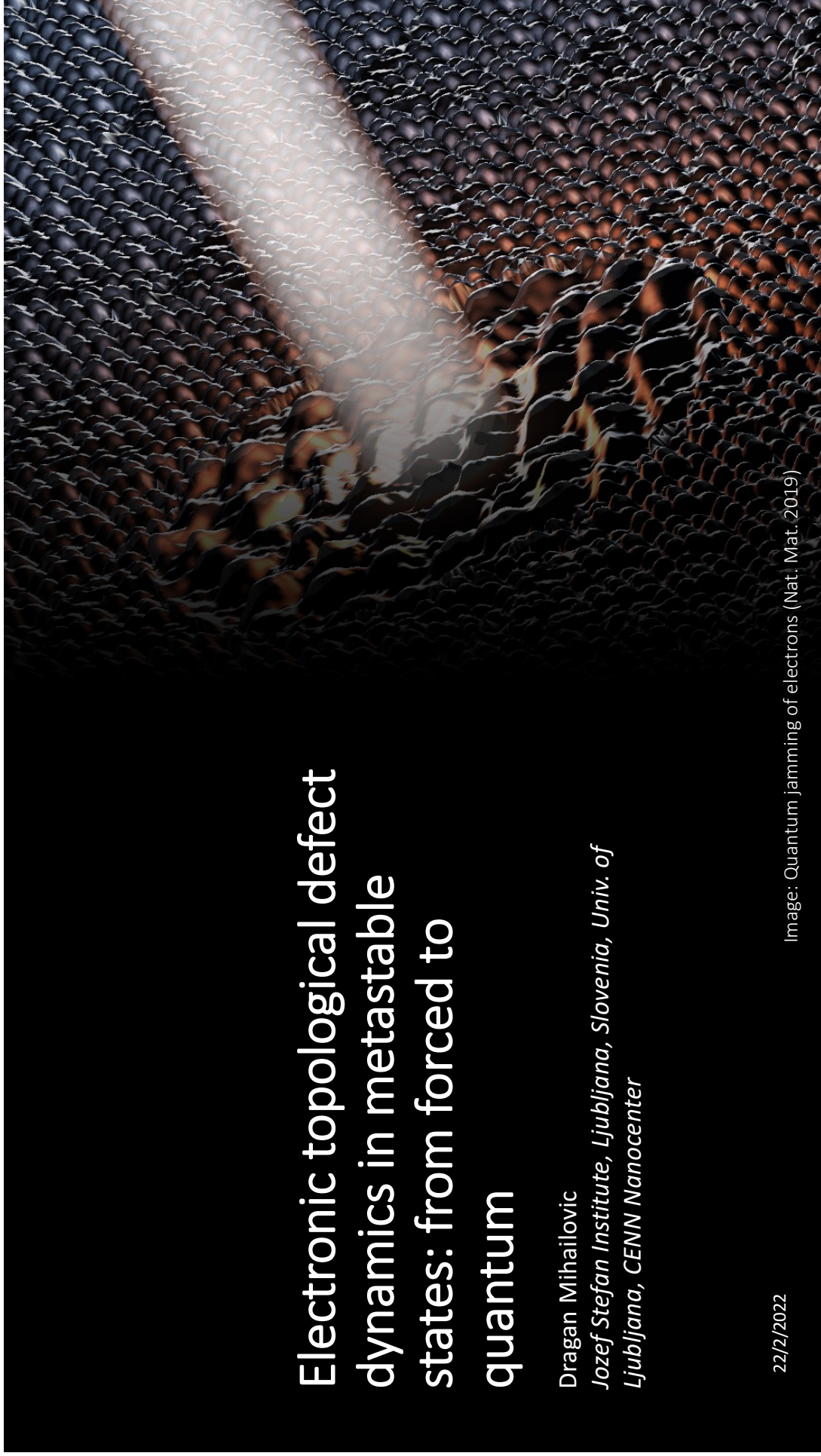


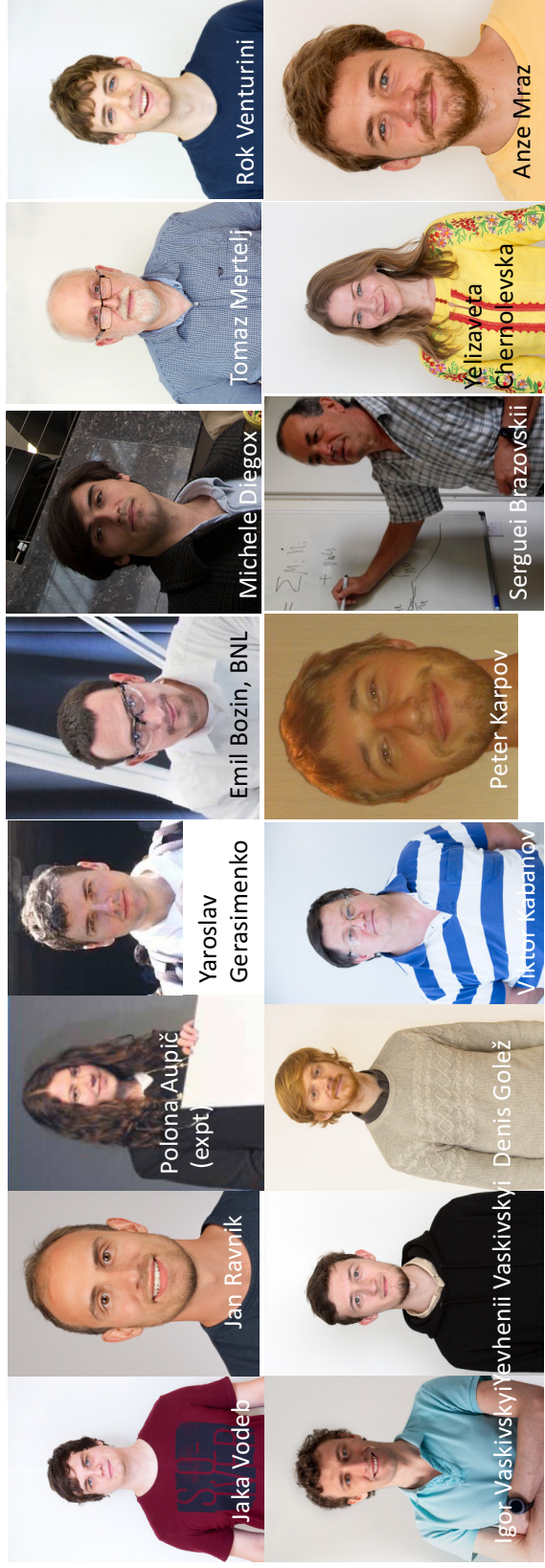
# Electronic topological defect dynamics in metastable states: from forced to quantum

Dragan Mihailovic  
*Jozef Stefan Institute, Ljubljana, Slovenia, Univ. of  
Ljubljana, CENN Nanocenter*

22/2/2022

Image: Quantum jamming of electrons (Nat. Mat. 2019)

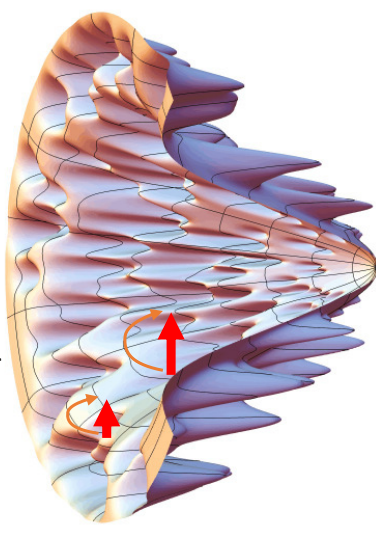




# Life exists (only) out of equilibrium

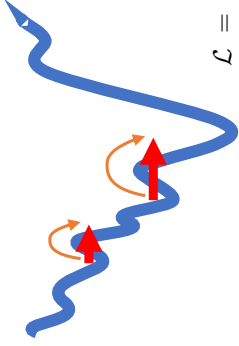


Protein folding bottlenecks  
(metastability – first order phase transitions)



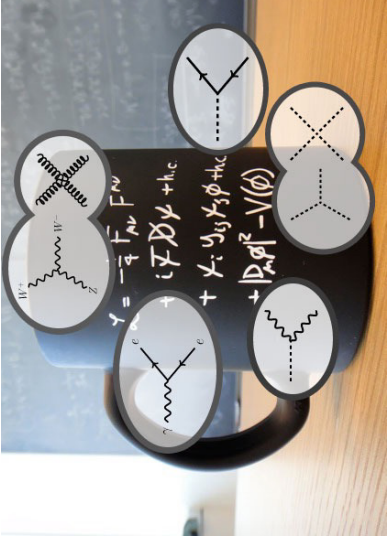
Edwin Schroedinger, What is life? (1944)

# The standard model



Particle decays

$$\begin{aligned}
 \mathcal{L} = & -\frac{1}{4}B_{\mu\nu}B^{\mu\nu} - \frac{1}{8}\text{tr}(\mathbf{W}_{\mu\nu}\mathbf{W}^{\mu\nu}) - \frac{1}{2}\text{tr}(\mathbf{G}_{\mu\nu}\mathbf{G}^{\mu\nu}) \\
 & + (\bar{\nu}_L, \bar{e}_L) \bar{\sigma}^\mu i D_\mu \begin{pmatrix} \nu_L \\ e_L \end{pmatrix} + \bar{e}_R \sigma^\mu i D_\mu e_R + \bar{\nu}_R \sigma^\mu i D_\mu \nu_R + (\text{h.c.}) \\
 & - \frac{\sqrt{2}}{v} \left[ (\bar{\nu}_L, \bar{e}_L) \phi M^e e_R + \bar{e}_R \bar{M}^e \bar{\phi} \begin{pmatrix} \nu_L \\ e_L \end{pmatrix} \right] \\
 & - \frac{\sqrt{2}}{v} \left[ (-\bar{e}_L, \bar{\nu}_L) \phi^* M^\nu \nu_R + \bar{\nu}_R \bar{M}^\nu \phi^T \begin{pmatrix} -e_L \\ \nu_L \end{pmatrix} \right] \\
 & + (\bar{u}_L, \bar{d}_L) \bar{\sigma}^\mu i D_\mu \begin{pmatrix} u_L \\ d_L \end{pmatrix} + \bar{u}_R \sigma^\mu i D_\mu u_R + \bar{d}_R \sigma^\mu i D_\mu d_R + (\text{h.c.}) \\
 & - \frac{\sqrt{2}}{v} \left[ (\bar{u}_L, \bar{d}_L) \phi M^d d_R + \bar{d}_R \bar{M}^d \bar{\phi} \begin{pmatrix} u_L \\ d_L \end{pmatrix} \right] \\
 & - \frac{\sqrt{2}}{v} \left[ (-\bar{d}_L, \bar{u}_L) \phi^* M^u u_R + \bar{u}_R \bar{M}^u \phi^T \begin{pmatrix} -d_L \\ u_L \end{pmatrix} \right] \\
 & + (D_\mu \bar{\phi}) D^\mu \phi - m_h^2 [\bar{\phi} \phi - v^2/2]^2/2v^2.
 \end{aligned}$$



(U(1), SU(2) and SU(3) gauge terms)

(lepton dynamical term)

(electron, muon, tauon mass term)

(neutrino mass term)

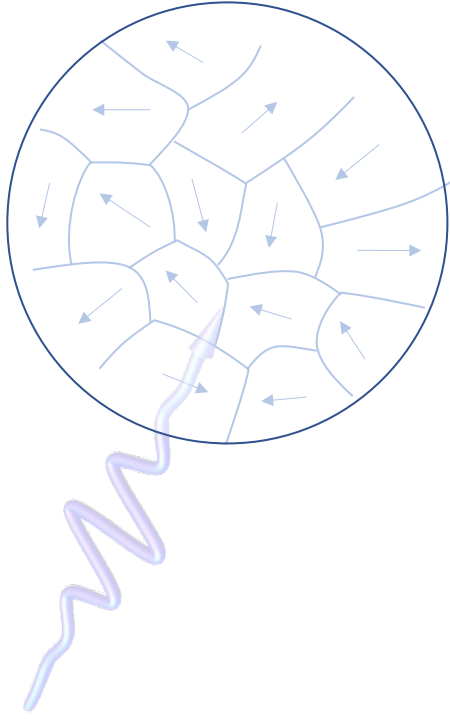
(quark dynamical term)

(down, strange, bottom mass term)

(up, charmed, top mass term)

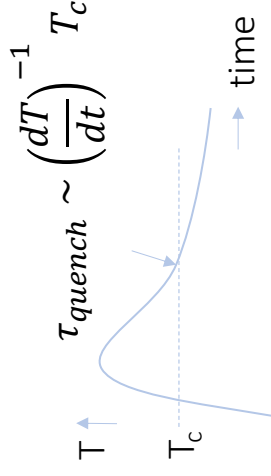
(Higgs dynamical and mass term) (

# Causality and the dynamics of emergent orders after a 2<sup>nd</sup> order PT



System size: laser spot, universe, etc.

The Kibble-Zurek Mechanism



The picture is naïve, assuming a common temperature, no interactions, etc.

Control of the outcome:



Tempering of steel:  
Control of defects and domains

- Tempering of system trajectories can controllably lead to different transition outcomes
- CONTROL KNOBS: spatial and temporal gradients, transient strain, tailored laser pulse sequences, etc.

