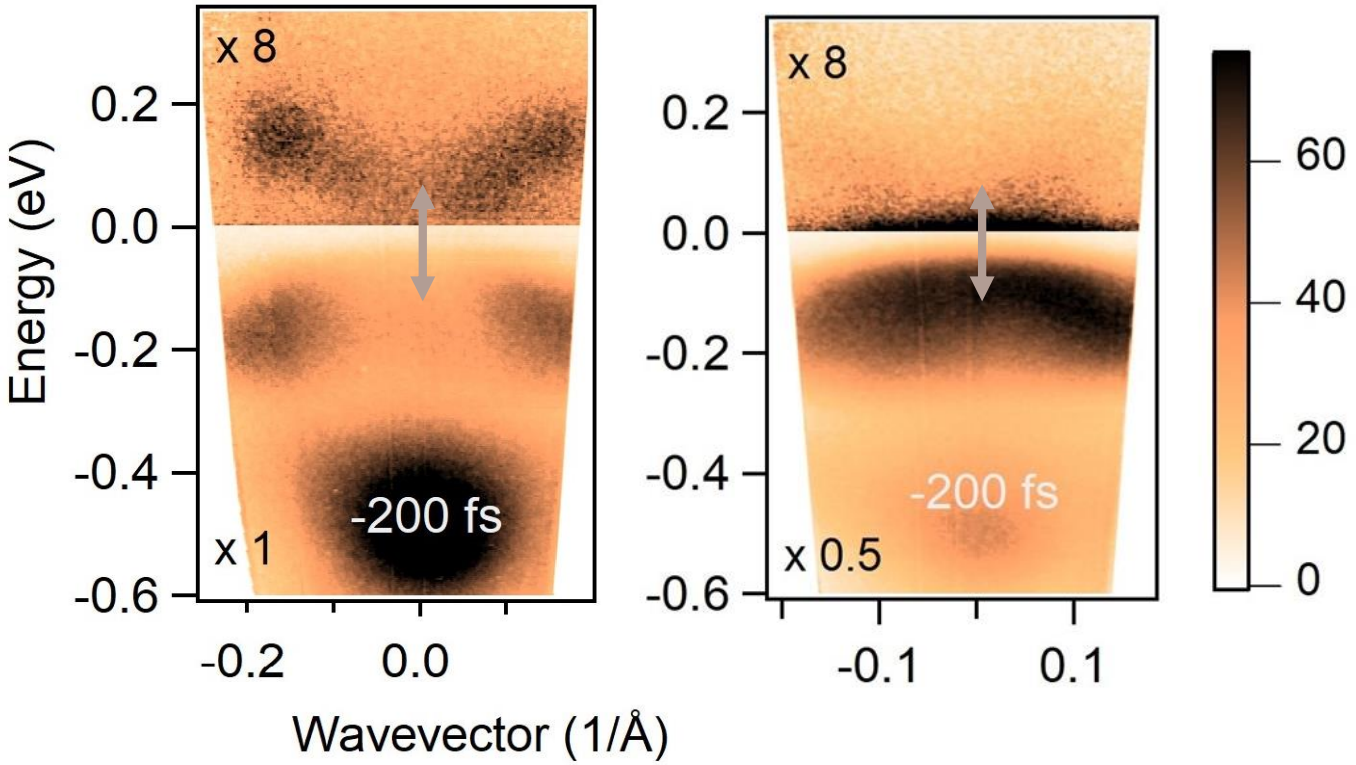
Stacking Order and ARPES

Y. D. Wang *et al.*, ***Nature Comm.*** **11**, 4215 (2020)



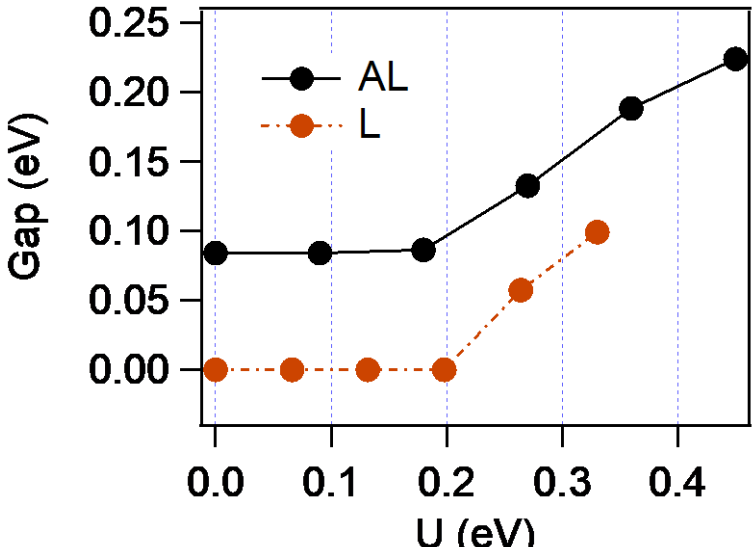
S Polarization

