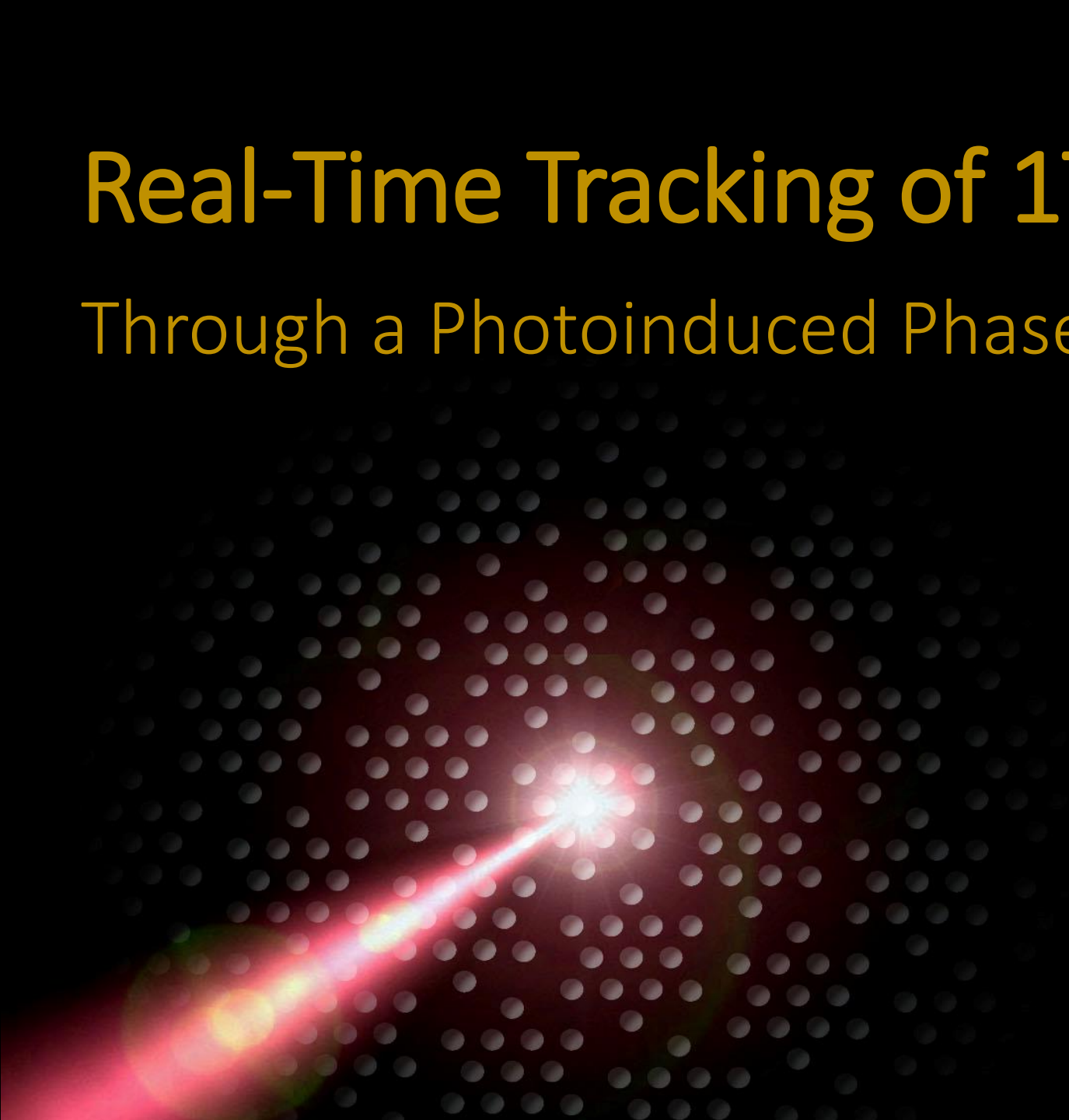
Real-Time Tracking of 1T-TaS_2

Through a Photoinduced Phase Transition



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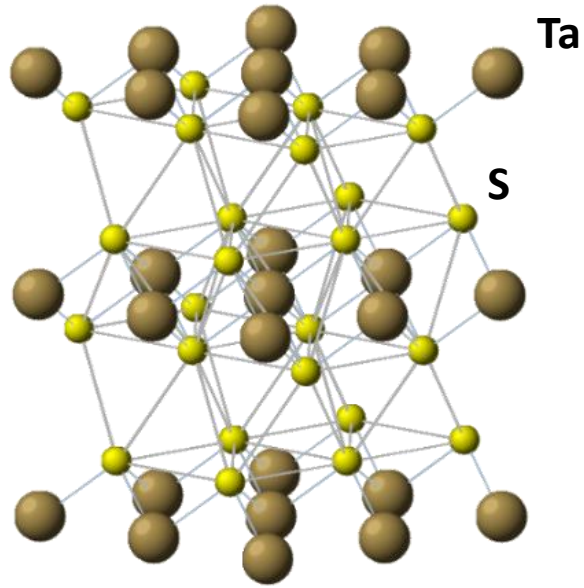
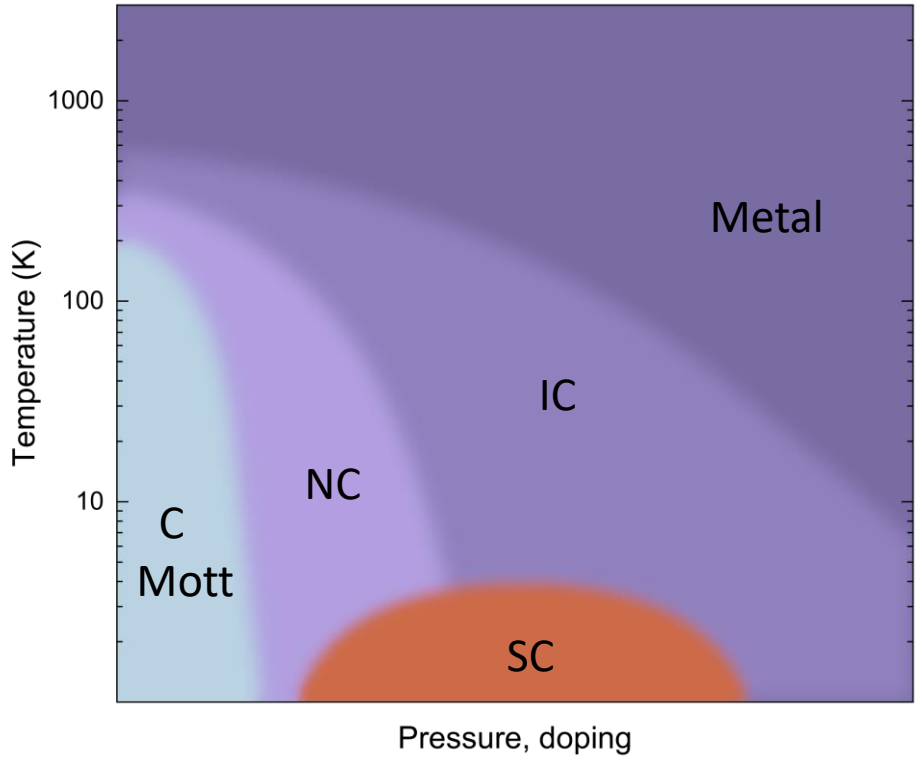
Outline

- Introduction
  - Recap: Hidden phases in 1T-TaS_2
  - Role of stacking order
- Stacking order in photoinduced states and its dynamics
- 1T-TaS_2 as an X-ray light modulator

1T-TaS_2: Thermodynamic case



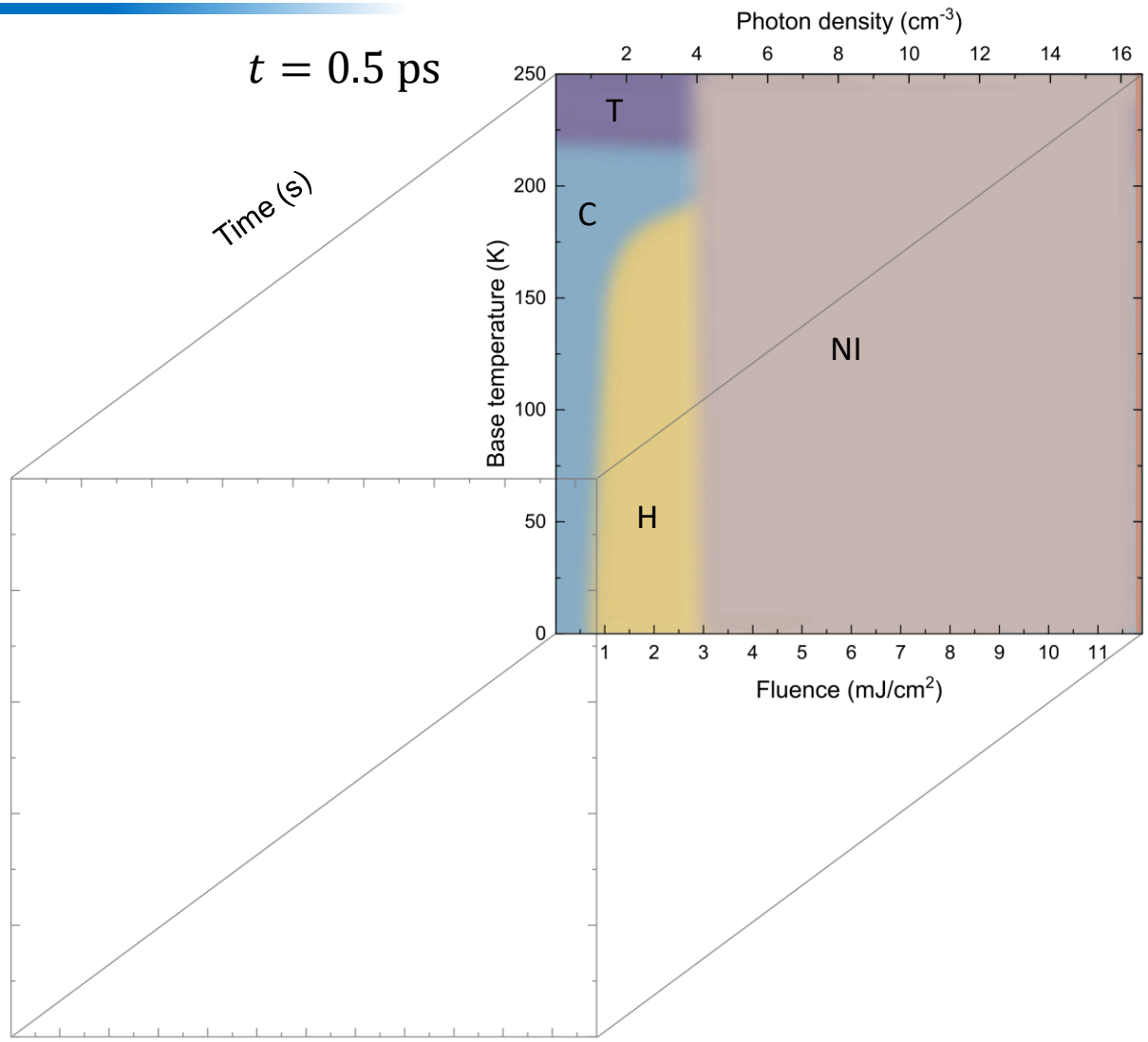


350 < T < 550 K: incommensurate CDW

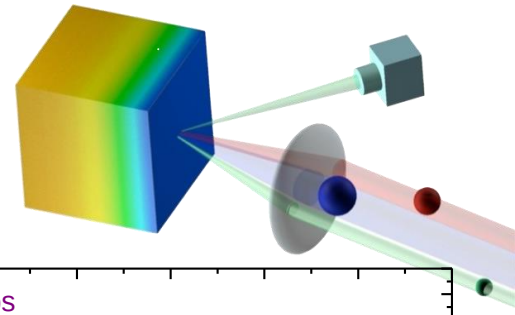
180 < T < 350 K: nearly - commensurate CDW