T. Kibble, J Phys a-Math Gen 9, 1387 (1976).  
W. Zurek, Nature 317, 505 (1985).

# Possible single transition outcomes

Starobinsky – Linde – Guth  
Kibble, Zurek, Volovik

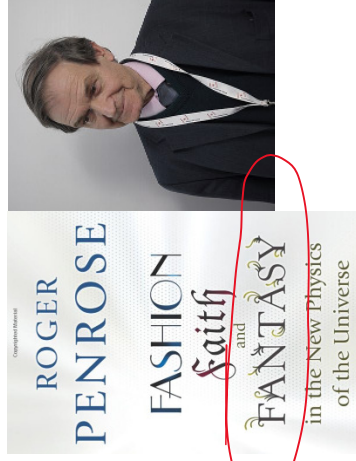
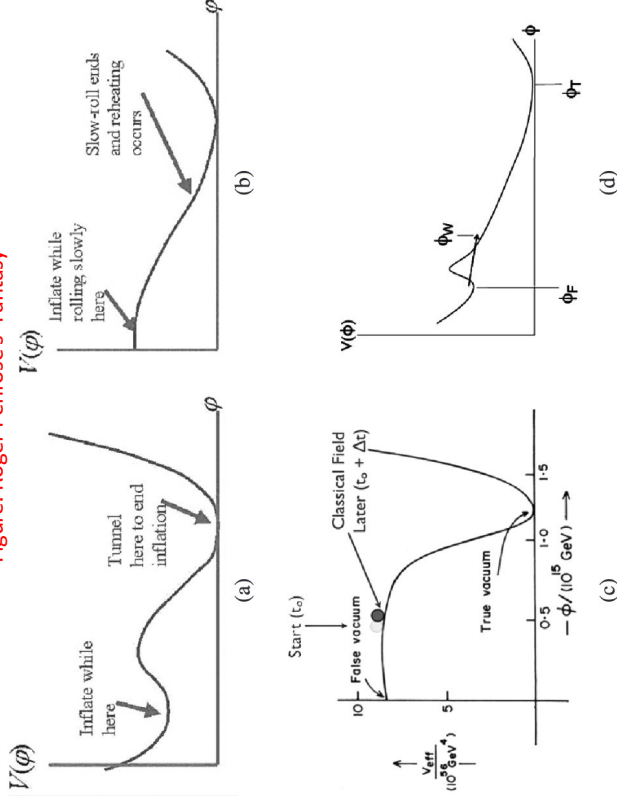


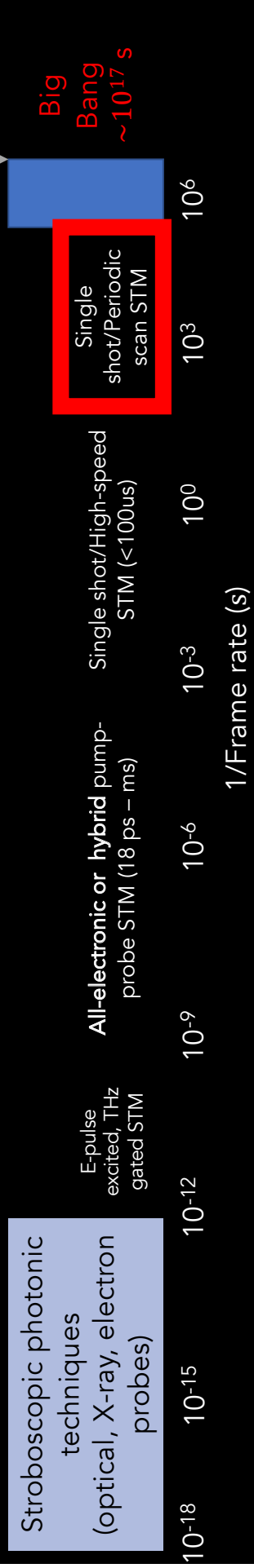
Figure: Roger Penrose's 'Fantasy'



We have little data over a vast range of timescales!

# Techniques for studying metastable, aperiodic, mesoscopic quantum structures

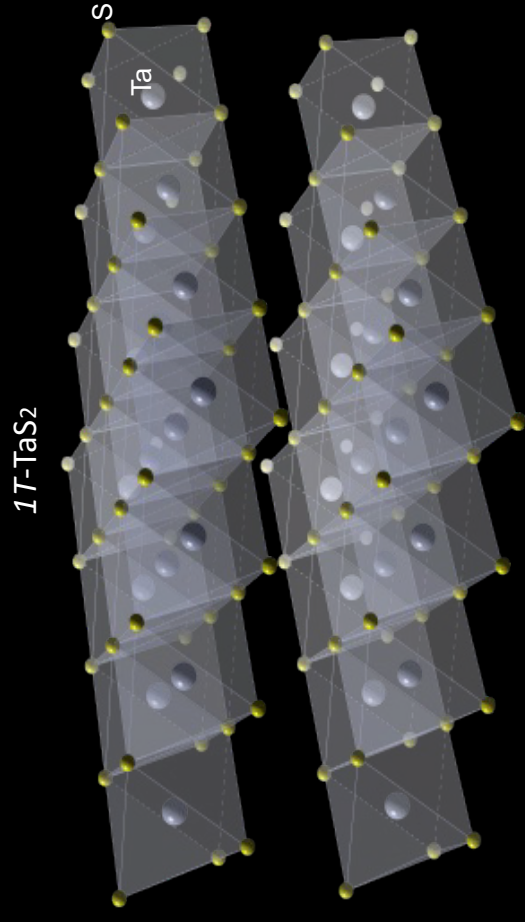
Human history (10<sup>12</sup> s)



# 1T-TaS<sub>2</sub> as a prototype system



Crystals of 1T-TaS<sub>2</sub> grown by Petra Sutar

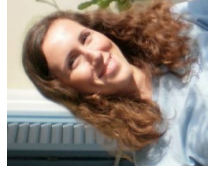
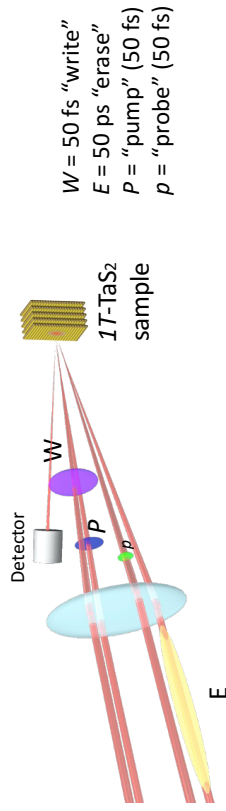


The threshold for localization, as defined by the dimensionless parameter,  $r_s = \frac{V}{t} = \frac{e^2 m^*}{\hbar^2 \sqrt{n}} \sim 30$  in 2D.

1T-TaS<sub>2</sub>, with  $m^* \sim 3 - 5m_e \rightarrow r_s = \frac{V}{t} = 70 \sim 100$ , is in the Wigner crystal regime



# Controllable metastable states in 1T-TaS<sub>2</sub>

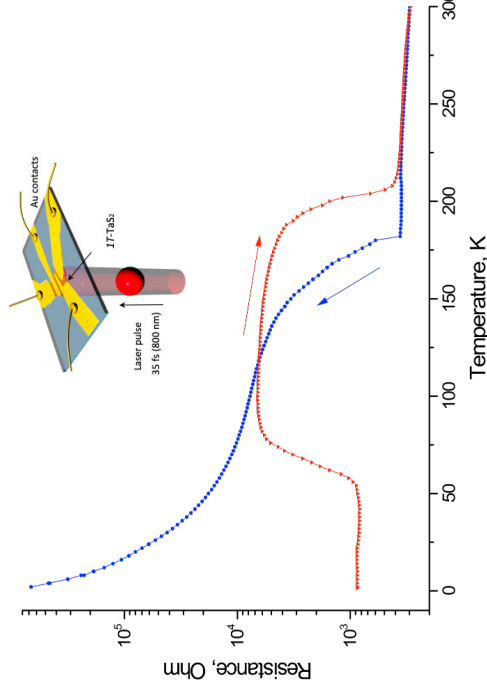


Ljupka Stojchevska

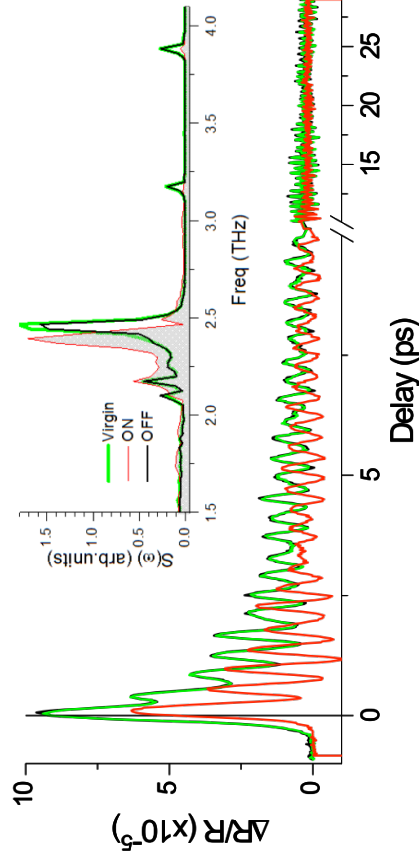


Igor Vaskivskiy

## Resistance change after a (single) 35 fs pulse



## CDW Collective mode frequency switching



# Charge Configuration Memory (CCM)

AN 2-TERMINAL ULTRAFAST ELECTRONIC NON-VOLATILE MEMORY CONCEPT FOR LOW-TEMPERATURE, ULTRA HIGH SPEED, LOW-ENERGY APPLICATIONS.

NANO LETTERS

pubs.acs.org/NanoLett



Letter

## Charge Configuration Memory Devices: Energy Efficiency and Switching Speed

Anze Mraz,\* Rok Venturini, Damjan Svetin, Vitomir Sever, Jan Aleksander Mihailovic, Igor Vaskivskiy, Bojan Ambrozic, Goran Drazic, Mária D'Antonio, Daniela Stormaiuolo, Francesco Tafuri, Dimitrios Kazazis, Jan Ravnik, Yasin Elkinci, and Dragan Mihailovic

Cite This: <https://doi.org/10.1021/acs.nanolett.2c01116>

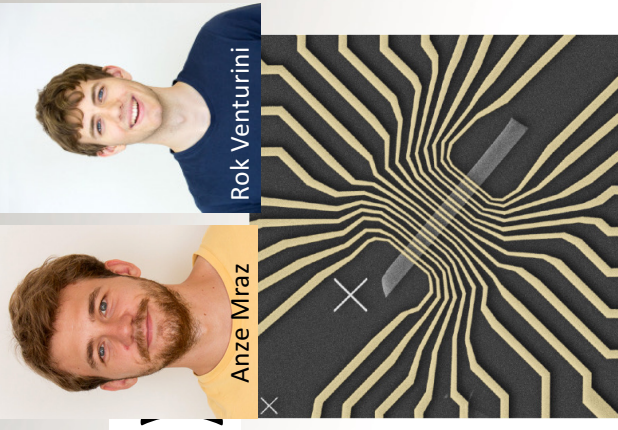


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Applied Physics Letters

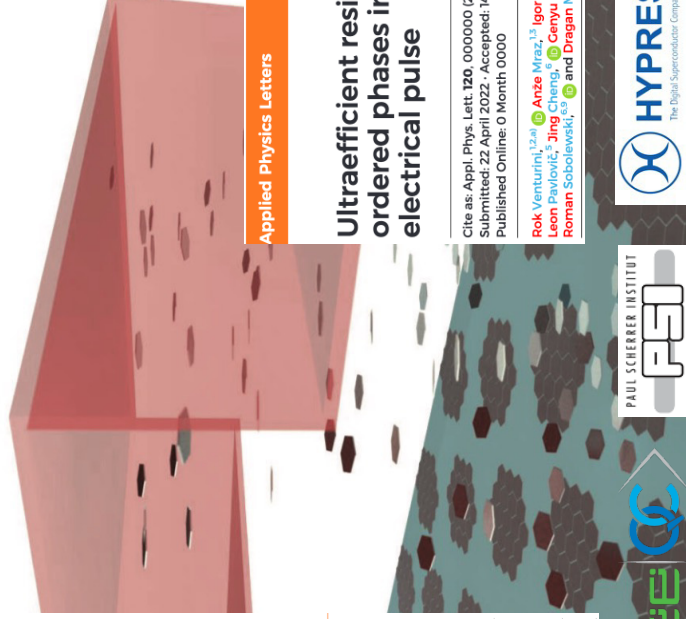
ARTICLE

scitation.org/journal/apl



Anze Mraz

Rok Venturini



## Ultrafast non-thermal and thermal switching in charge configuration memory devices based on 1T-TaS<sub>2</sub>

Cite as: Appl. Phys. Lett. **119**, 013106 (2021); doi: 10.1063/5.0052311  
Submitted: 30 March 2021 · Accepted: 31 May 2021  
Published Online: 8 July 2021

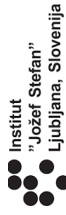
D. Mihailovic,<sup>1,2,a</sup> D. Svetin,<sup>1,4</sup> I. Vaskivskiy,<sup>1,2</sup> R. Venturini,<sup>1,4</sup> B. Lipovsek,<sup>1,4</sup> and A. Mraz,<sup>1,3</sup>



Letter



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Institut  
"Jožef Stefan"  
Ljubljana, Slovenia



COSYLAB  
CONFLECT SYSTEM LABORATORY



Applied Physics Letters

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## Ultraefficient resistance switching between charge ordered phases in 1T-TaS<sub>2</sub> with a single picosecond electrical pulse

Cite as: Appl. Phys. Lett. **120**, 000000 (2022); doi: 10.1063/5.0096850  
Submitted: 22 April 2022 · Accepted: 14 June 2022 ·  
Published Online: 0 Month 0000

Rok Venturini,<sup>1,2,a</sup> Anze Mraz,<sup>1,3</sup> Igor Vaskivskiy,<sup>1,2</sup> Yevhenii Vaskivskiy,<sup>1,2</sup> Damjan Svetin,<sup>1,4</sup> Tomaz Mertelj,<sup>1,2</sup> Leon Pavlovič,<sup>5</sup> Jing Cheng,<sup>6</sup> Cenyu Chen,<sup>6</sup> Priyanthi Amarasinghe,<sup>7</sup> Syed B. Qadi,<sup>8</sup> Sudhir B. Trivedi,<sup>7</sup> Roman Sobolewski,<sup>5,9</sup> and Dragan Mihailovic<sup>1,4,a</sup>