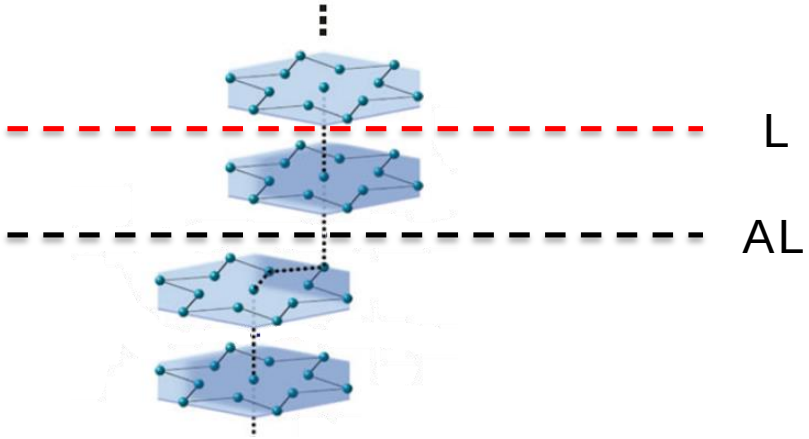
Gap 0.15 eV



Polarization dependence questions a simple Mott scenario

Dimerization and correlations



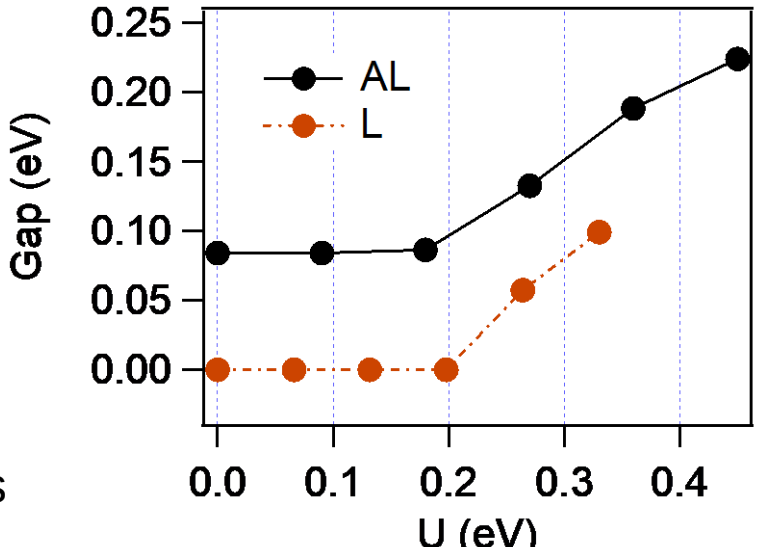


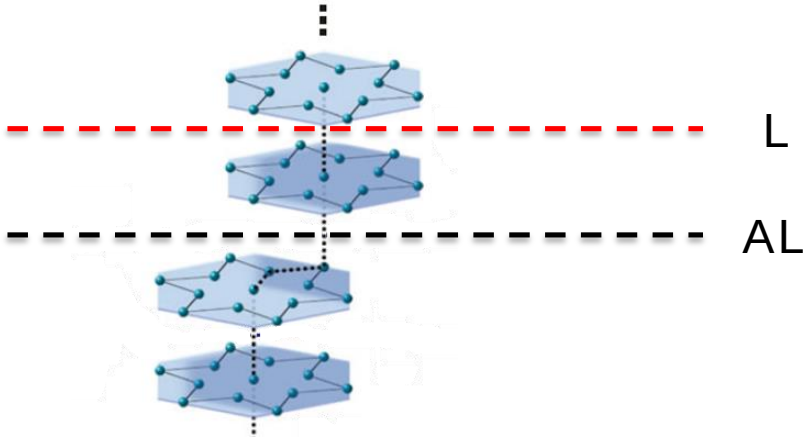