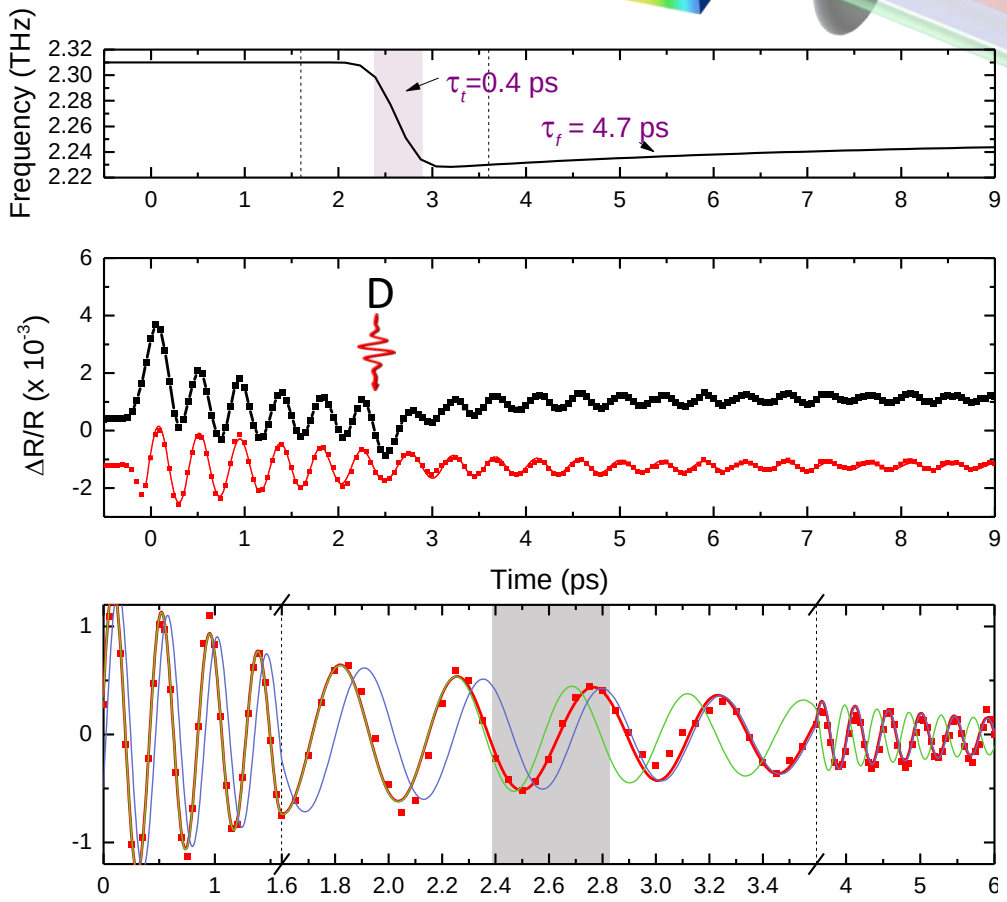
T < 180 K: commensurate CDW & Mott

1T-TaS_2: Photo doping



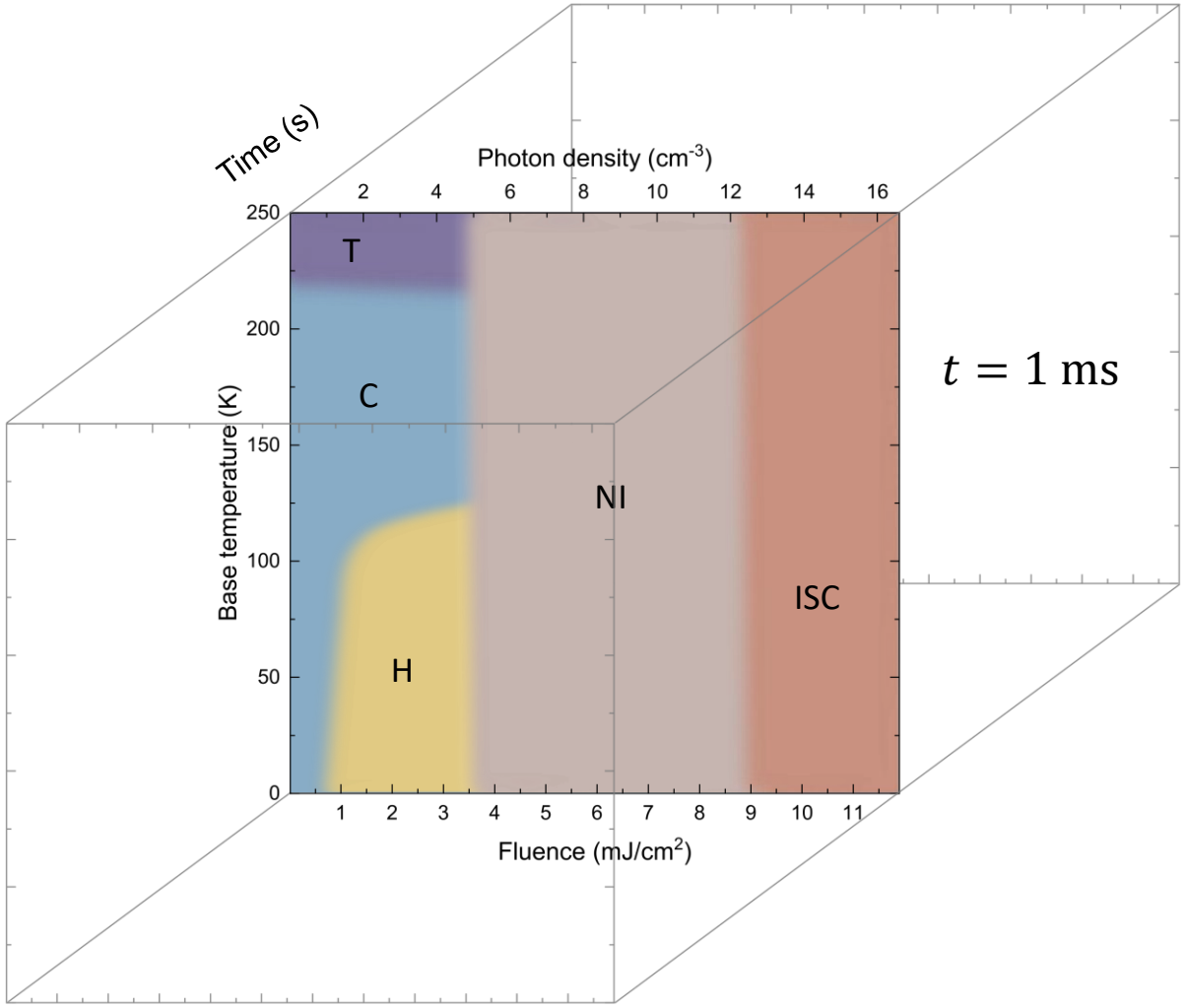
Ravnik *et al.*, Nat Comm. **12**, 2323 (2021)



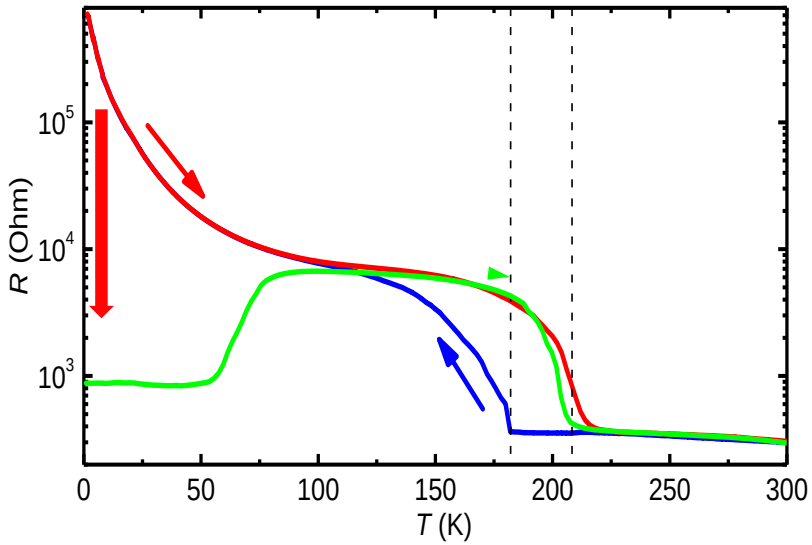


Ravnik, IV *et al.*, PRB **97**, 075304 (2018)