Letter



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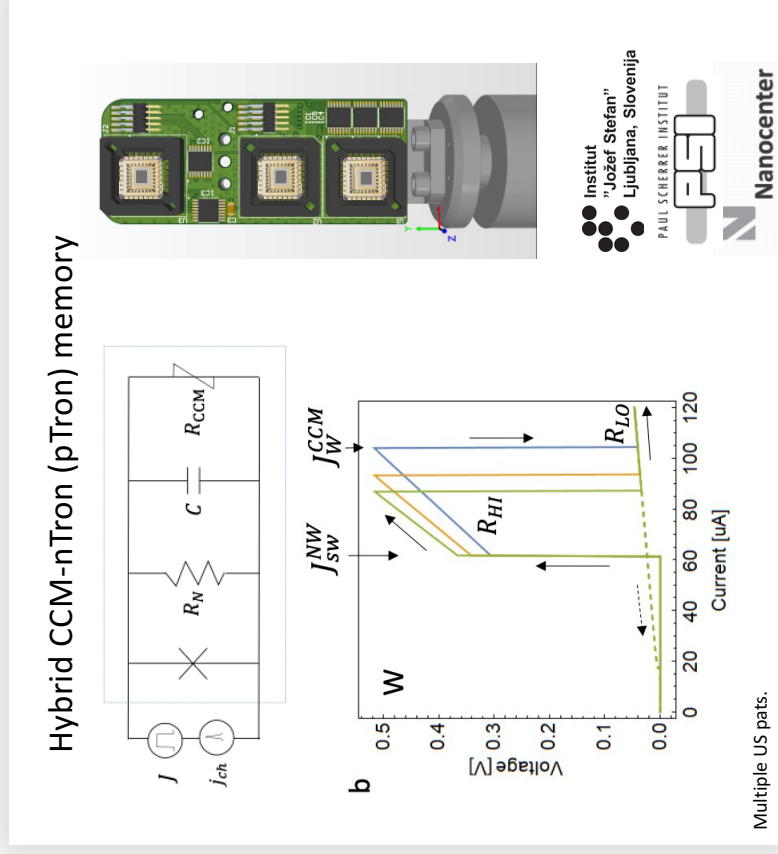
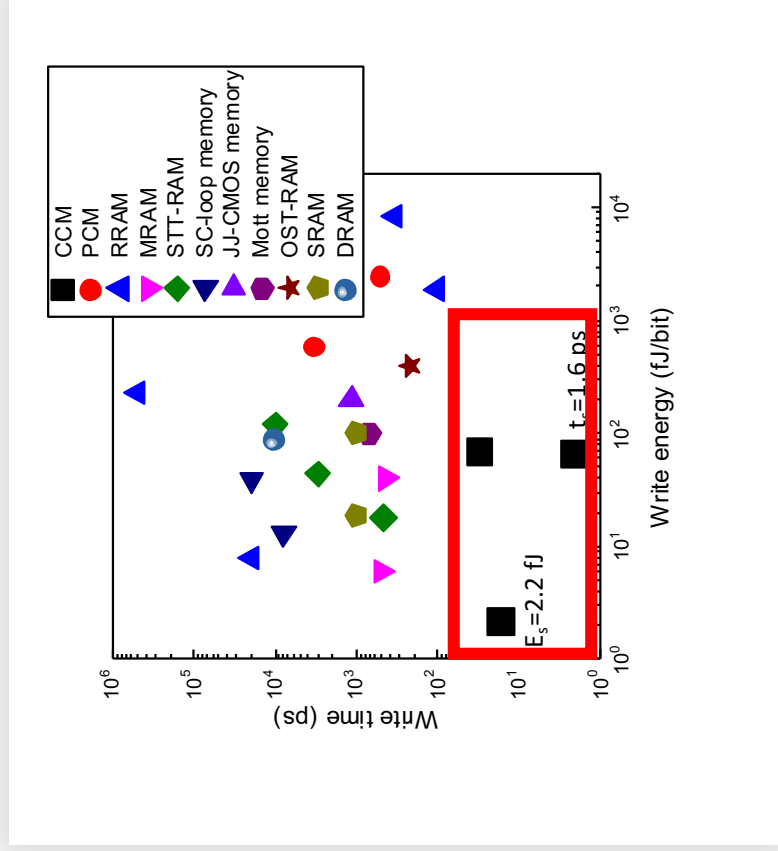


Expert Center

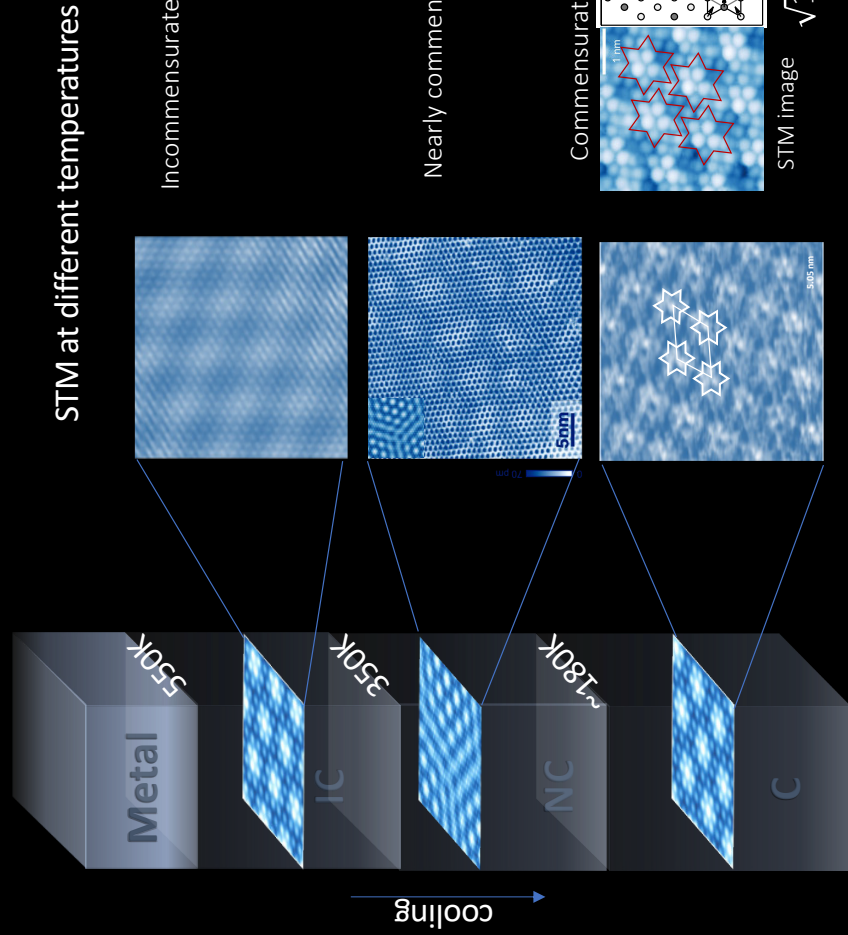


Crossmark

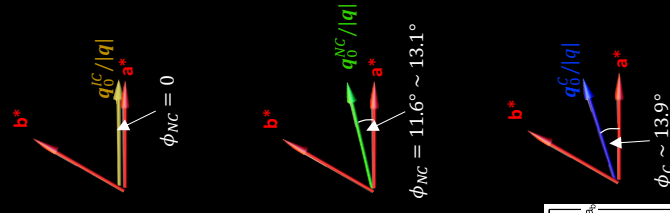
# Ultra-fast, ultra-efficient cryo-memory



# 1T-TaS<sub>2</sub> under equilibrium conditions



Ordering vector



Incommensurate CDW

Nearly commensurate

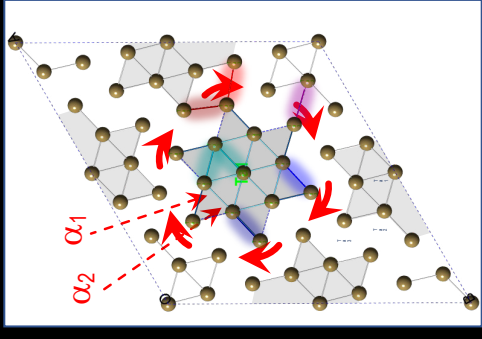
Commensurate CDW

STM image  $\sqrt{13} \times \sqrt{13}$

A Wigner crystal of polarons

Structural X-ray PDF study  
10K - 600K

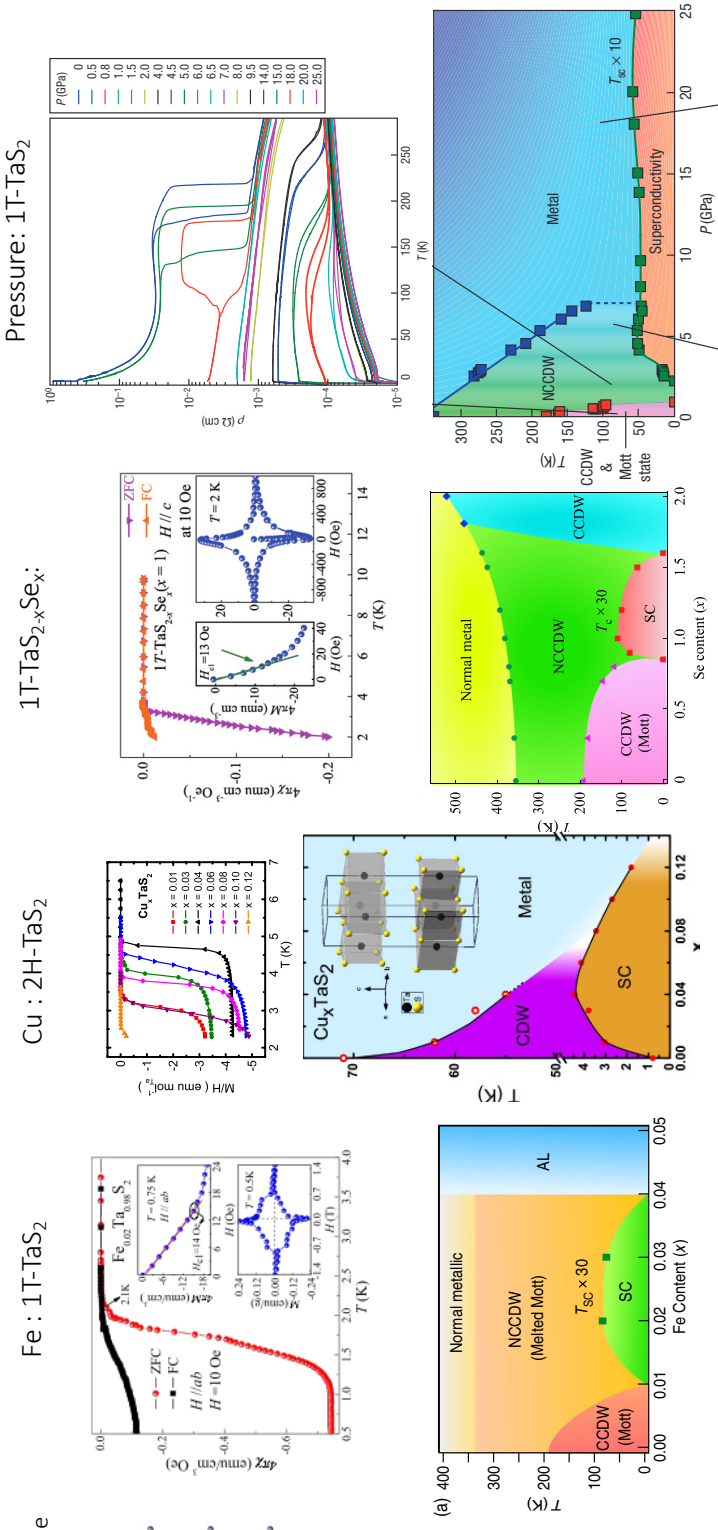
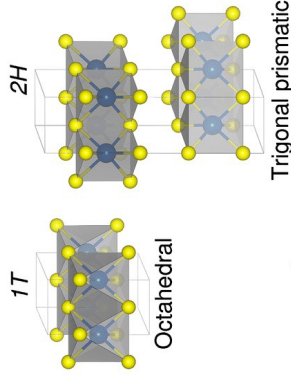
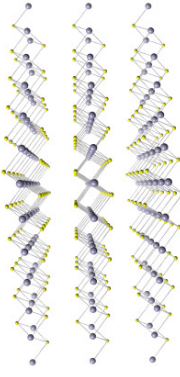
Chiral Ta displacements



Emil Bozin, BNL  
2022, to be published

# The many phases in TaS<sub>2</sub>: Multiple structural and charge-density-wave states, superconductivity under pressure, and/or (Fe,Cu,Na or Se...?) doping.