Dimerization and correlations

0.09 eV

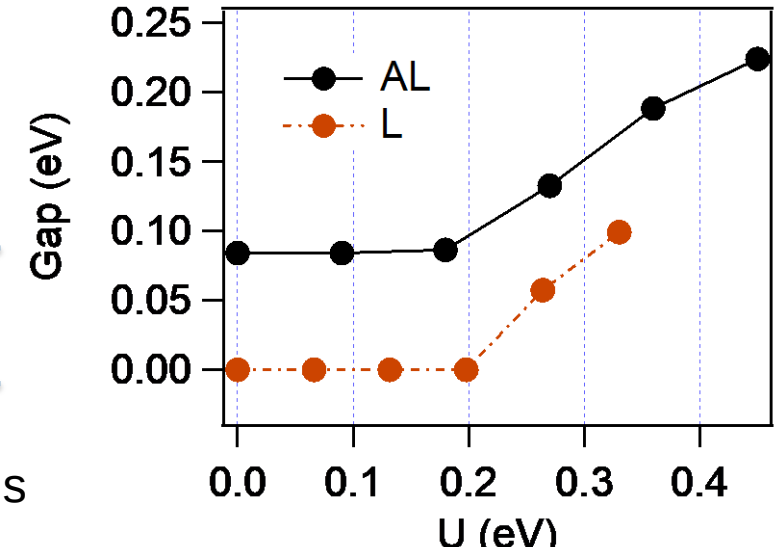
0 eV

No Correlations





Dimerization and correlations



0.09 eV

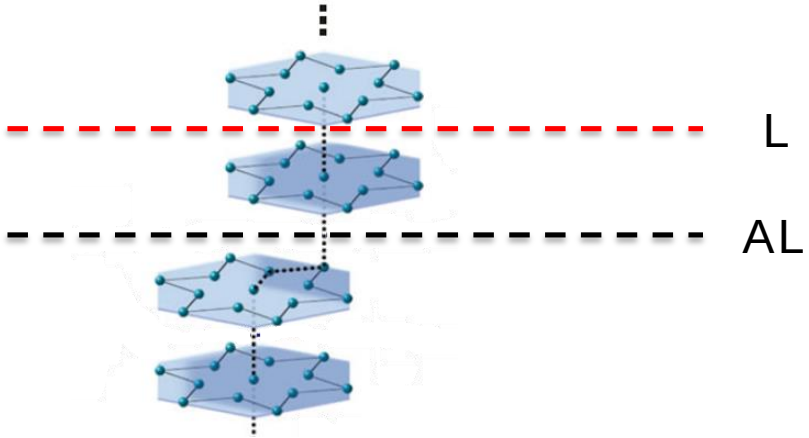
0 eV