1T-TaS_2: Photo doping

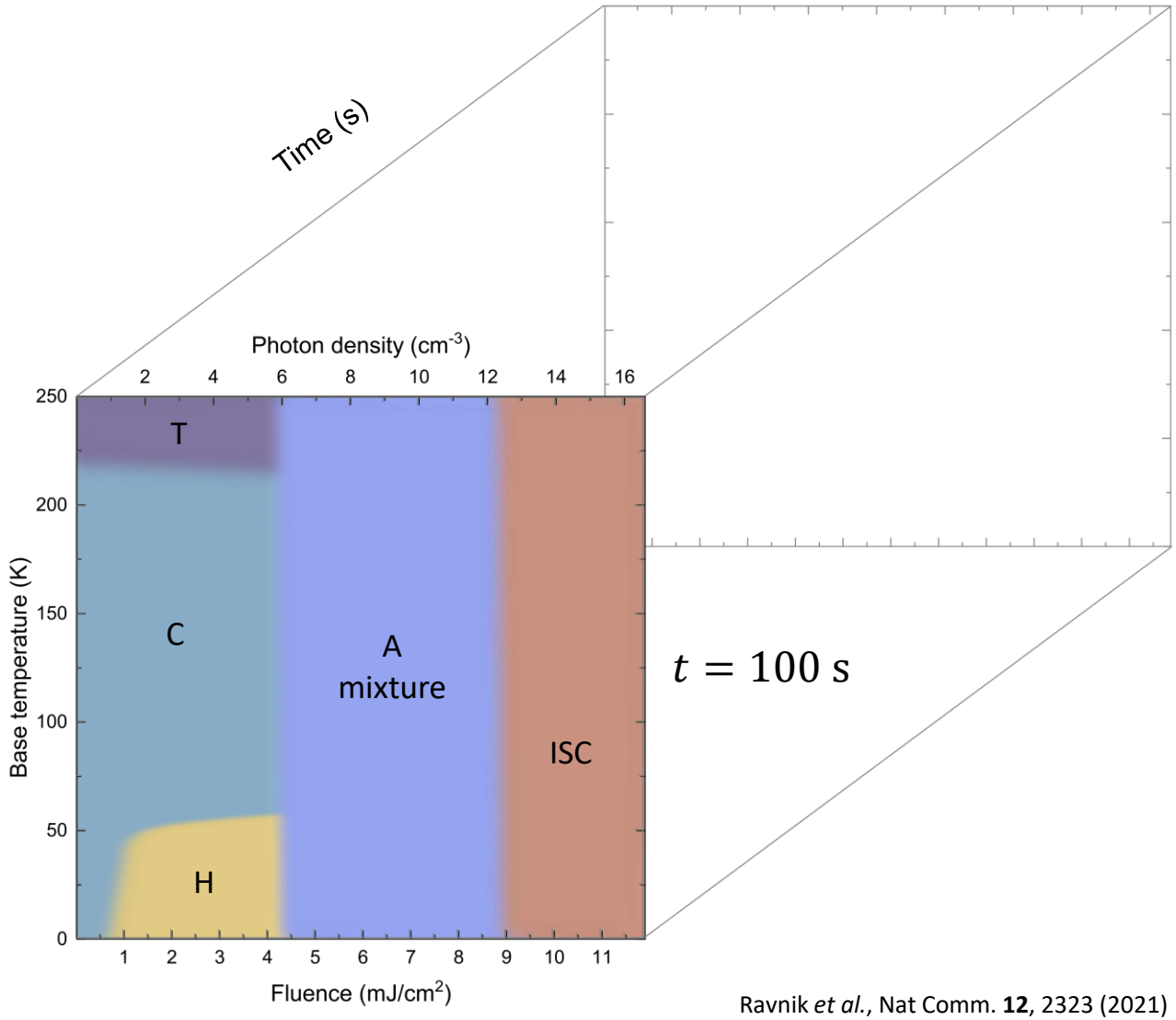


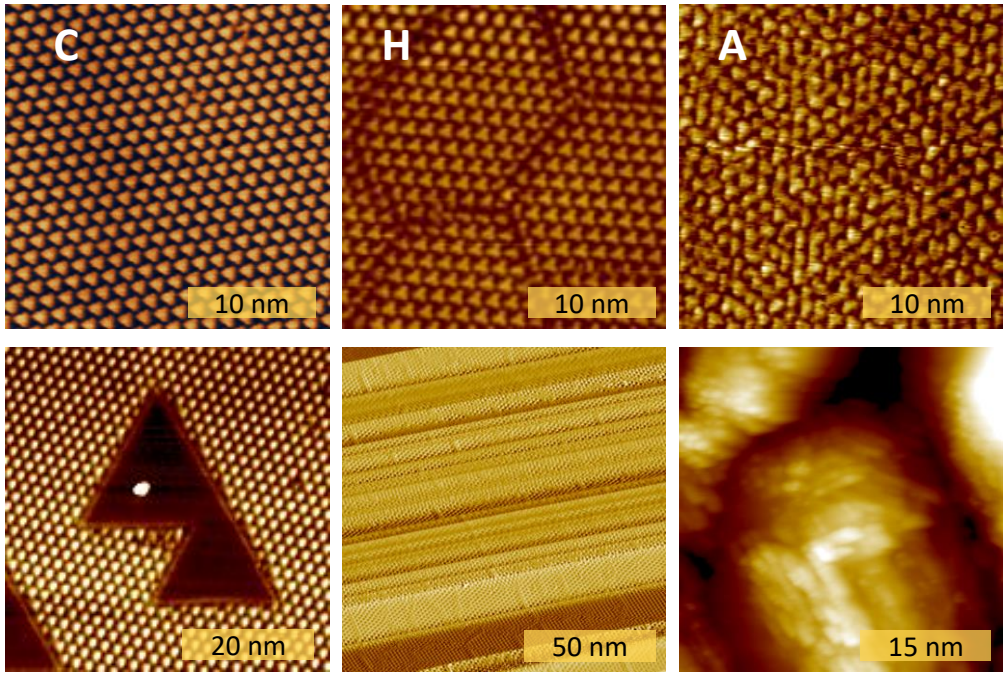
Ravnik *et al.*, Nat Comm. **12**, 2323 (2021)



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

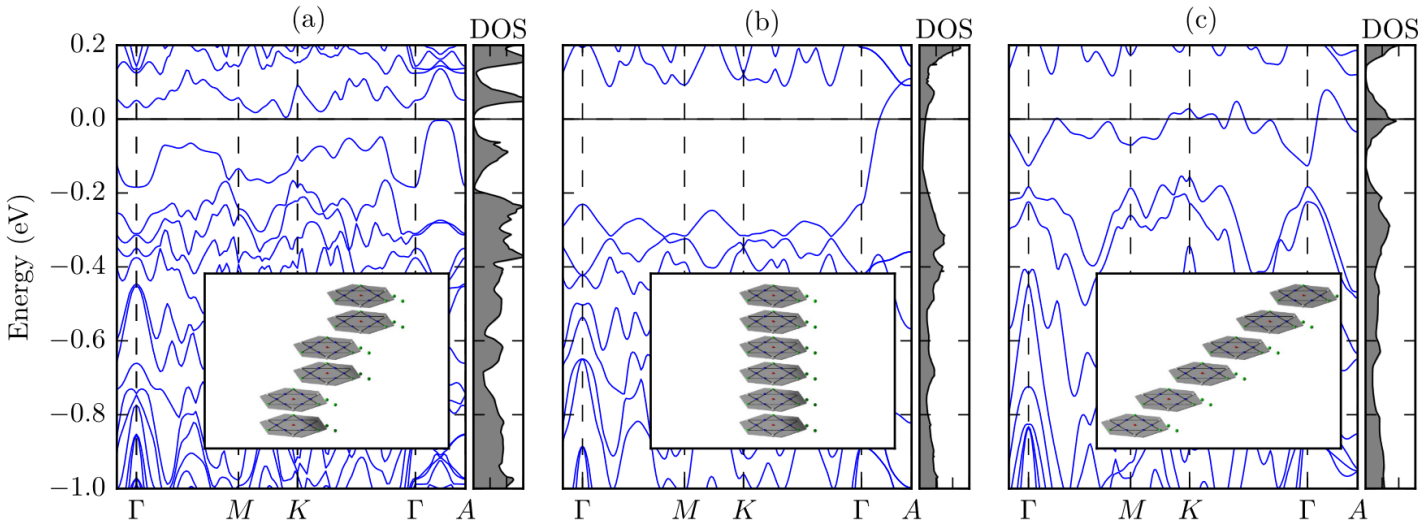
1T-TaS_2: Photo doping



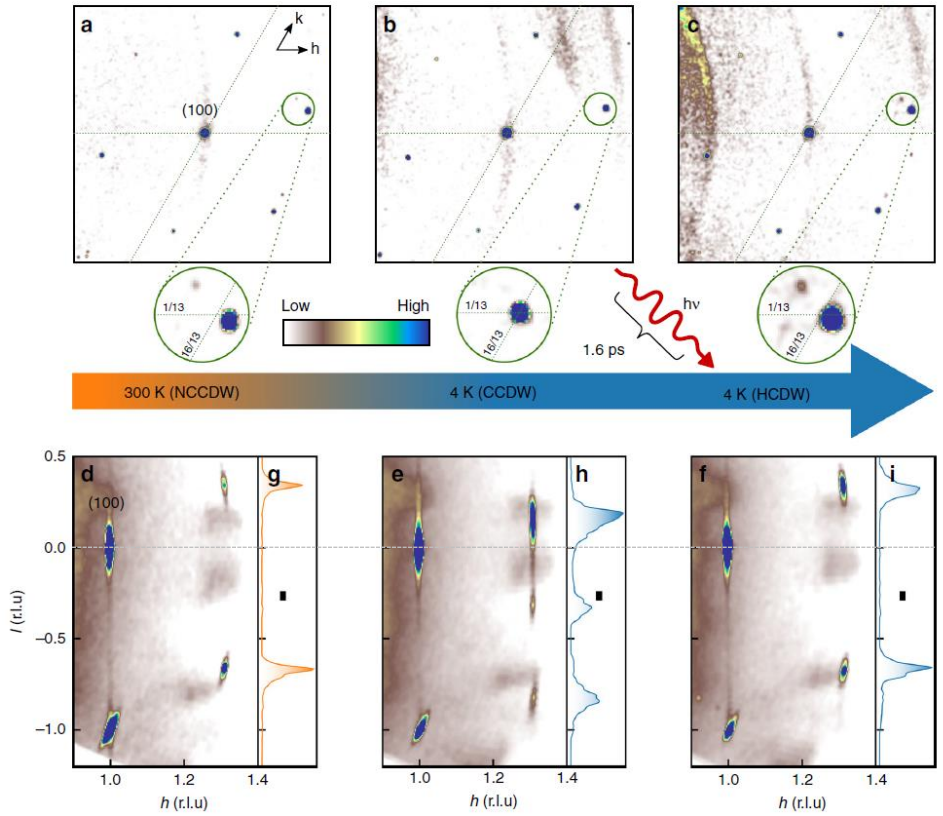


Ravnik *et al.*, Nat Comm. **12**, 2323 (2021)