The 1T polytype of TaS<sub>2</sub> is metastable  
( $T_{c\uparrow}=550\text{K}$ ,  $T_{c\downarrow}=1100\text{K}$ )



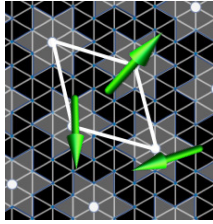
Li et al. EPL 2012

Wagner et al (PRBB 2008)

Liu et al. APL 2013

Sipos et al (Nat.Mat. 2008)

# The 'quantum spin liquid' state of 1T-TaS<sub>2</sub>

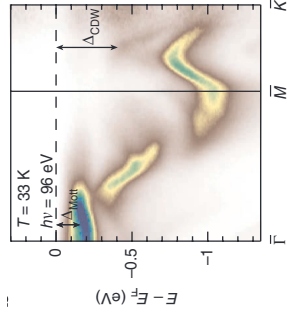


$\sqrt{13} \times \sqrt{13}$  superlattice

Charge gap 0.3 ~ 0.4 eV

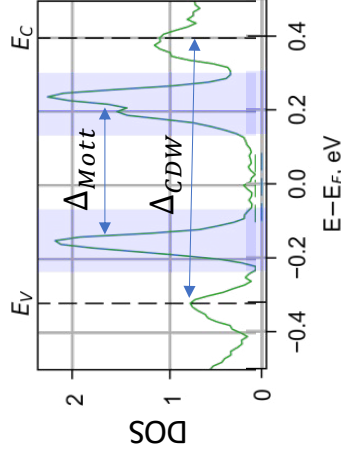
ARPES

Hellmann et al., Nat. Comm. 2012



STM

Gerashimenko, 2017



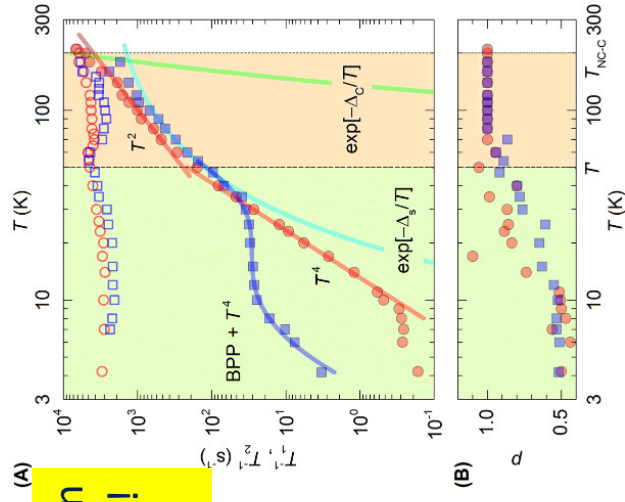
nature  
physics

ARTICLES  
PUBLISHED ONLINE 31 JULY 2017 | DOI:10.1038/NPHYS422

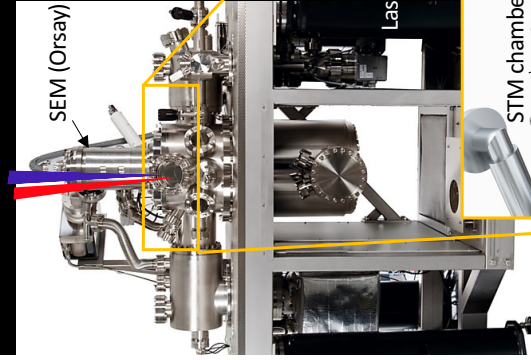
A high-temperature quantum spin liquid with polaron spins

Martin Klanjšek<sup>1</sup>, Andrej Zorko<sup>1</sup>, Rok Žitko<sup>1</sup>, Jernej Mravlje<sup>1</sup>, Zvonko Jagličić<sup>2,3</sup>, Pabitra Kumar Biswas<sup>4</sup>, Peter Prelovšek<sup>1,5</sup>, Dragan Mihailović<sup>2,5</sup> and Denis Arčon<sup>1,5\*</sup>

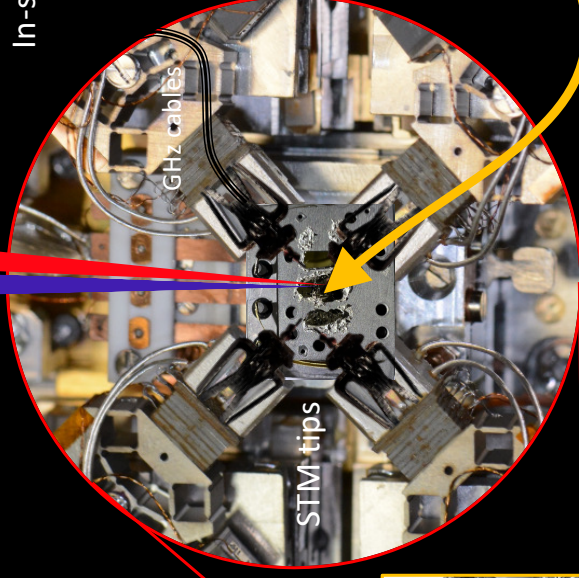
NQR Spin relaxation is gaples 50~180K! ( $1/T_1 \sim T^2$ )



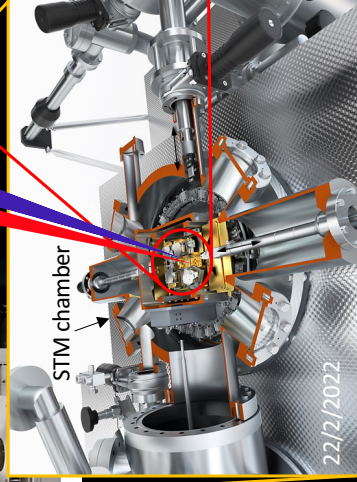
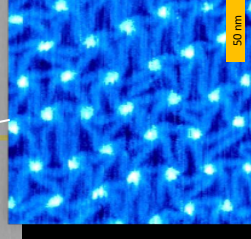
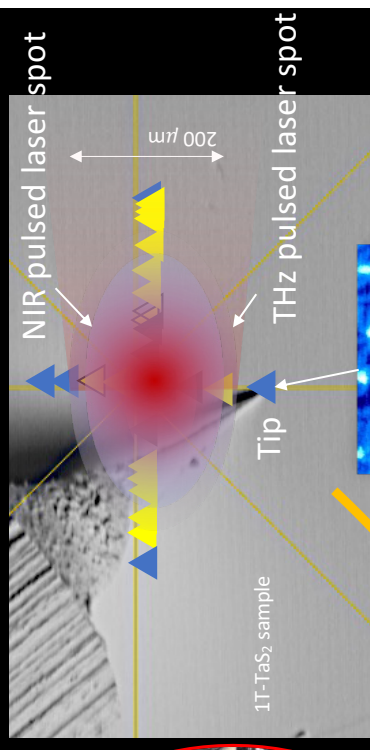
# The workhorse: a time-resolved 4-probe STM/SEM microscope.



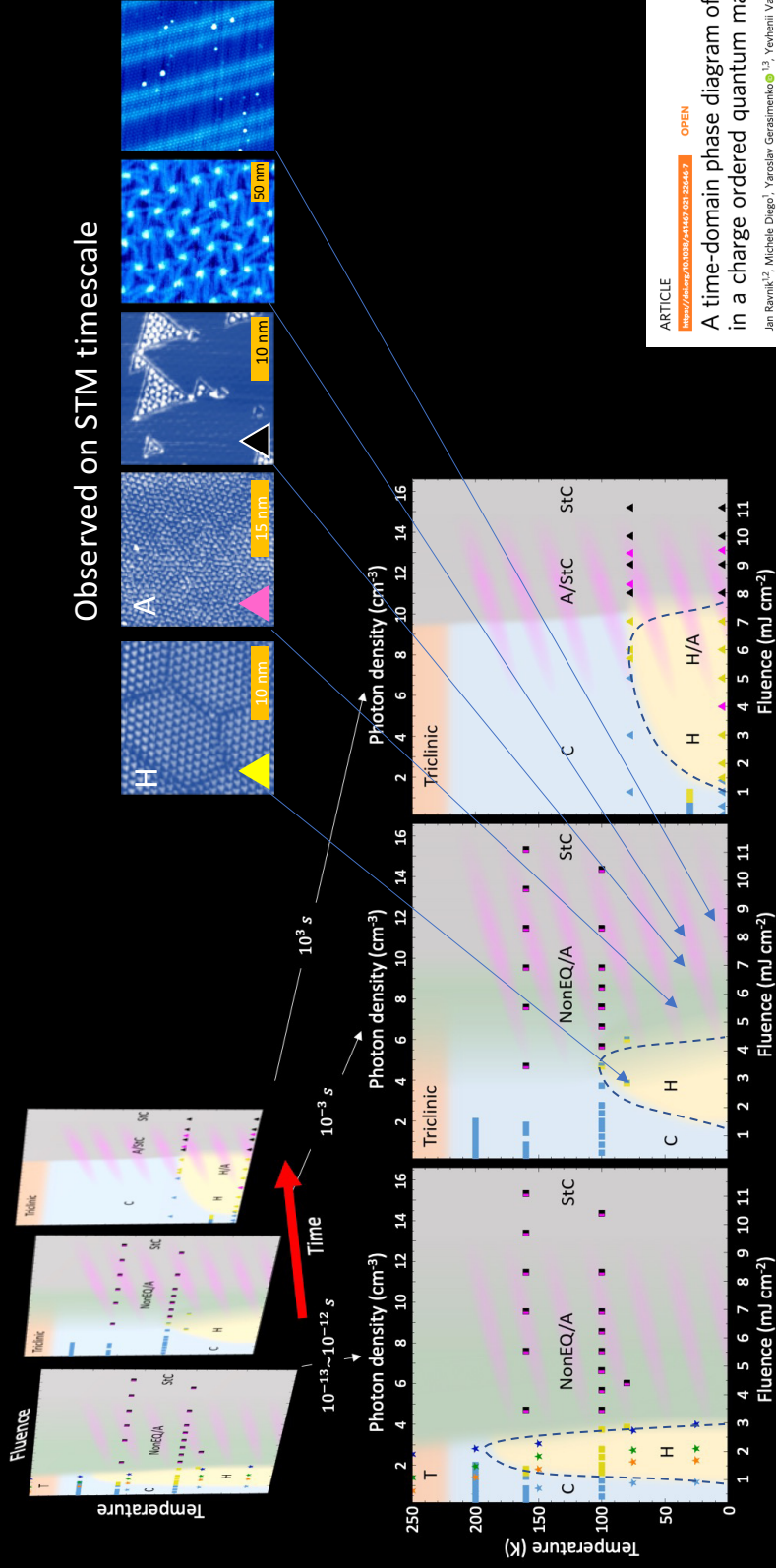
Laser / THz beams



In-situ SEM image of 1T-TaS<sub>2</sub> sample and STM tip, 4 K



# A time-domain phase diagram in 1T-TaS<sub>2</sub>



Observed on STM timescale

ARTICLE  
<https://doi.org/10.1038/s41467-021-23223-7> OPEN

A time-domain phase diagram of metastable states in a charge ordered quantum material

Jan Ravnik<sup>1,2</sup>, Michele Diogo<sup>1</sup>, Yaroslav Gerasimenko<sup>1,3</sup>, Yevhenii Vastivskiy<sup>1</sup>, Igor Vaskivskiy<sup>1,3</sup>, Tomaz Mertelj<sup>1,3</sup>, Jaka Vodeb<sup>1</sup> & Dragan Mihailovic<sup>1,3,4</sup>



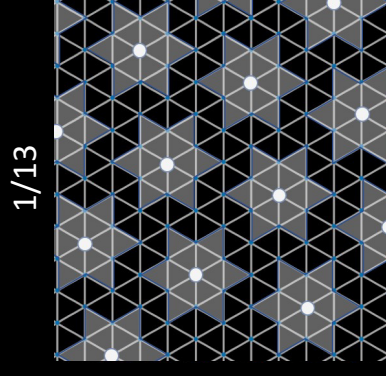
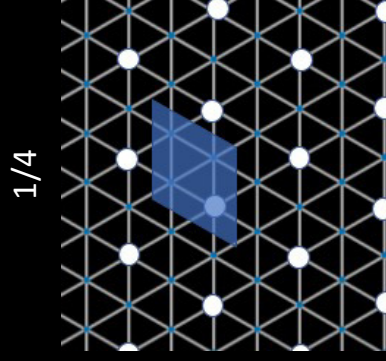
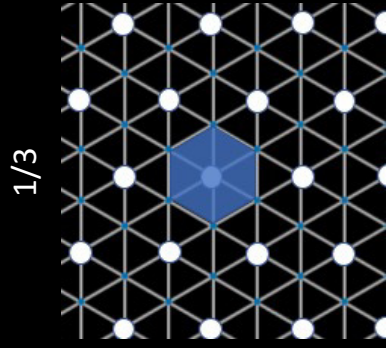
The problem of characterizing metastable states that evolve during measurements



Jacques Henri Lartigue, 1913  
(4x5 Speed Graphic camera with  
focal plane shutter)

# Commensurate CDWs in dichalcogenides as polaronic Wigner crystals\* ( $r_s = V/t \sim 70$ )

Sparse electron ordering on a triangular lattice



- Vodeb, J. et al. *New J Phys* **21**, 083001–16 (2019).

- Drummond and Needs, *Phys. Rev. Lett.* (2009)

- Camjayi,, Haule, Dobrosavljević & Kotliar, *Nat Phys* **4**, 932–935 (2008).

\* a Mott-Wigner-polaronic state in 1T-TaS<sub>2</sub>

**OPEN** Modeling of networks and globules of charged domain walls observed in pump and pulse induced states

Petr Karpov<sup>1</sup> & Serguei Brazovskii<sup>1,2,3</sup>

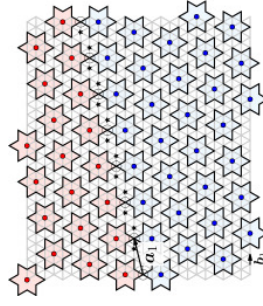
<sup>1</sup>23 November 2017  
<sup>2</sup>...  
<sup>3</sup>...