No Correlations

0.22 eV

0.1 eV

With Correlations



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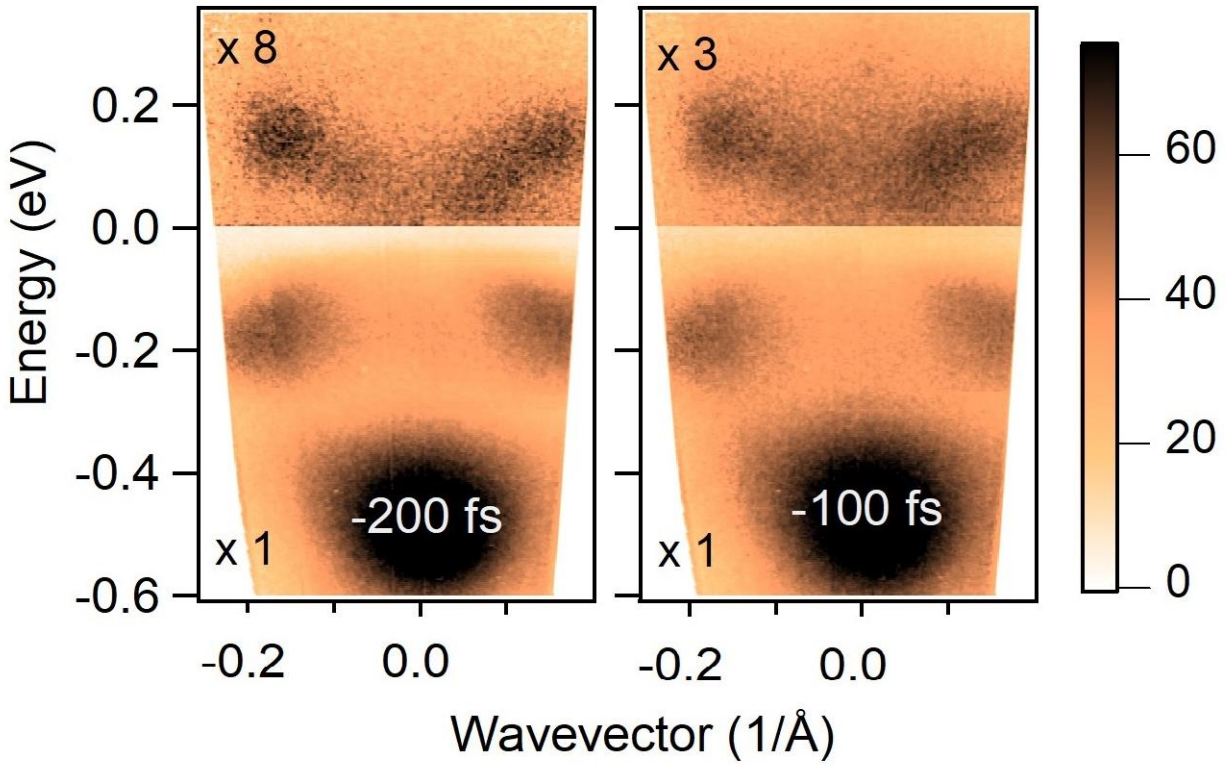
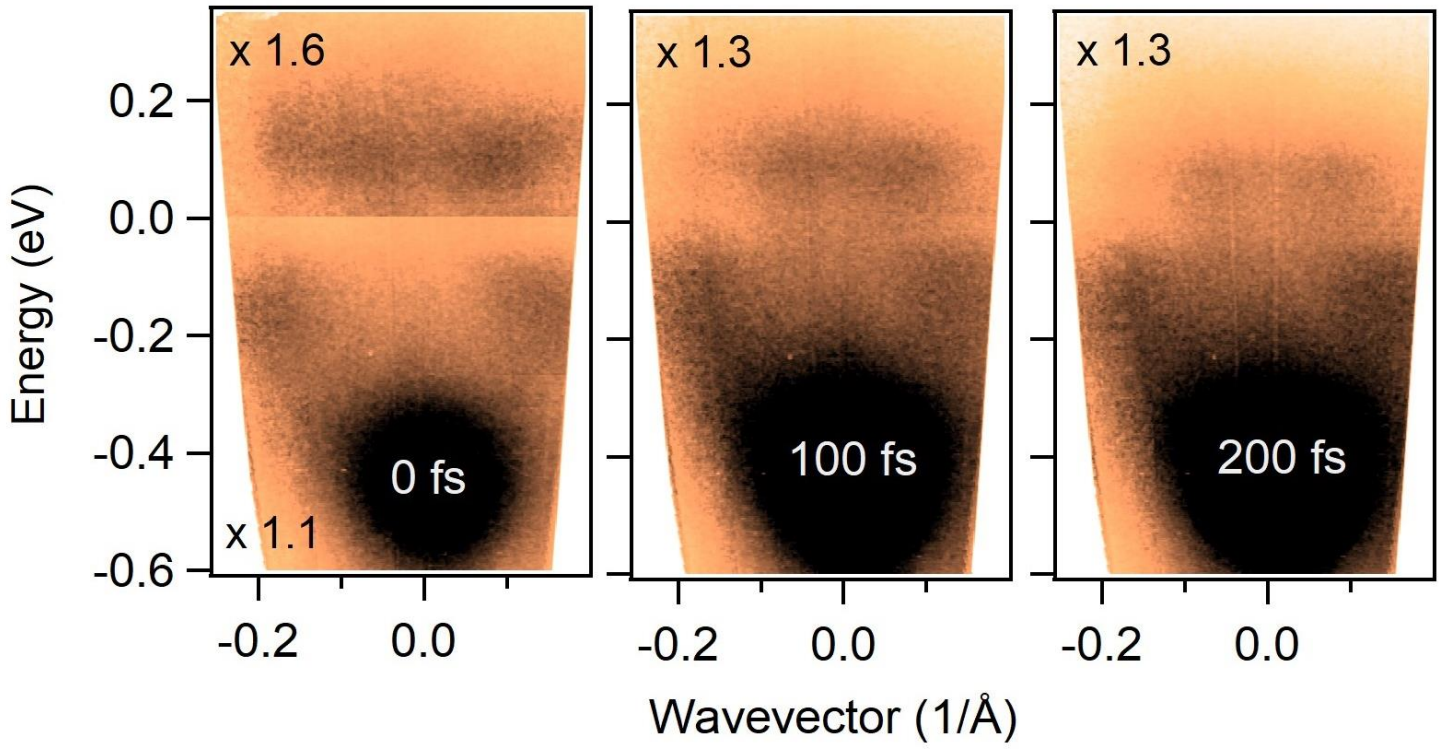
Collapse of the CDW