Out-of-plane ordering of polarons



Ritschel *et al.*, Phys. Rev. B **98**, 195134 (2018)

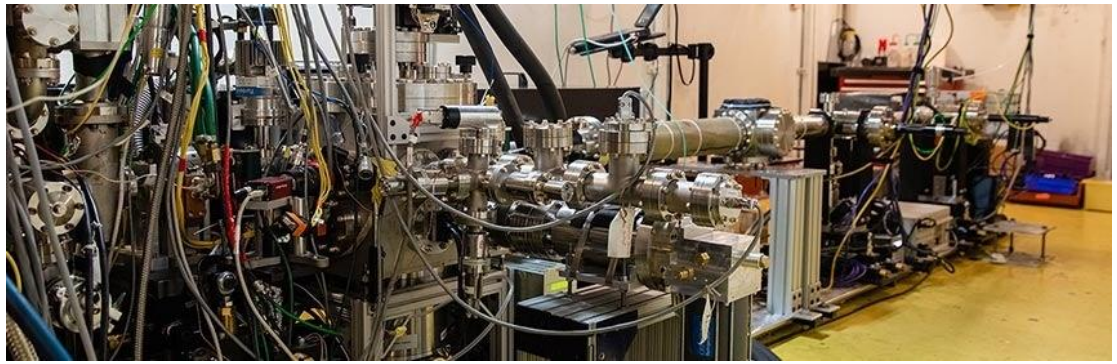


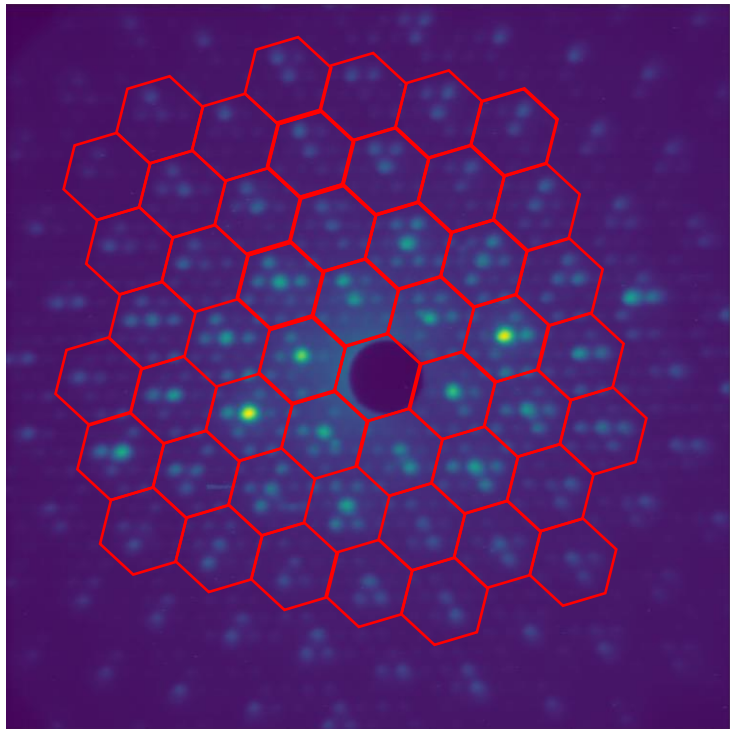
Stahl *et al.*, Nat. Comm. (2019)

- **IC and NC**: $3 \times c_0$ periodicity
- **C state**: bilayers + partially disordered
- **H state**: similar to NC?
- **A state**: ???

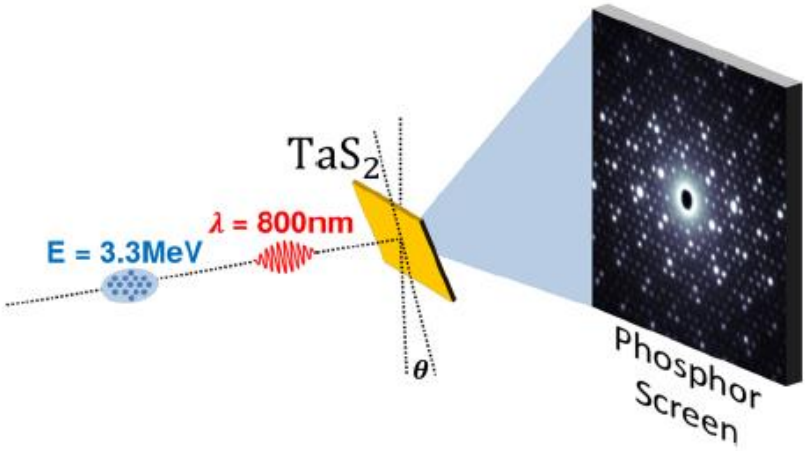
MeV UED: experiment

- Short de Broglie wavelength ($< 10^{-3}$Å @ 3MeV)
  -> flat Ewald sphere
- Large penetration depth
- Large scattering cross section
  -> relatively easy to measure