Charged lattice gas model with only Coulomb interactions

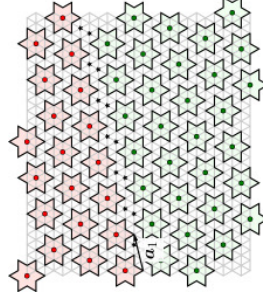
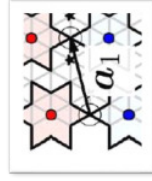
$$H = \sum_{i,j} U_{ij} n_i n_j,$$

Thomas-Fermi screening:

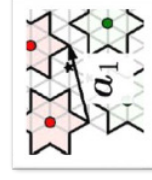
$$U_{ij} = e^2 \frac{\exp(-r/l_s)}{|\mathbf{r}_i - \mathbf{r}_j|} ;$$



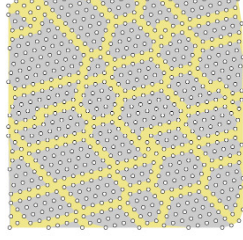
(a)  $q = +e/13$



(b)  $q = +2e/13$



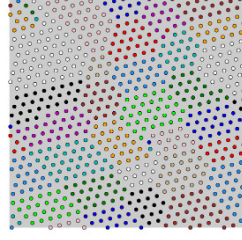
MC simulations Experiment



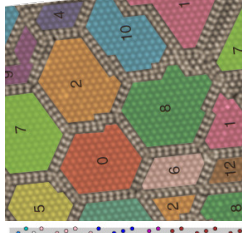
(a)  $N_v = 17$  voids,  $\nu_v = 2.3\%$  - domain walls



(b)



(c)  $N_v = 17$  voids,  $\nu_v = 2.3\%$



(d)

# MC simulation of Polaronic Wigner crystals

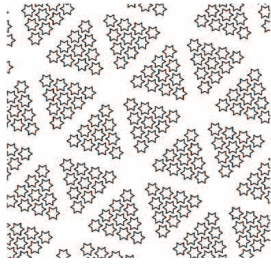
Charged lattice gas model with screened coulomb interaction:

$$\mathcal{H} = \sum_{i < j} V(i, j) n_i n_j,$$

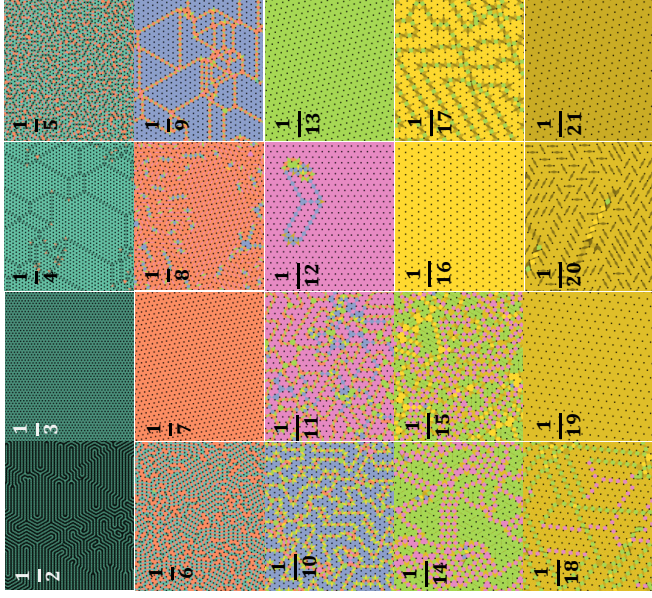
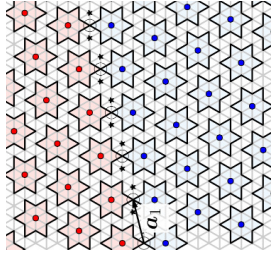
where

$$V(i, j) = V_0 \frac{\exp(-r_{ij}/r_s)}{r_{ij}}$$

Hole-doped



Electron-doped



Magic filling fractions lead to ordered Wigner crystalline phases

System	$f$	Phase
2H-Fe <sub>0.33</sub> TaS <sub>2</sub>	1/3	crystal
1T-TiSe <sub>2</sub>	1/4	crystal
1T-Cu <sub>0.08</sub> TiSe <sub>2</sub>	1/4.2	domain state
2H-Fe <sub>0.33</sub> TaSe <sub>2</sub>	1/4	crystal
2H-Fe <sub>0.33</sub> NbSe <sub>2</sub>	1/4	crystal
2H-TaS <sub>2</sub>	1/9	crystal
2H-TaSe <sub>2</sub>	1/9	crystal
2H-NbSe <sub>2</sub>	~ 1/9	domain state
1T-TaS <sub>2</sub>	1/13	crystal
PD 1T-TaS <sub>2</sub>	1/12.6	domain state
1T-TaSeS	1/12.6	domain state
1T-Ta <sub>0.99</sub> Fe <sub>0.01</sub> S <sub>2</sub>	1/12.6	domain state
1T-Nb <sub>0.04</sub> TaS <sub>2</sub>	~ 1/13	domain state
1T-Nb <sub>0.07</sub> TaS <sub>2</sub>	~ 1/13	domain state
PD 1T-TaS <sub>2</sub>	1/11	amorphous state
1T-Nb <sub>0.1</sub> TaS <sub>2</sub>	~ 1/11	possible amorphous state
4Hb-TaS <sub>2</sub>	1/13	crystal
1T-TaSe <sub>2</sub>	1/13	crystal
1T-Ti <sub>0.07</sub> Ta <sub>0.93</sub> Se <sub>2</sub>	1/12.6	domain state
4Hb-TaSe <sub>2</sub>	1/13	crystal
1T-NbSe <sub>2</sub>	1/13	crystal
1T-VSe <sub>2</sub>	1/16	crystal

Stojchevska et al.,  
Science (2014)

Karpov & Brazovskii,  
Sci Rep (2018).

Vodeb et al., New J. Phys. (2019)

10.1088/1367-2630/ab3057

# Configurational quantum charge liquid

$$\psi = |\text{img1}\rangle + |\text{img2}\rangle + \dots$$

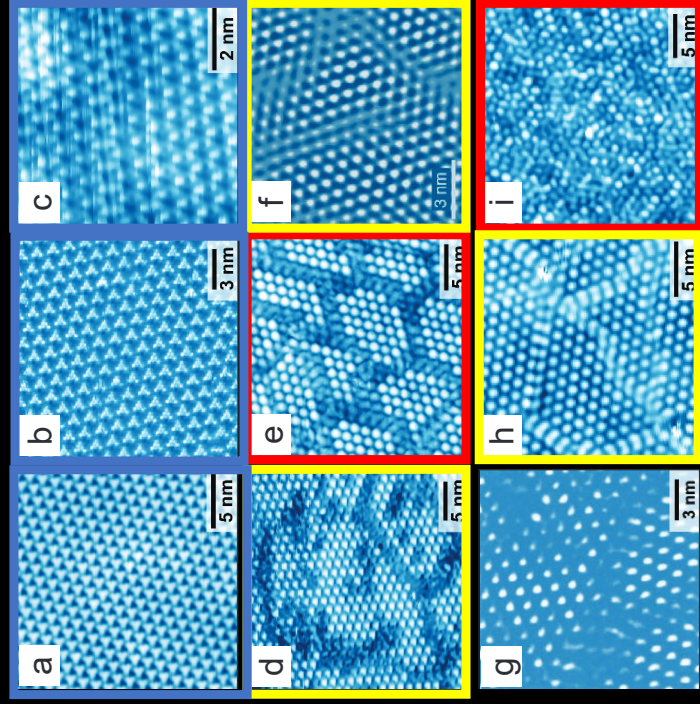
- Domain states are configurationally (nearly) degenerate.<sup>1</sup>
- There is a large configurational entropy
- Which configuration wins is determined by Quantum Darwinism<sup>2</sup>, and interaction with the environment

1. Vodeb et al., *New J. Phys.* (2019)

2. e.g. W. Zurek, *Rev. Mod. Phys.* (2003).

3. Coppersmith et al *Phys. Rev. B* (1982).

# Scanning tunneling microscopy (STM) of some doped and photodoped TMDs



## Legend: Superconductors

Superconductors under pressure

Light-induced metastable

Undoped:  $f_m$  = integer filling fraction

a) 1T-TaS<sub>2</sub> ( $f_m = 1/13$ ),

b) 1T-TaSe<sub>2</sub> ( $f_m = 1/13$ )

c) 1T-TiSe<sub>2</sub> ( $f_m = 1/4$ ).

Doped:  $f_m$  in between integer filling fractions

d) 1T-Ta<sub>0.99</sub>Fe<sub>0.01</sub>S<sub>2</sub> ( $f \approx 1/12.6$ ),

e) photodoped 1T-TaS<sub>2</sub> (fluence  $F \approx 1 \text{ mJ/cm}^2$ ,  $f \approx 1/12.6$ ),

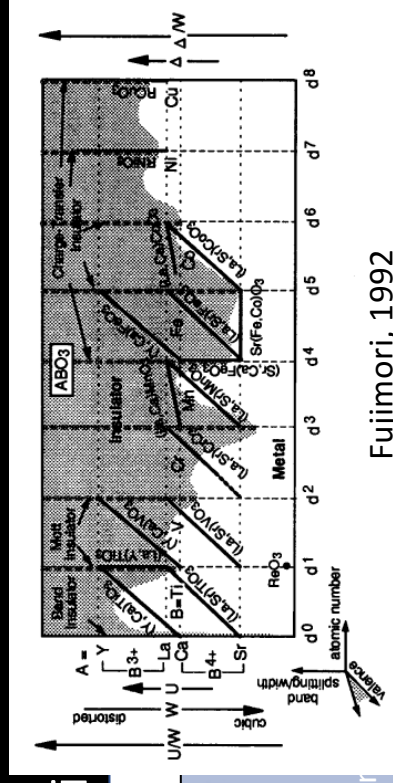
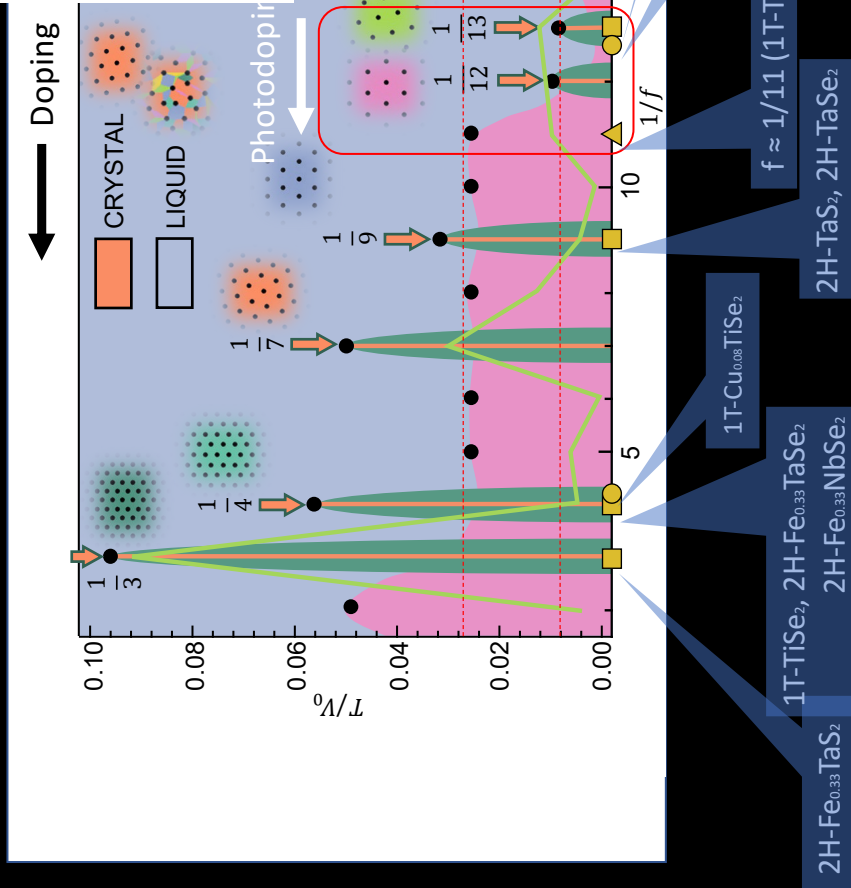
f) 1T-Cu<sub>0.08</sub>TiSe<sub>2</sub> ( $f \approx 1/4.2$ ),

g) 1T-Ti<sub>0.07</sub>Ta<sub>0.93</sub>Se<sub>2</sub> ( $f \approx 1/12.6$ )

h) 1T-TaSeS ( $f \approx 12.6$ ).

i) glassy state in photodoped metastable 1T-TaS<sub>2</sub>

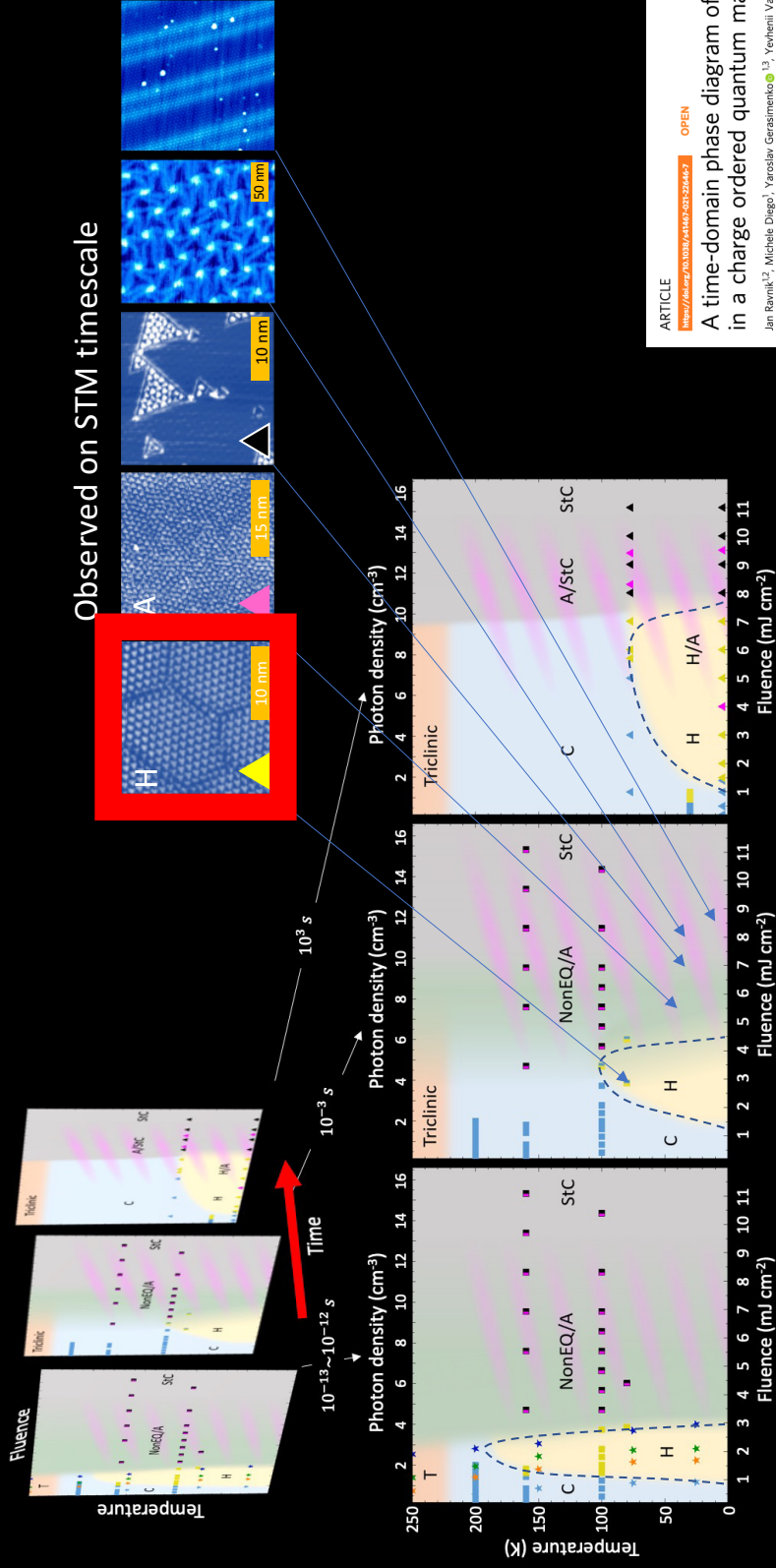
# Phase diagram of Wigner crystals in Transition Metals