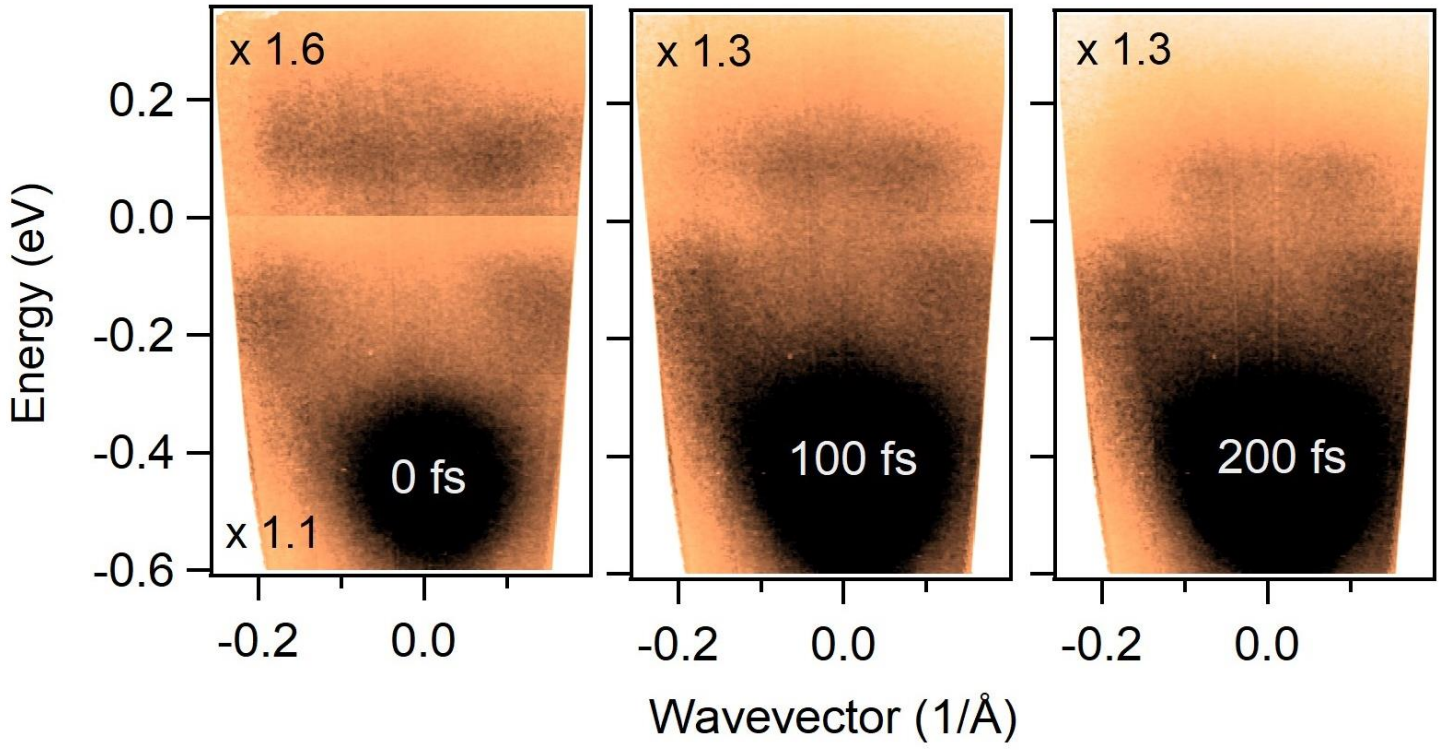


Collapse of the CDW



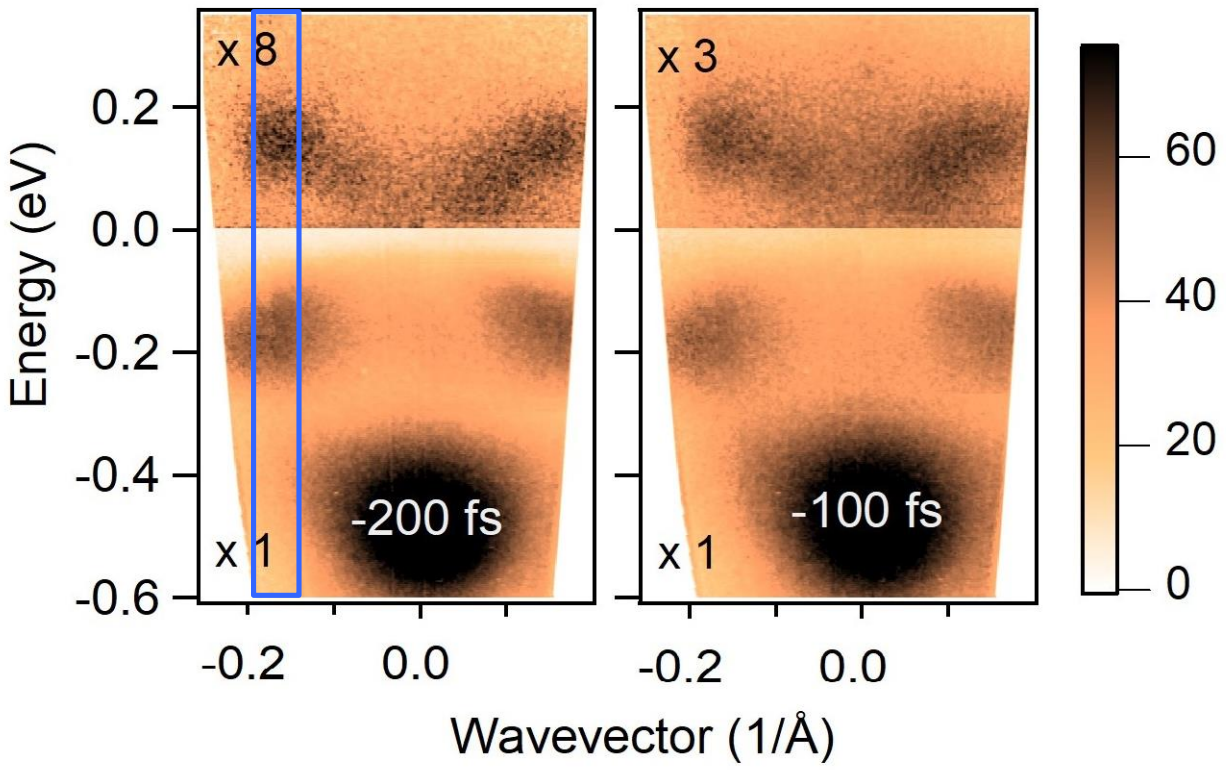
Collapse of the CDW

Photoexcitation flattens the dispersion of electronic states near to the Fermi Level