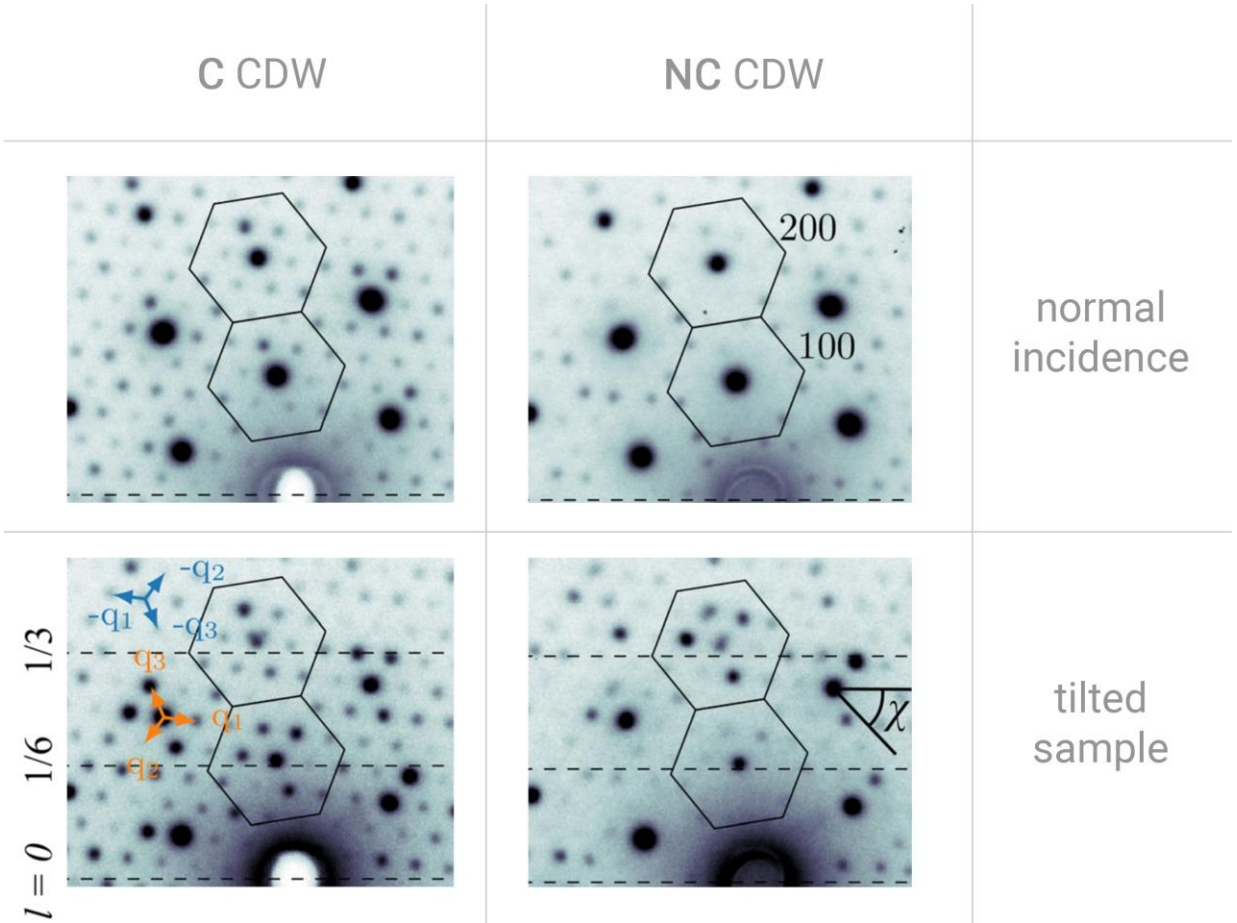


Out-of-plane stacking in UED

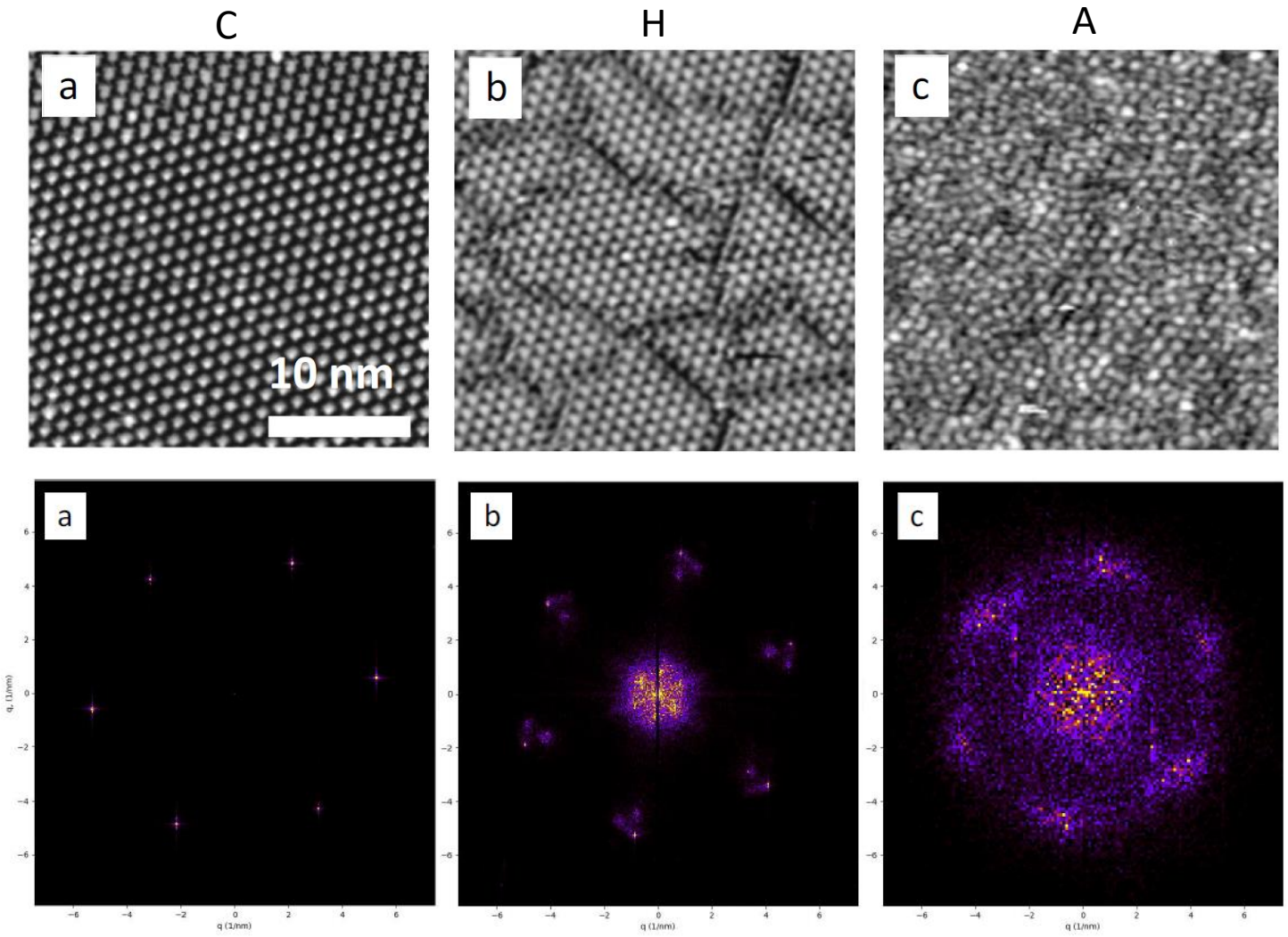


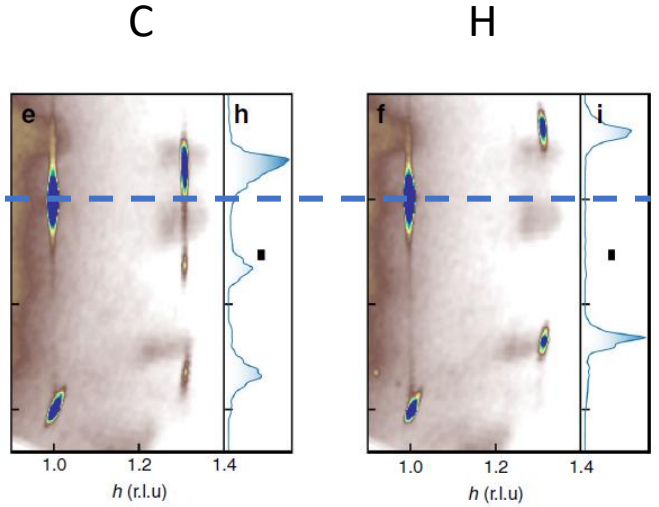
Le Guyader *et al.*, Struct Dyn (2017)

- $l = 0$: $I_C > I_{NC}$
- $l = {}^1/_6$: $I_C > I_{NC}$
- $l = {}^1/_3$: $I_C < I_{NC}$



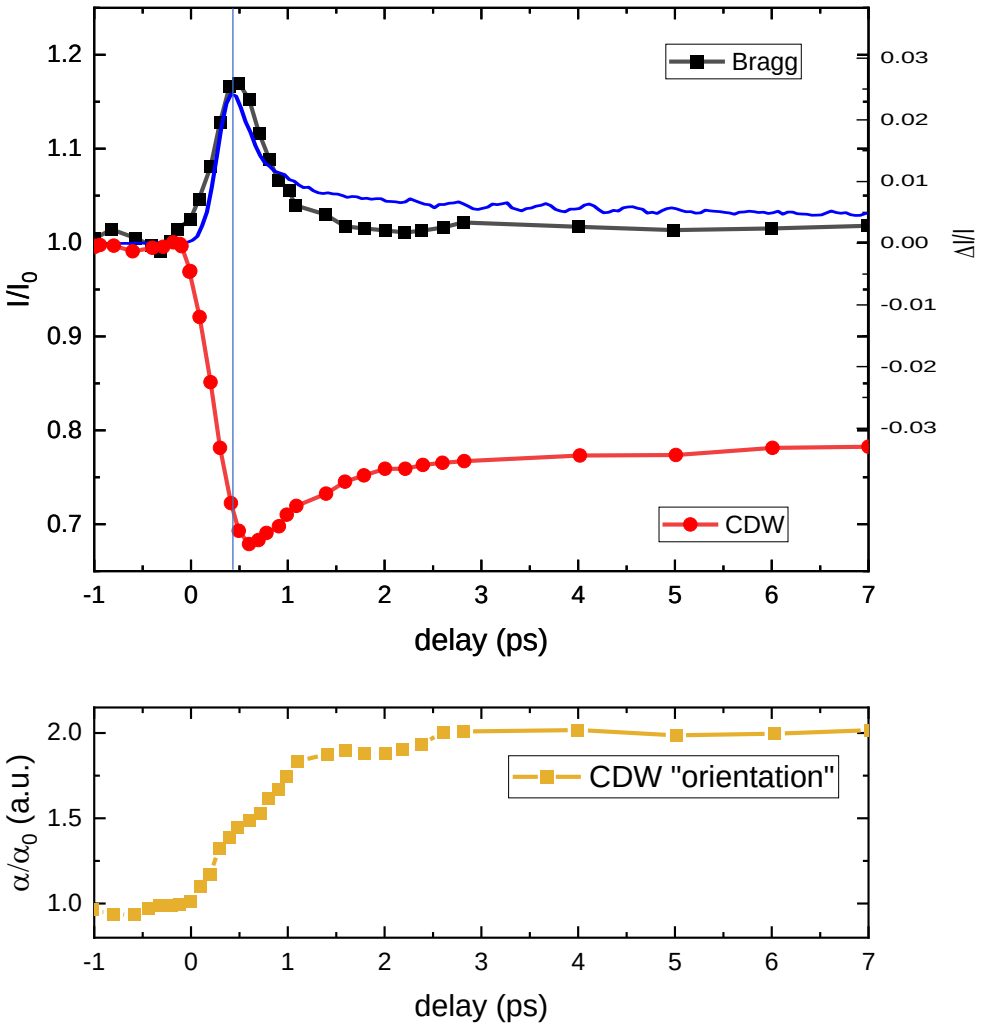
Photoinduced states: what to expect





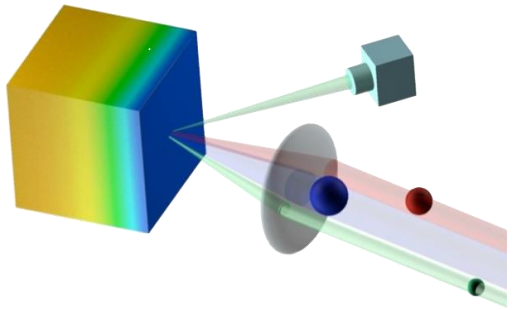
Stahl *et al.*, Nat. Comm. (2019)

How fast is the transition to the H state?

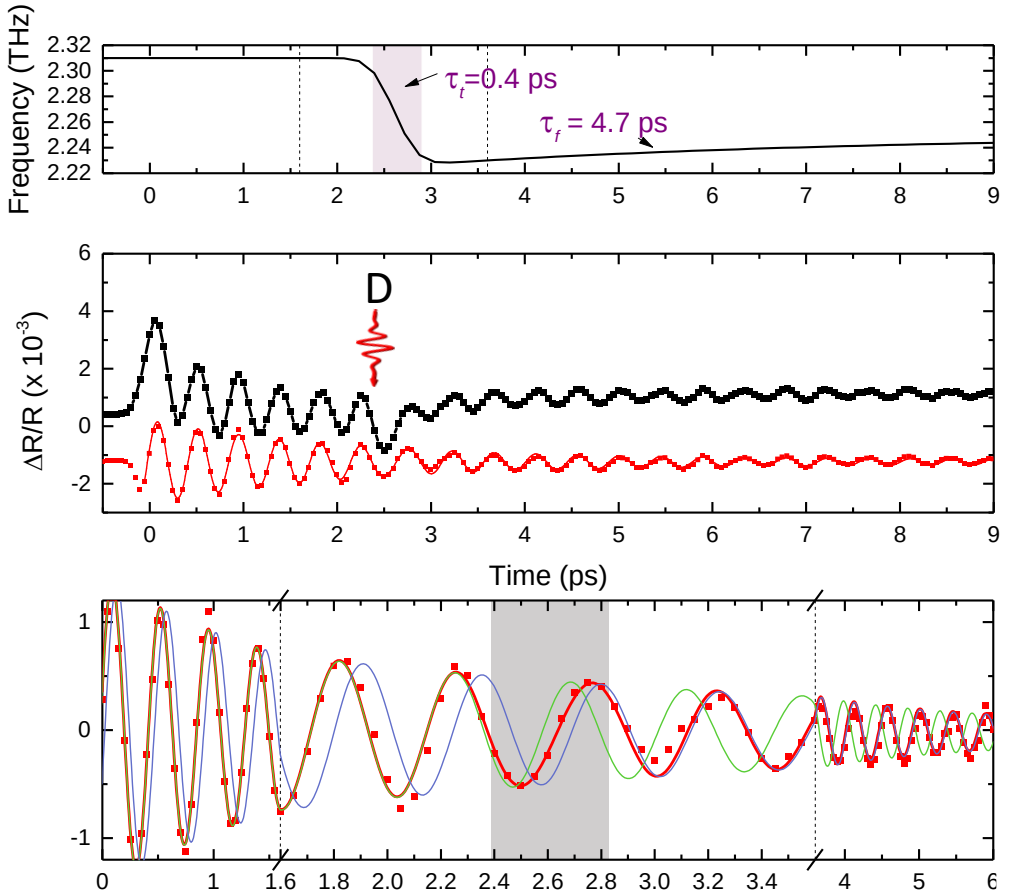


- Bragg: ~ 400 fs increase
- CDW satellites: ~600 fs decay
- CDW “reorientation”: ~1 ps

How fast is the transition to the H state?