Fujimori, 1992

Vodeb et al, *New J. Phys.*, (2019)

# A time-domain phase diagram in 1T-TaS<sub>2</sub>



ARTICLE

OPEN

<https://doi.org/10.1038/s41467-021-23223-7>

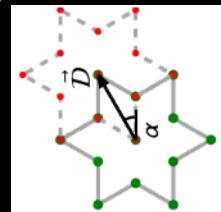
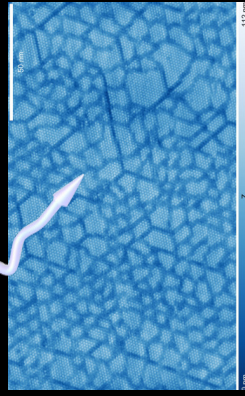
A time-domain phase diagram of metastable states in a charge ordered quantum material

Jan Ravnik<sup>1,2</sup>, Michele Diogo<sup>1</sup>, Yaroslav Gerasimenko<sup>1,3</sup>, Yevhenii Vaskivskiy<sup>1</sup>, Igor Vaskivskiy<sup>1,3</sup>, Tomaz Mertelj<sup>1,3</sup>, Jaka Vodeb<sup>1</sup> & Dragan Mihailovic<sup>1,3,4</sup>

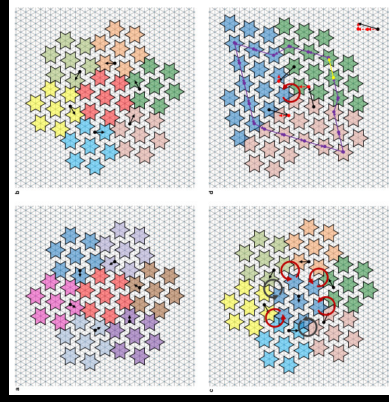
NATURE COMMUNICATIONS | (2021)12:23223 |



# The photoinduced hidden state: chiral domain order



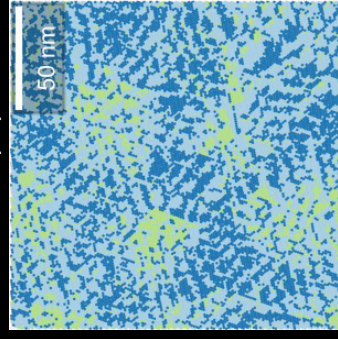
Displacement vector  $\vec{D}$  between adjacent domains



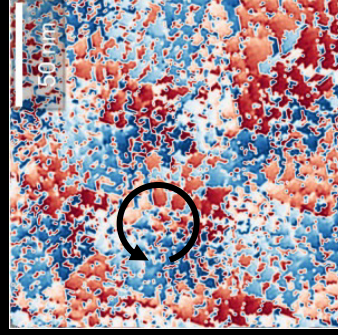
Experimental STM data

Displacement distance  $|\vec{D}|$

$\alpha$

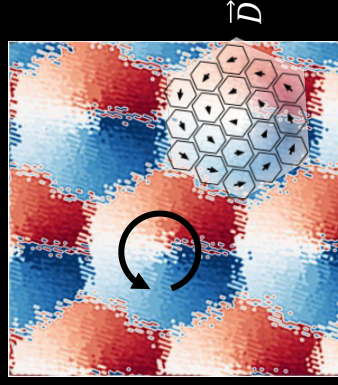


0 a  $a\sqrt{3}$   
 $\vec{D}$ , atomic units



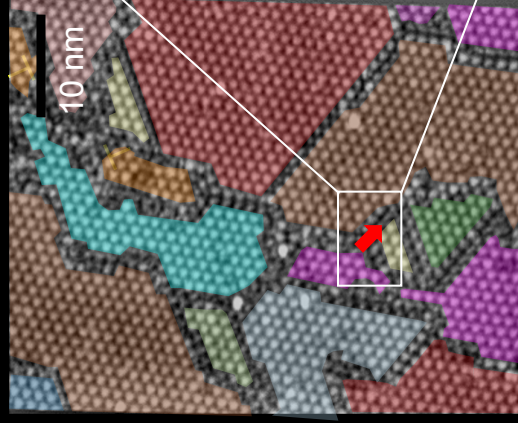
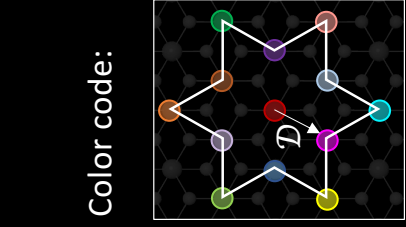
-180 0 180  
Direction  $\alpha$ , deg.

Simulation of  $\alpha$

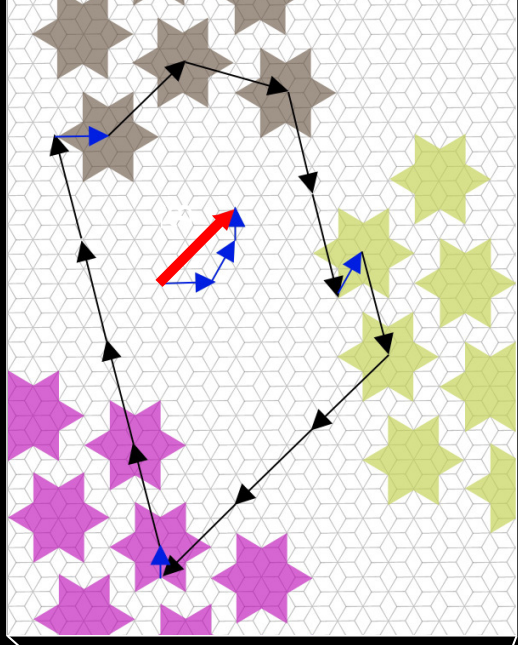


$\vec{D}$

# Topologically non-trivial vertices in the 'hidden' state

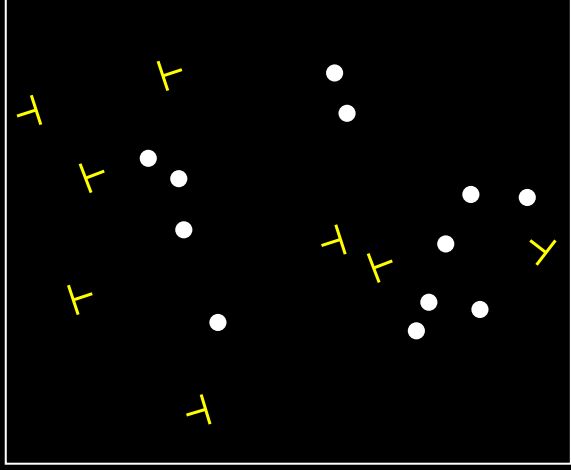
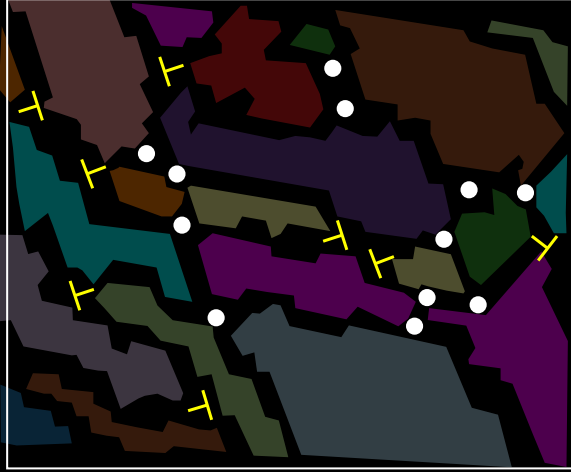
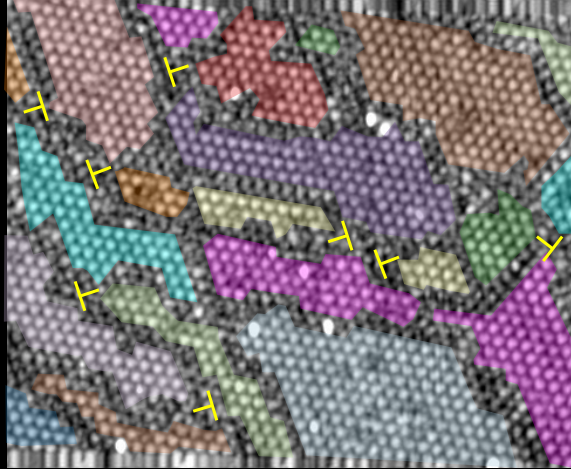


Burgers' vector constructions



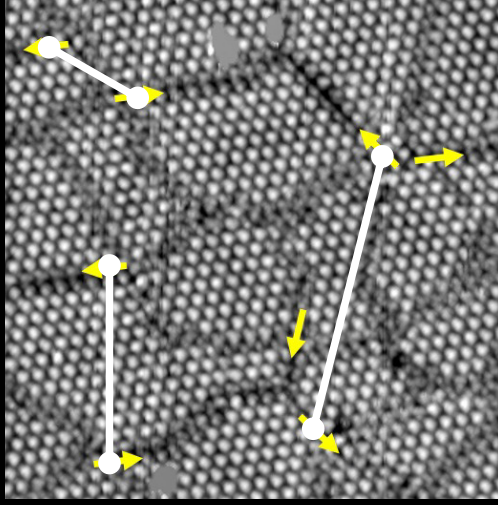
The H state has topologically protected defects where  $\vec{B} \neq 0$

# Vertices as dislocations



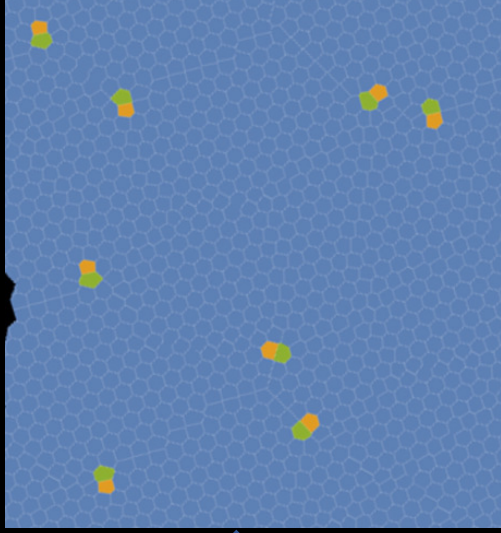
# Wigner-Seitz cell constructions of the CDW superlattice: Charge is associated with $B \neq 0$ defects

STM image of H state



Burgers vectors

Wigner-Seitz construction of H state



Disclinations



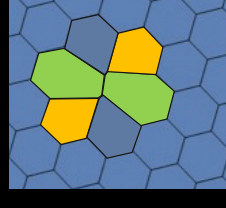
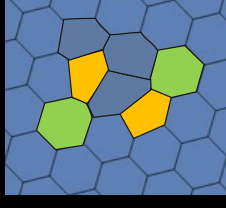
Dislocations



Add 1 electron:



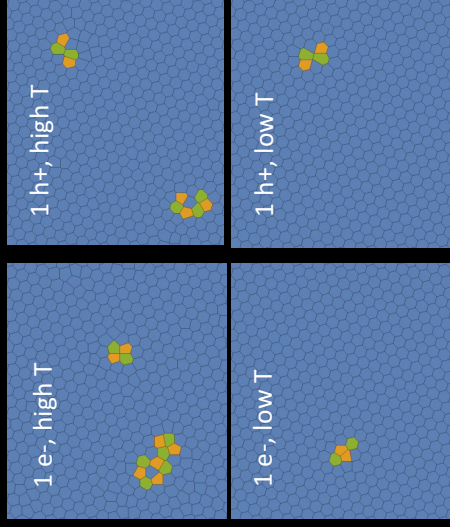
Add 1 hole:



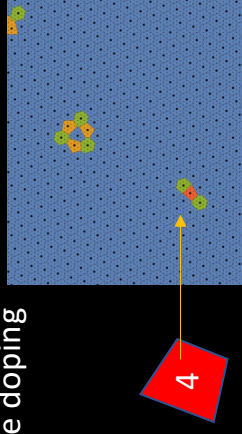
# CLG Monte Carlo simulation and experiment (Wigner-Seitz constructions)