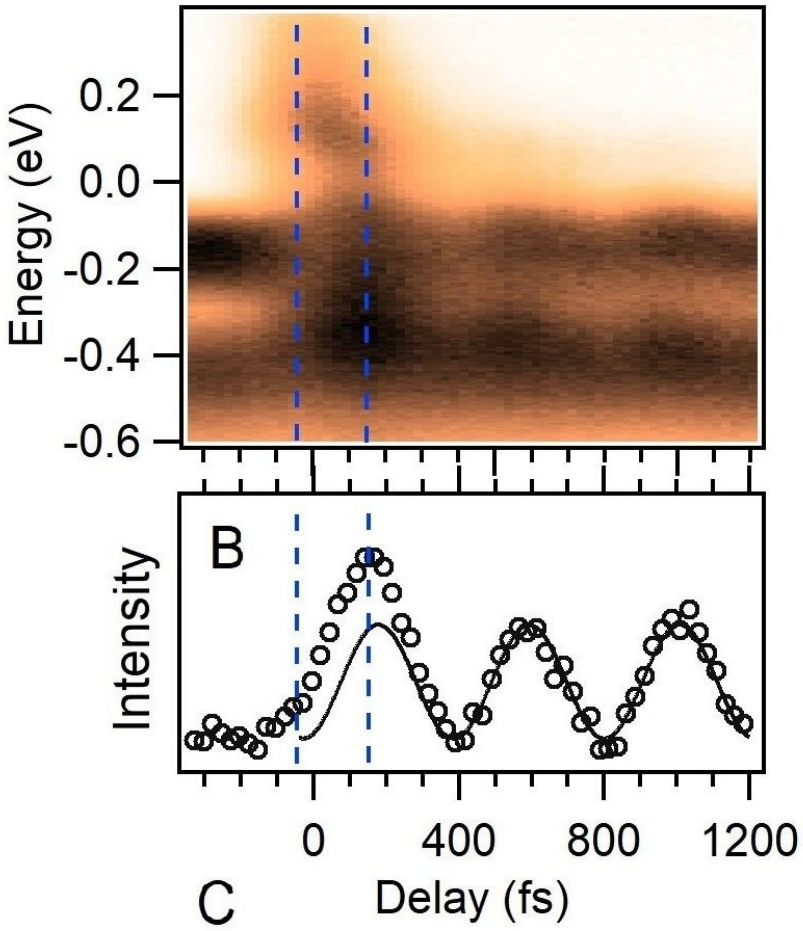


CDW fluctuations localize electronic states in nanodomains

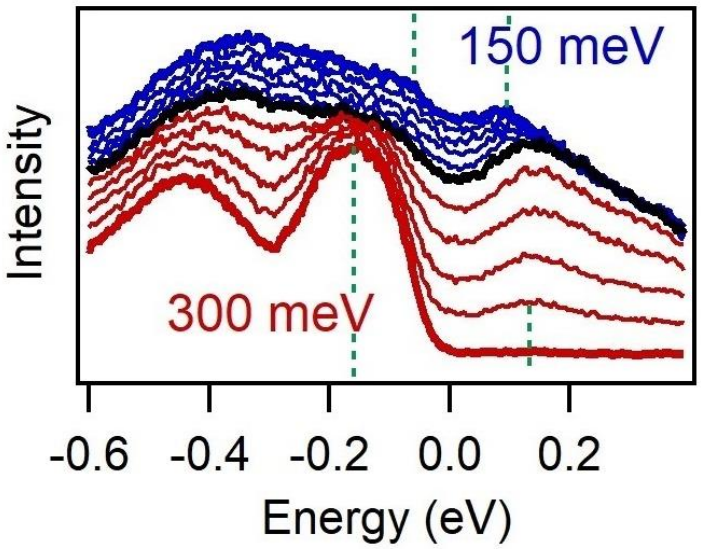
Collapse of the CDW



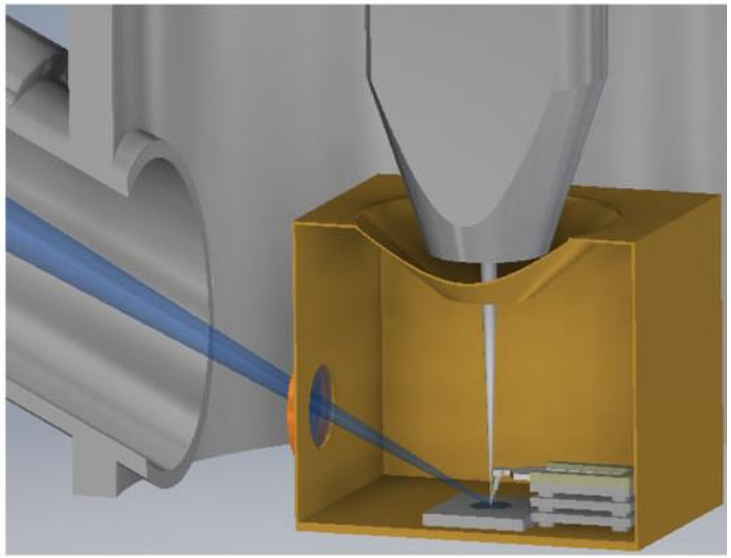
Gap dynamics

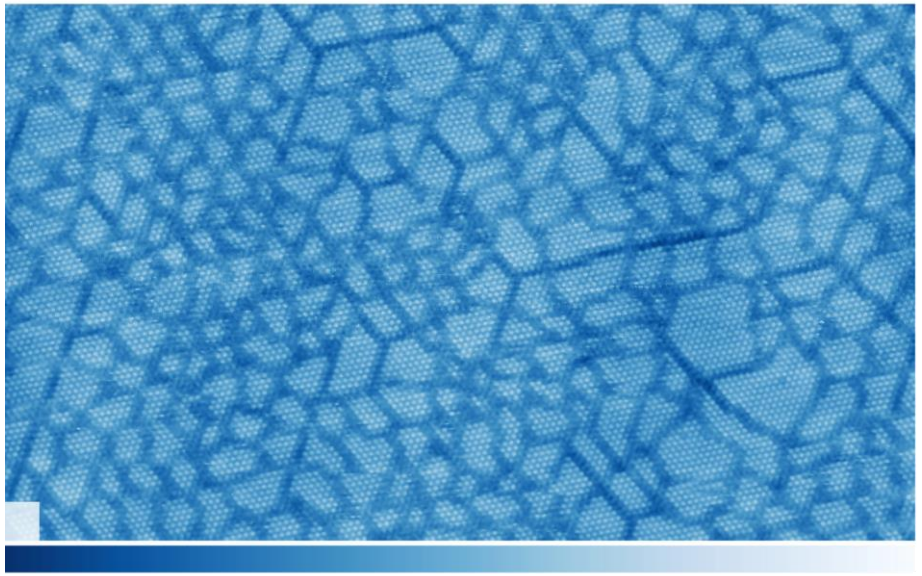


Coherent: schrinking of LMPB-UMPB distance in ½ period of the CDW mode



The Hidden phase





L. Stojchevska *et al.*, ***Science*** *344, 177 (2014)*

Yaroslav A Gerasimenko *et al.*, ***npj Quantum Materials*** *4, 32 (2019)*

Conclusions

In plane chirality switch at the metal insulator transition

Control by laser beams and applied stress

Interplay of Coulomb repulsion and dimerization.

Electron localization during the photoinduced phase transition.

Thanks

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