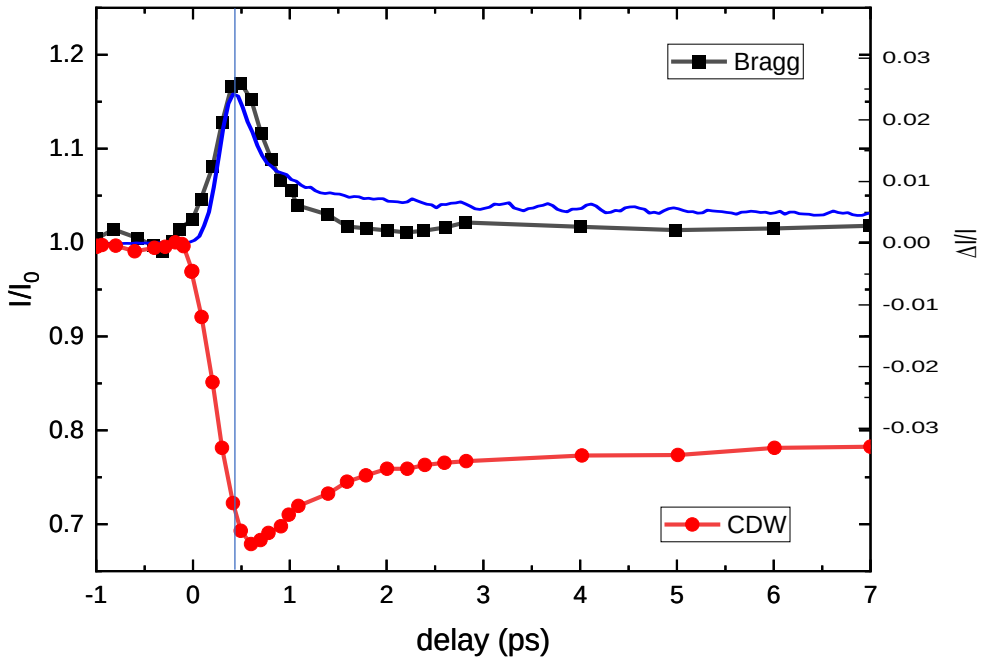


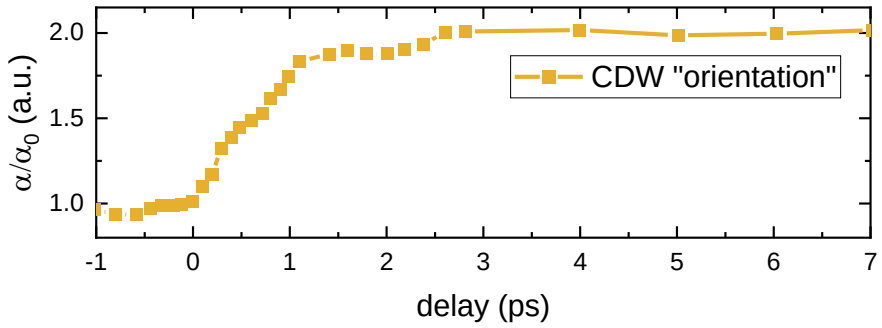
Ravnik, IV *et al.*, PRB **97**, 075304 (2018)



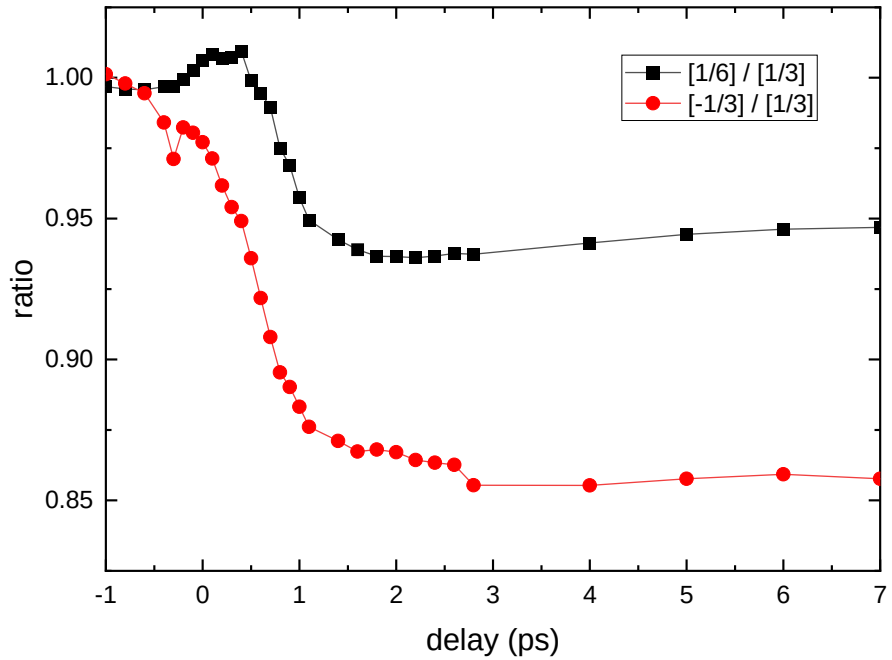
How fast is the transition to the H state?

Integrated along l

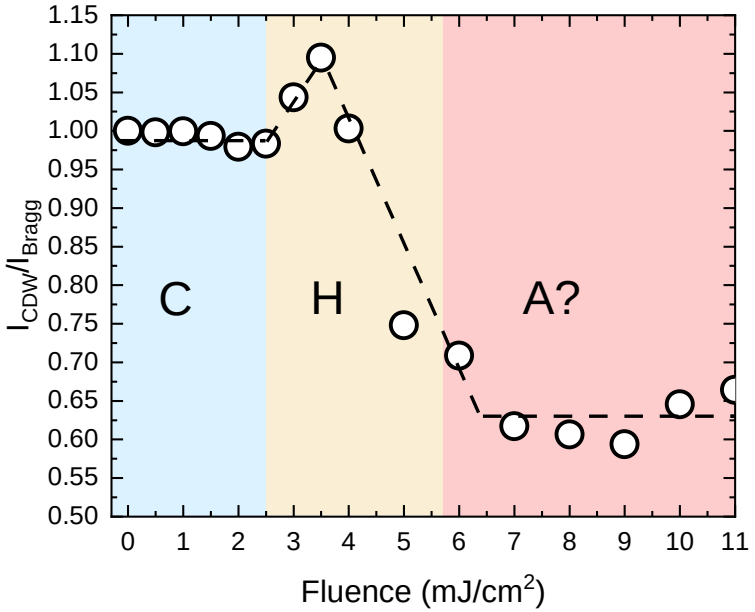




l-resolved



Static case ($l = 0$: $I_C > I_{NC}$)



Normal incidence (static measurement):

- **Increase** at moderate fluence -> H state
- **Decrease** at high fluence -> A state

Stacking in the **H state** is not the same as in the NC/IC states!

UED: Summary

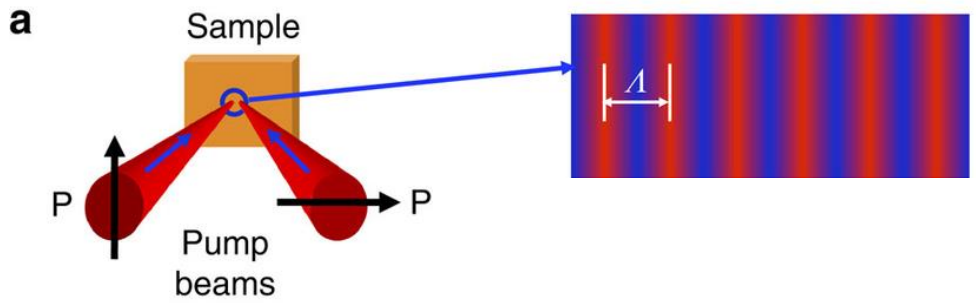
- The stacking in the H state is different both from C and NC/IC
- Restacking occurs within 1 ps– comparable to the change of AM observed in optics.
- The A state is disordered along c-axis.
- What is the time-scale for the A state transition?

1T-TaS_2: is it… a panacea?

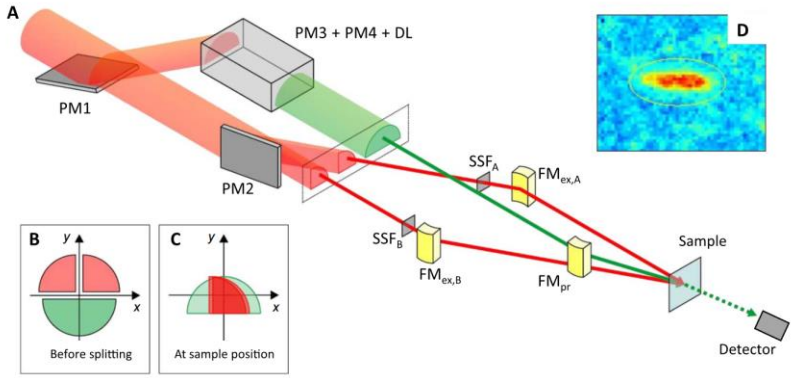
- Memory device *(D. Mihailovic group)*
- Electronic logical gate *(Y. Iwasa group)*
- Ink for printing the electronic circuits *(doi: 10.1021/acsnano.2c00378)*
- Humidity sensor *(doi: 10.1039/C9TC02785H)*
- Passive photonic device, switch/diode *(doi: 10.1016/j.jallcom.2019.07.343)*
- Optical neural networks *(Yuning Wang, thesis)*
- ……

Part II: *1T-TaS_2*-based ultrafast X-ray modulator

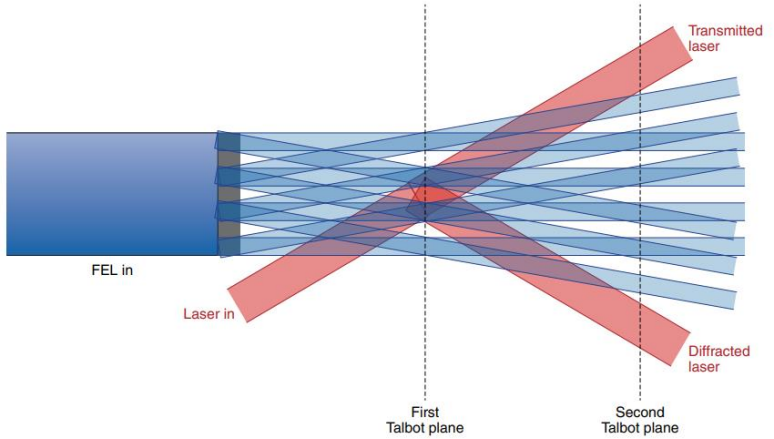
Transient grating experiment



- Electron dynamics
- Spin dynamics
- Phonon dynamics
- Heat transport
- …..