MC calculation of a polaronic Wigner crystal (CLG)

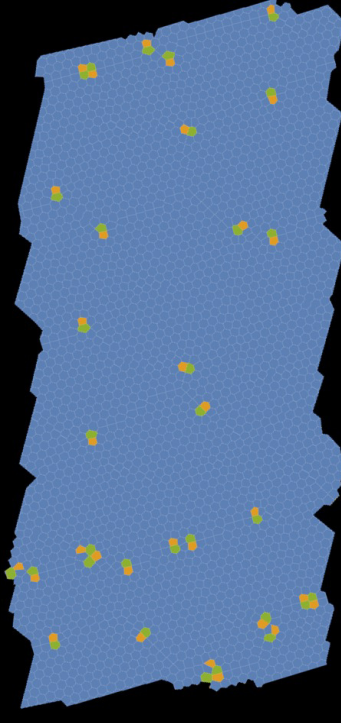
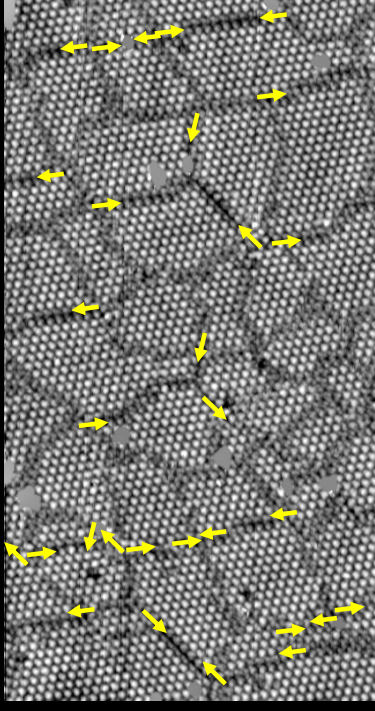
Single particle doping



Multiple particle doping



STM of H state (4K)

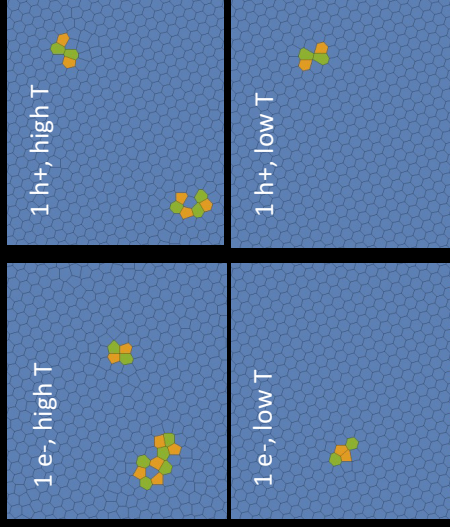


Experiments show that the electrons are topologically entangled objects.

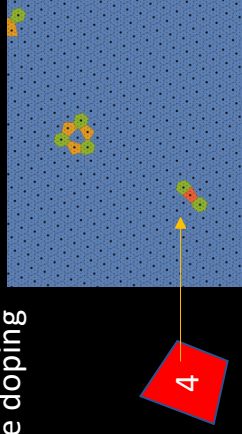
# CLG Monte Carlo simulation and experiment (Wigner-Seitz constructions)

MC calculation of a polaronic Wigner crystal (CLG)

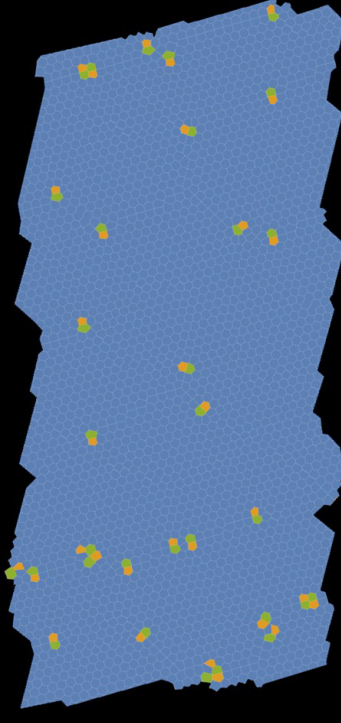
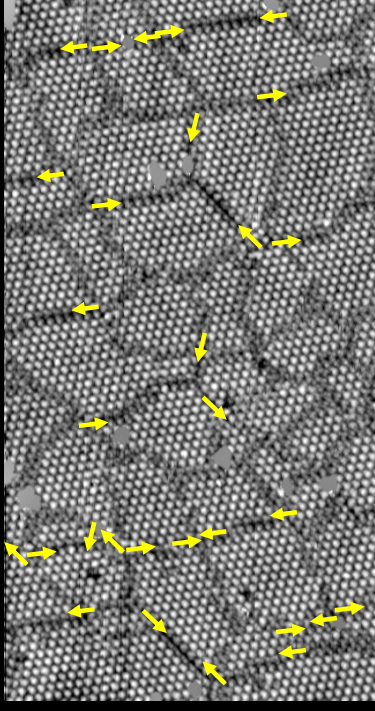
Single particle doping



Multiple particle doping

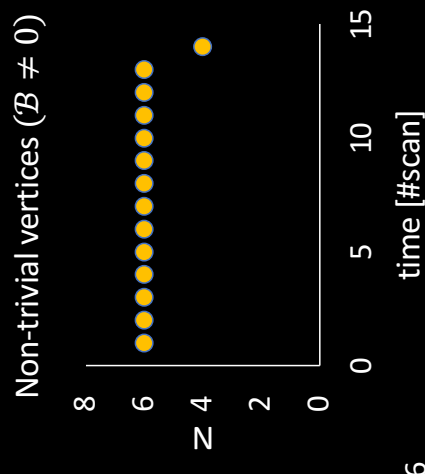
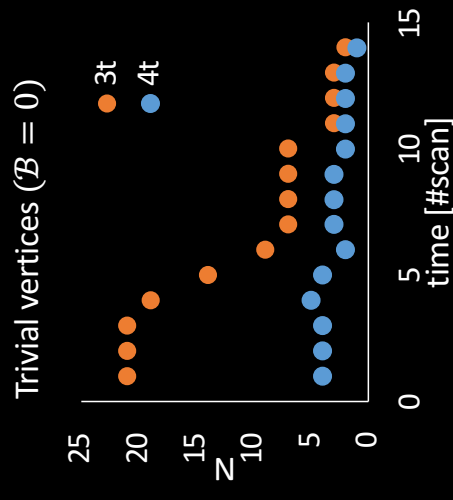
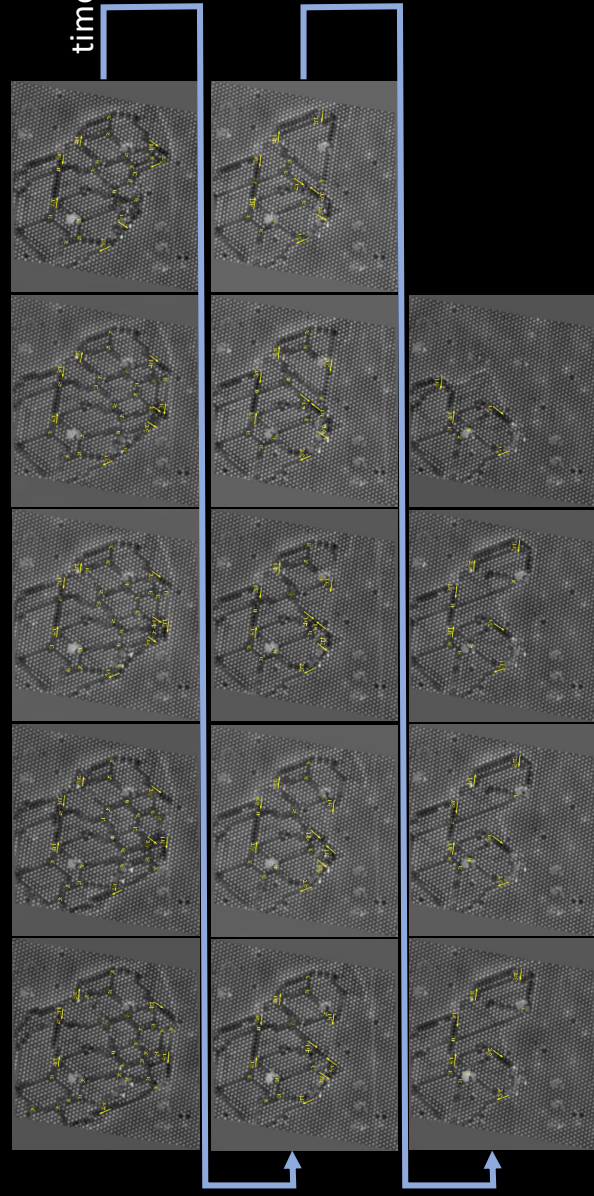


STM of H state (4K)



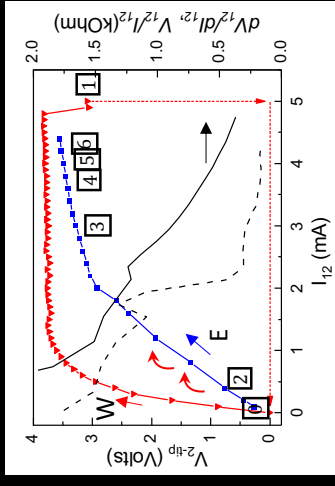
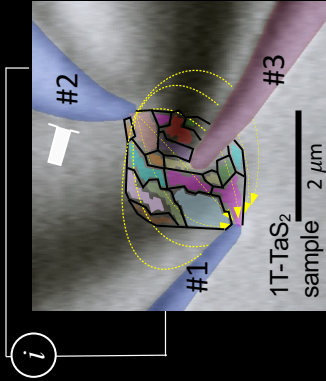
Experiments show that the electrons are topologically entangled objects.

# Defect dynamics: spontaneous relaxation through configurational states

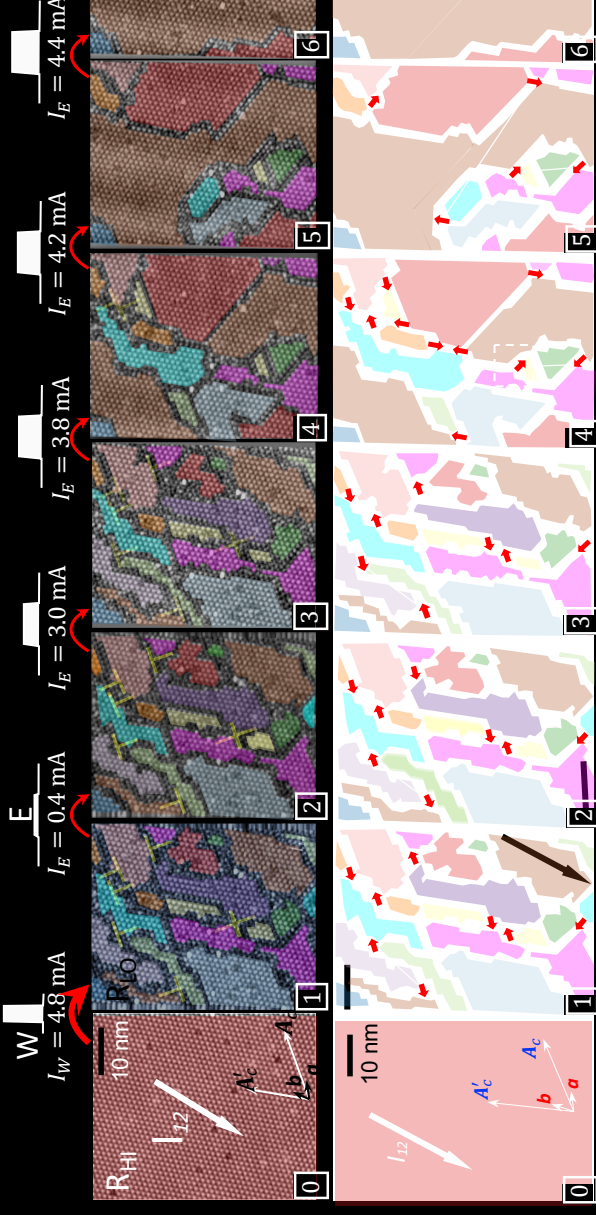
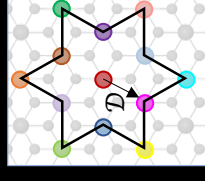


Conclusion: Topologically non-trivial defects stabilize the 'hidden' domain state

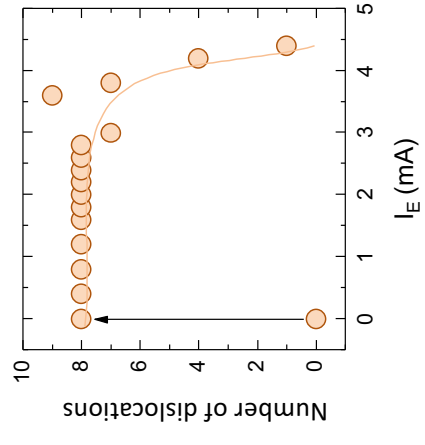
# Defect dynamics under applied electric field