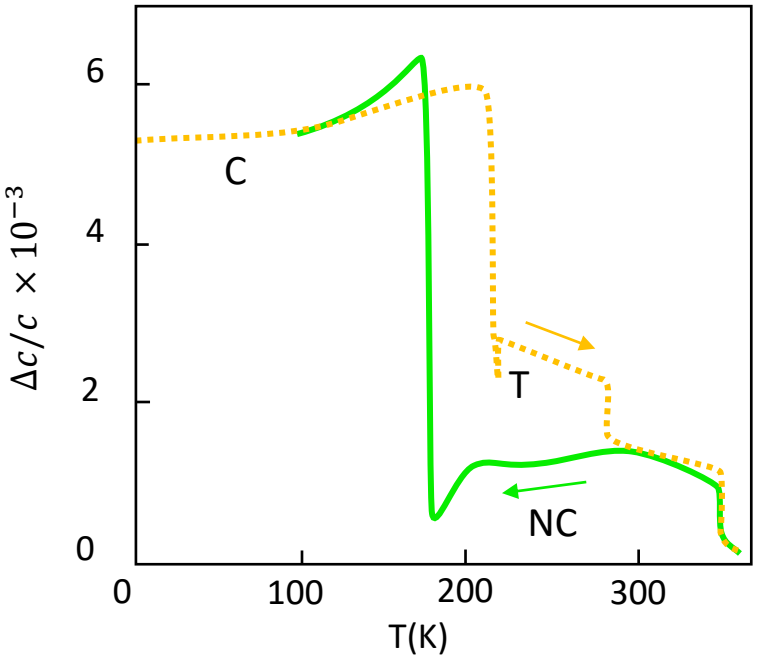


Bencivenga *et al.*, Sci. Adv. **5**, 5805 (2019)



Martin Beye, Nat. Phot. **15**, 490 (2021)

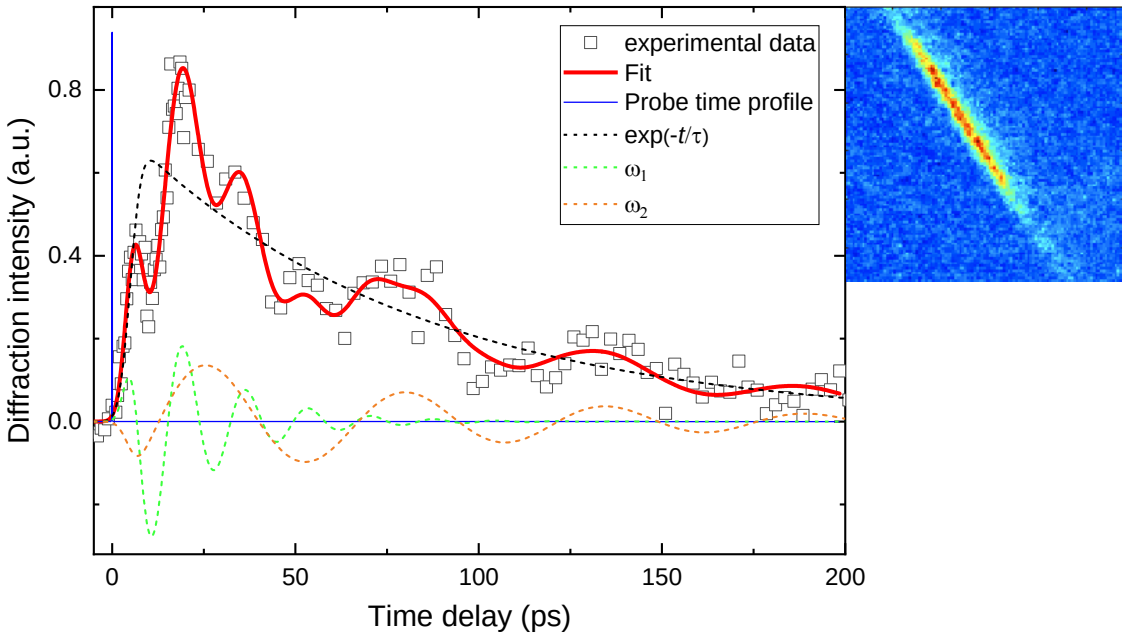
c-axis vs. temperature

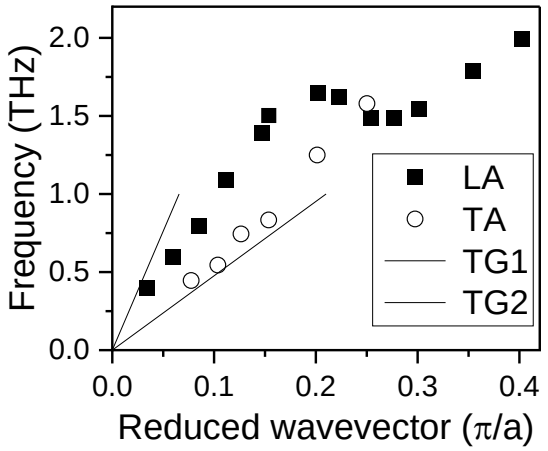


0.5% change of the lattice constant upon the phase transition!

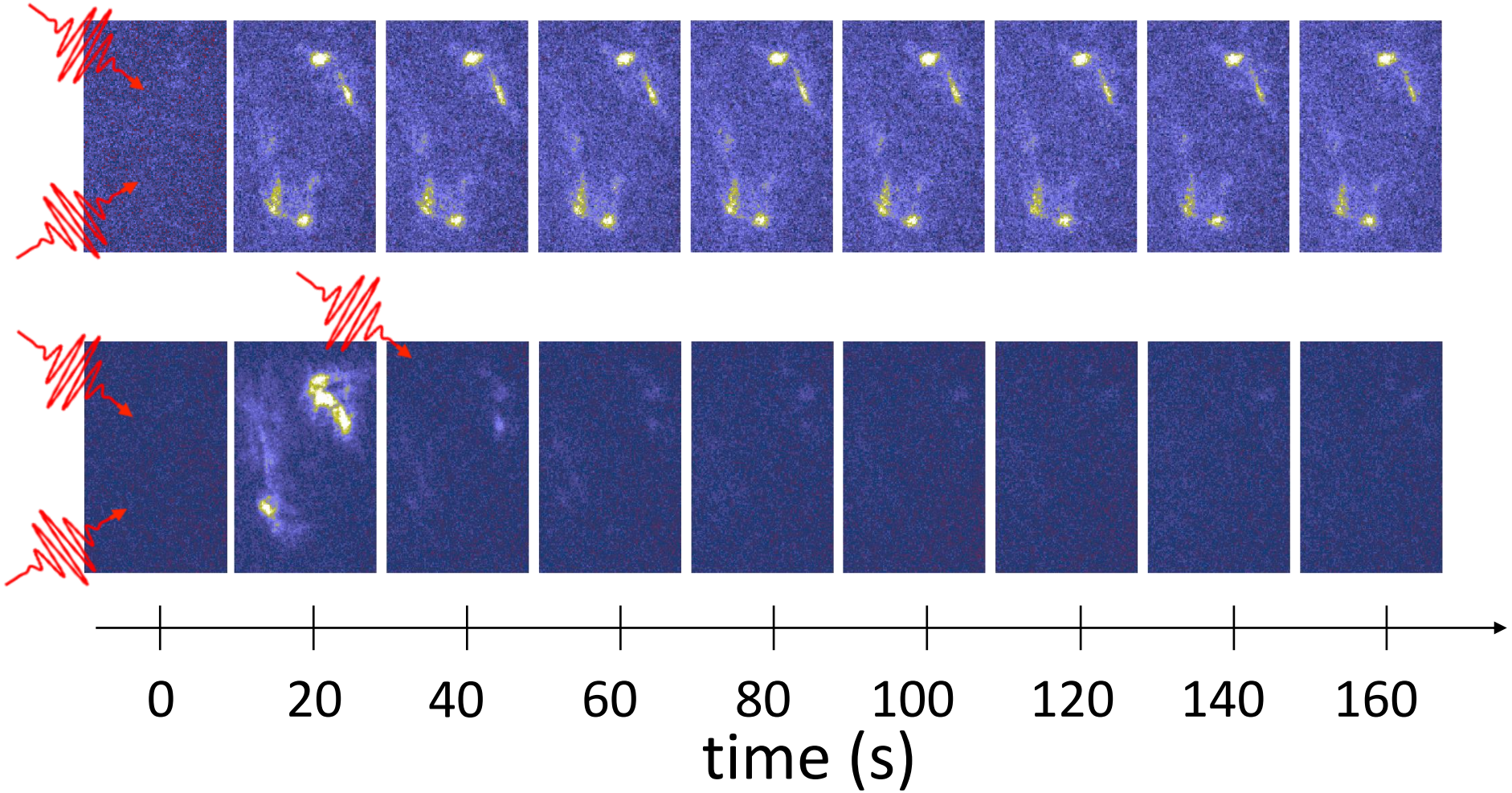
replotted from:
Sezerman *et al.,* Solid State Communications, **36**, 9 (1980)

Transient grating: room temperature

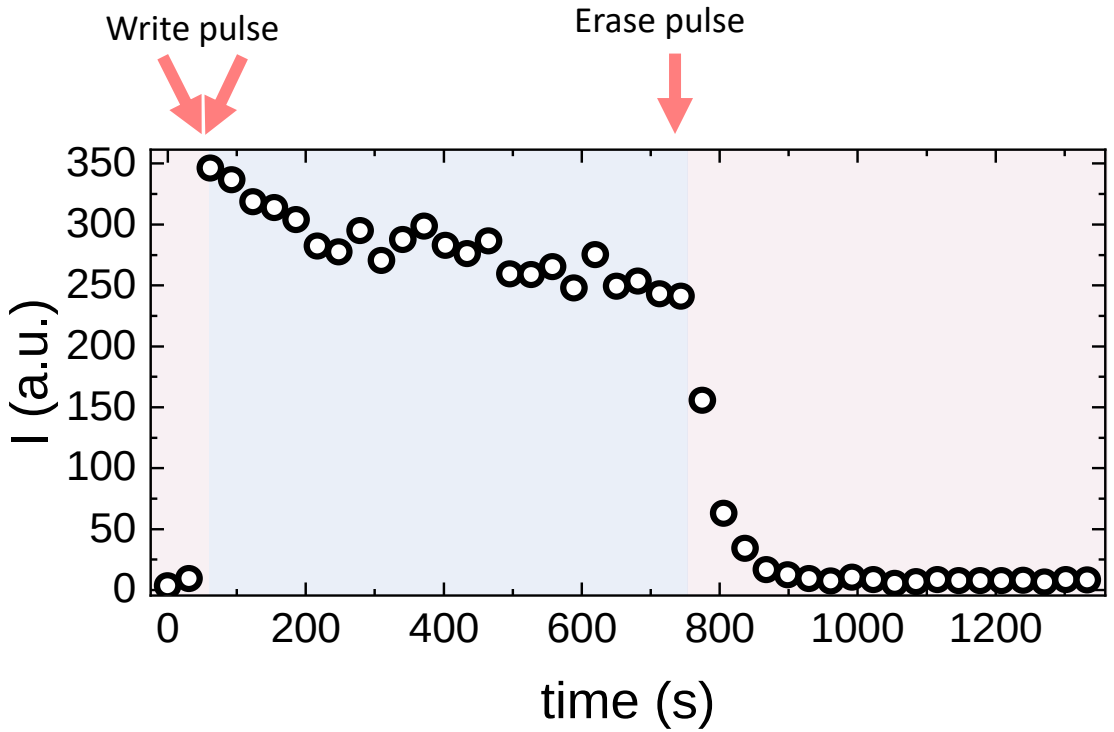


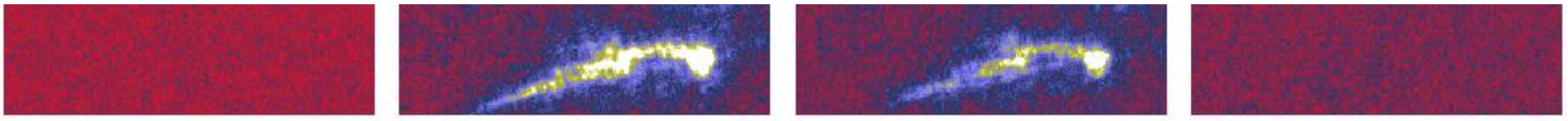


“Transient” grating: 100 K



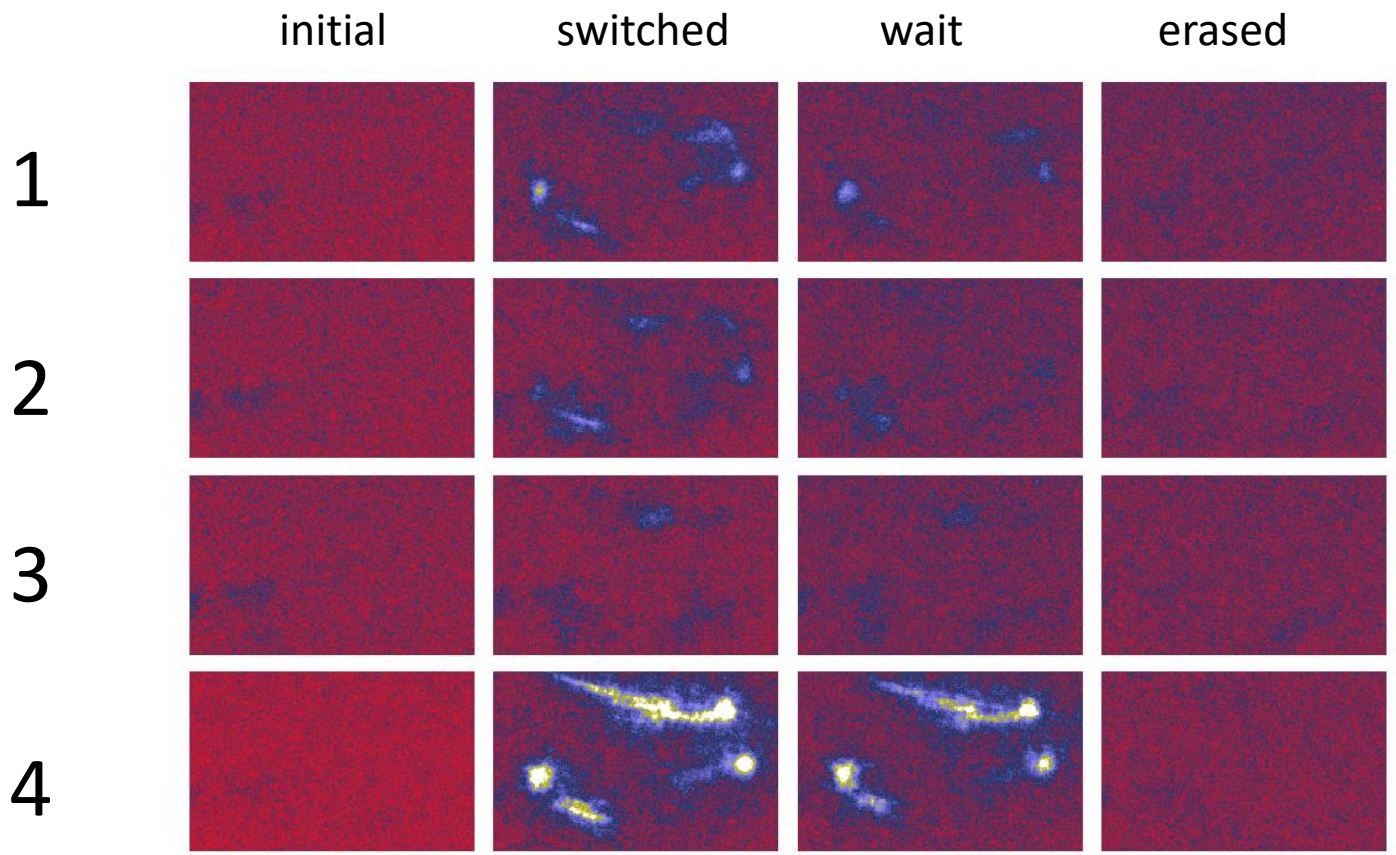
“Transient” grating: 100 K



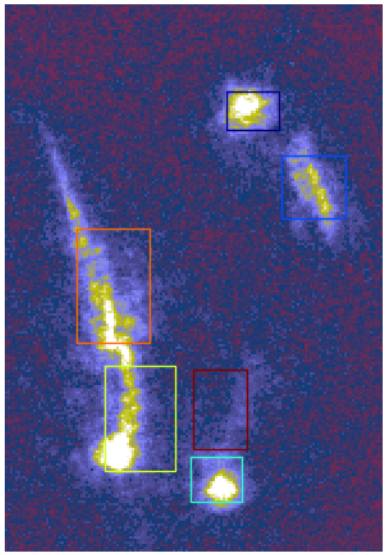


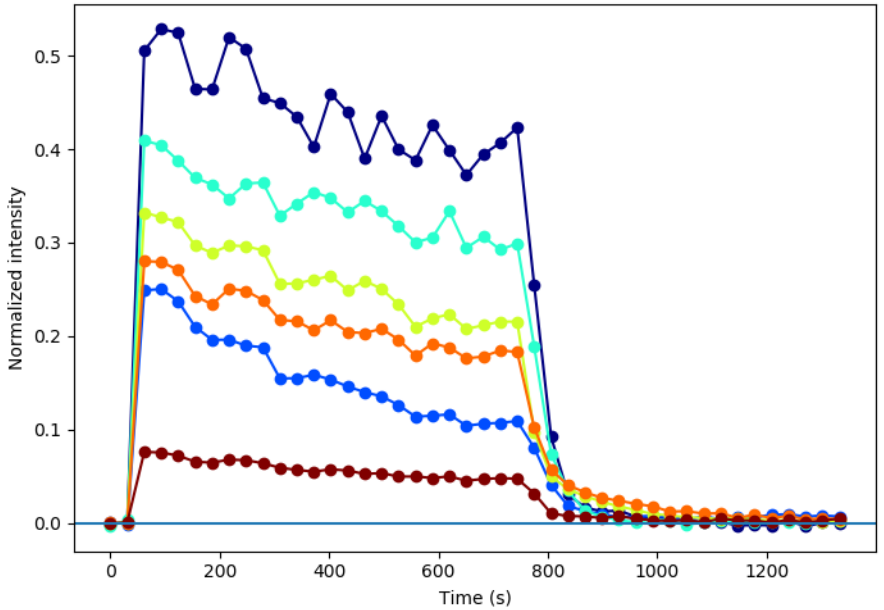
Initial | Switched | After ~ 10 min | Erased

Transient grating: repeatability



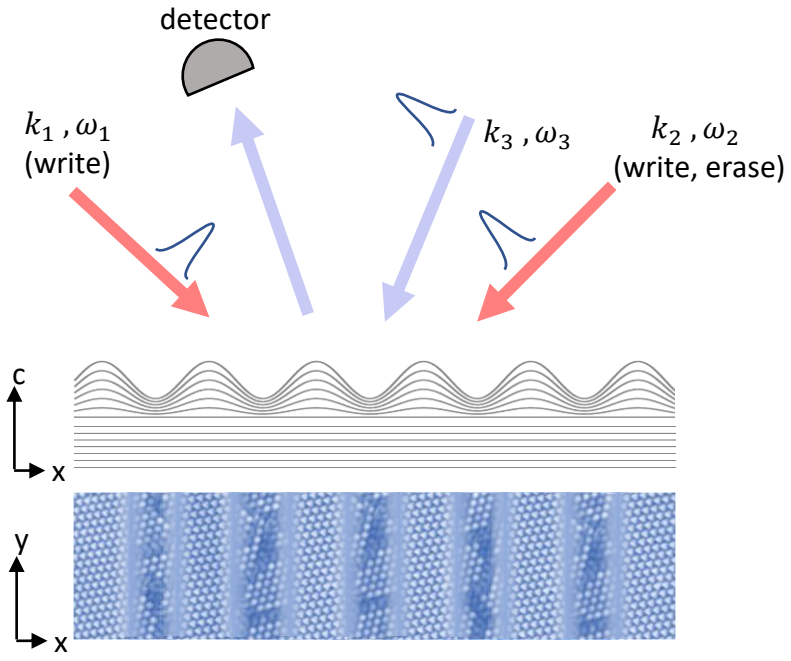
Relaxation dynamics





Each individual spot relaxes at slightly different rate – **strain**!

Efficiency of the 1T-TaS_2 grating



$$\eta = \frac{I_d}{I_0} = RJ_1^2\left\{\frac{4\pi h}{\lambda}\right\}$$

R – reflectivity
J – Bessel function
h – height of modulation
λ – phonon wavelength

Efficiencies of % are achievable

Thank you for attention