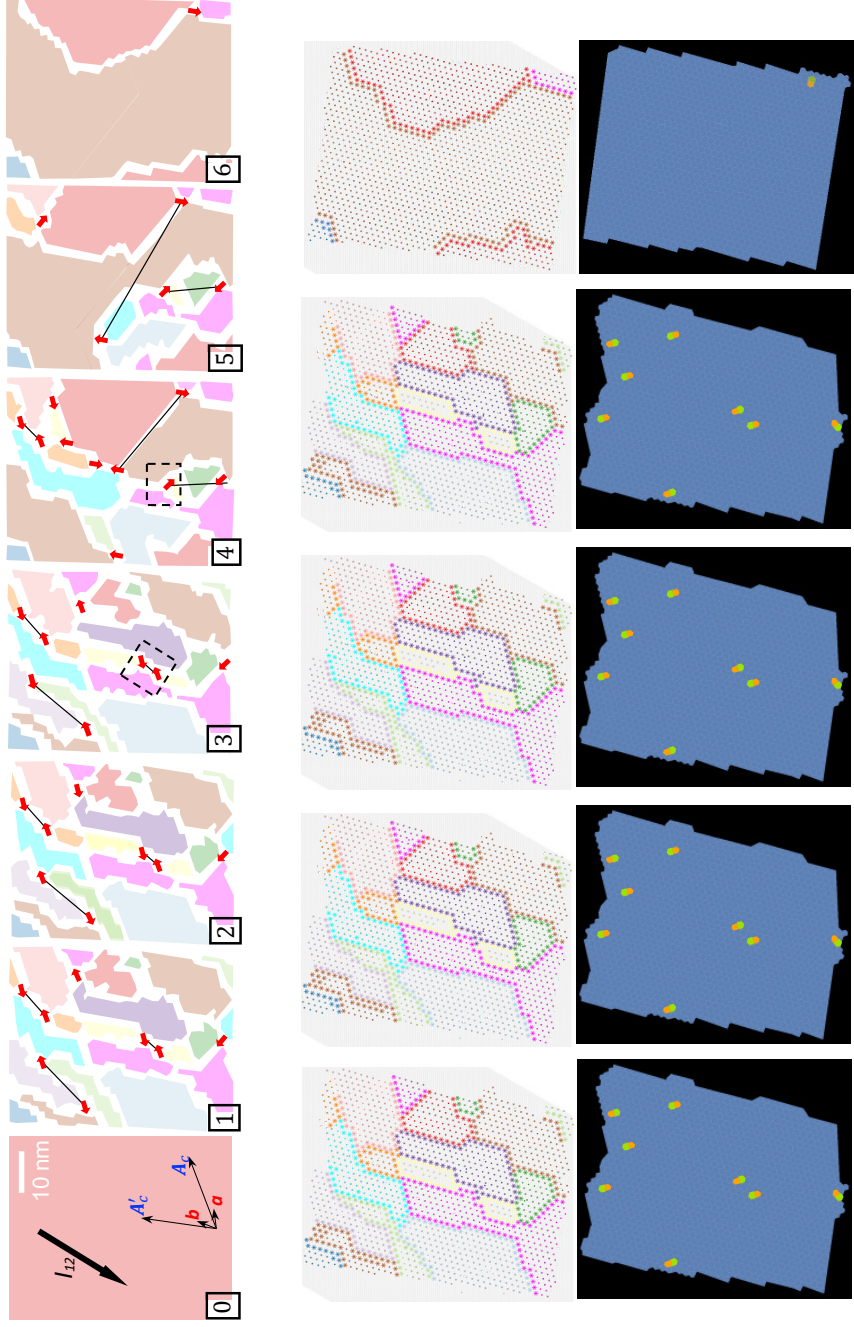
Displacement vectors: colour code



Non-trivial defect annihilation

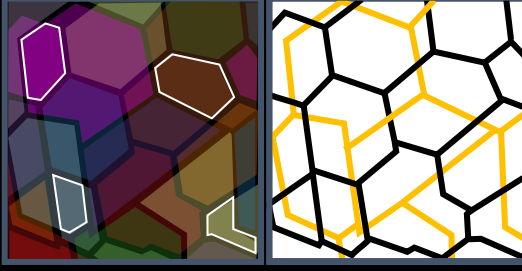






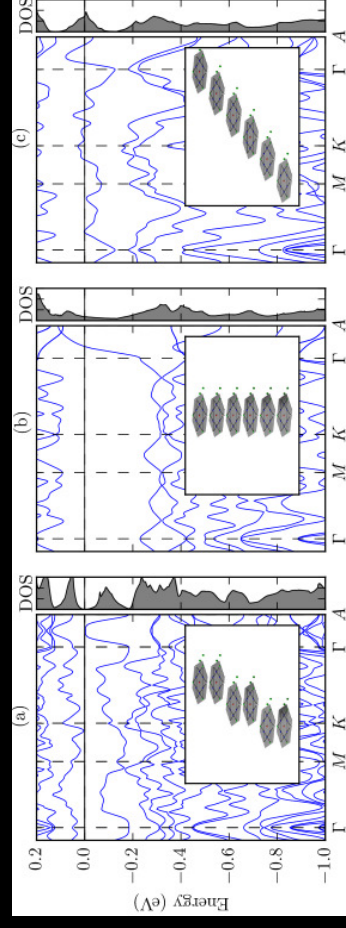
# Interlayer ordering

Occasionally, the CDWs are stacked without a phase shift



From experiment

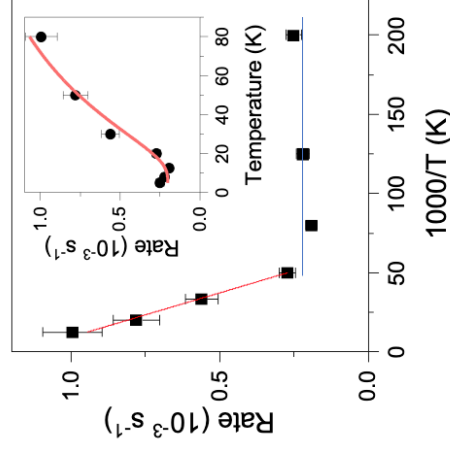
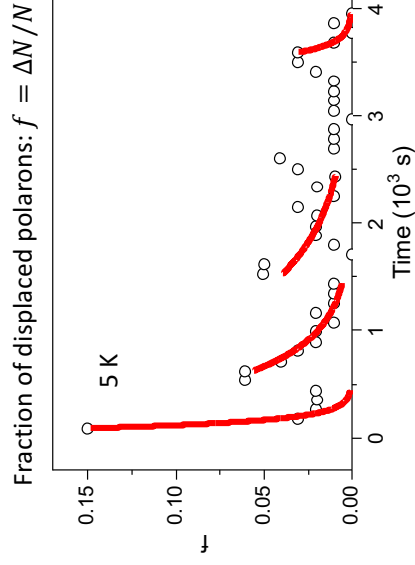
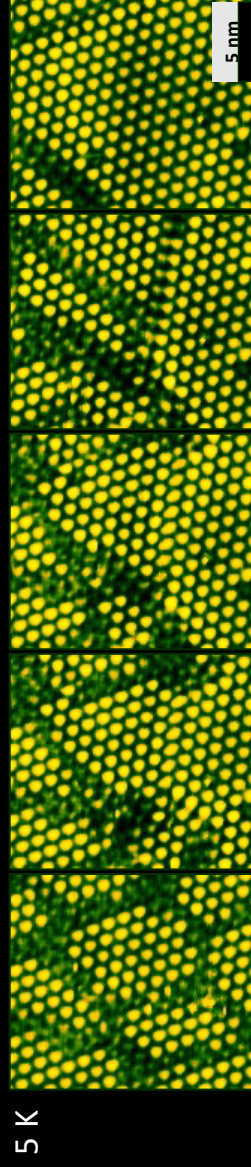
Band structure calculations



1. Butler, C. J., Yoshida, M., Hanaguri, T. & Iwasa, Y. Mottness versus unit-cell doubling as the driver of the insulating state in 1T-TaS<sub>2</sub>. *Nat Commun* **11**, 2477 (2020).
2. Stahl, Q. *et al.* Collapse of layer dimerization in the photo-induced hidden state of 1T-TaS<sub>2</sub>. *Nat Commun* **11**, 1–7 (2020).
3. Ritschel, T., Berger, H. & Geck, J. Stacking-driven gap formation in layered 1T-TaS<sub>2</sub>. *Phys Rev B* **98**, 1–8 (2018).

# Quantum tunneling between configurational states

time →



Total relaxation rate (fit):

$$R(T) = R_q + R_0 \exp\left(-\frac{E_B}{k_B T}\right)$$

Quantum tunneling Activated hopping

WKB estimate of the tunneling rate

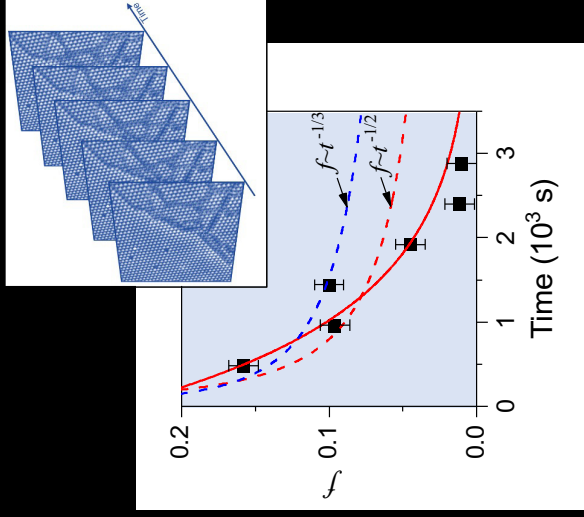
$$R_q = \nu \exp\left(-2W\sqrt{2m^*E_b}/\hbar^2}\right)$$

For a 1000 electron domain,

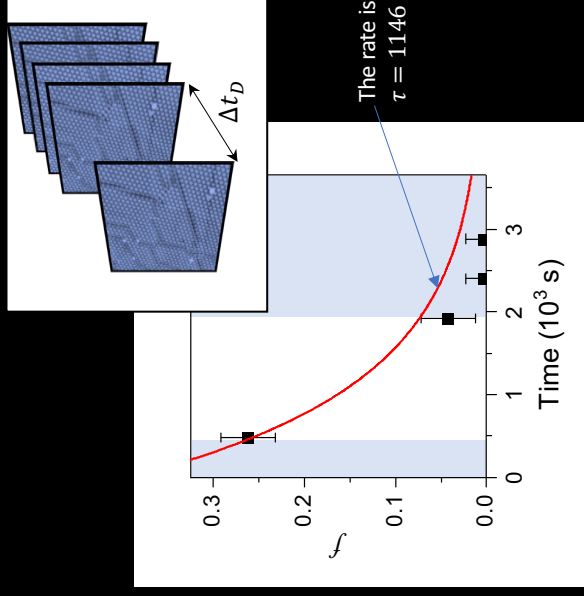
$$R_q = 2.2 \pm 0.3 \times 10^{-4} \text{ s}^{-1} \text{ (reasonable)}$$

# Tip-enhanced relaxation?

Relaxation **with** tip scanning



Relaxation with **NO** tip scanning

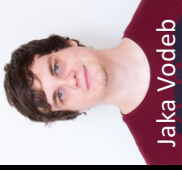


The rate is similar: a fit gives  $\tau = 1146 \pm 38$  s (for both)



Schroedinger's cat measurements

# D-wave annealing (direct embedding)



Jaka Vodeb

Quantum annealing using the transverse field Ising model:

$$H = -\frac{A(s)}{2} \left( \sum_i \sigma_i^x \right) + \frac{B(s)}{2} \left( \sum_i h_i \sigma_i^z + \sum_{i>j} J_{i,j} \sigma_i^z \sigma_j^z \right)$$

Annealing protocol:

$$H = -AH_x + BH_z$$

$$Z = \text{Tr}(\exp(-\beta H))$$

$$\beta H = \beta A \left( -H_x + \frac{B}{A} H_z \right)$$

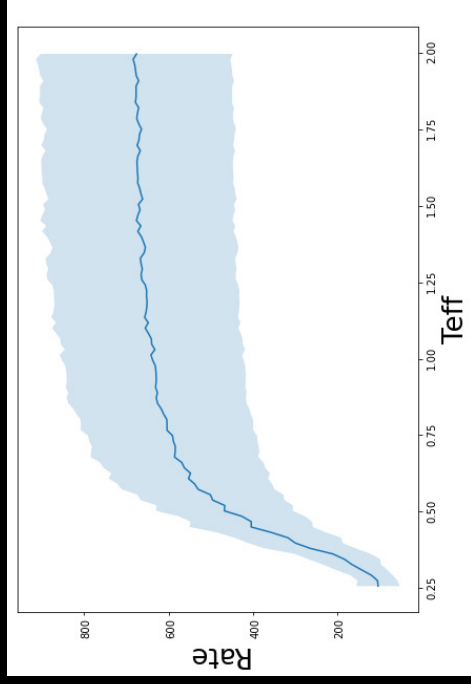
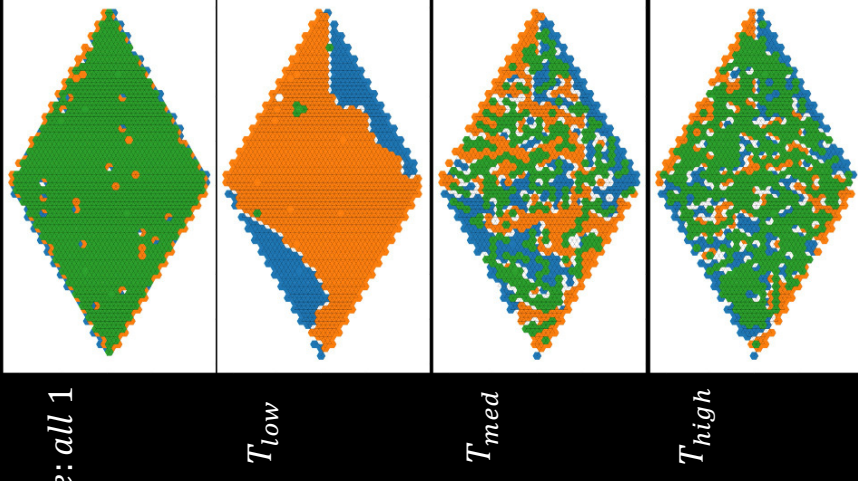
$$\frac{A}{k_B T} = \frac{1}{T_{eff}} \quad T_{eff} = \frac{k_B T}{A}$$

Temperature scale:

$$T = 16 \text{ mK}$$

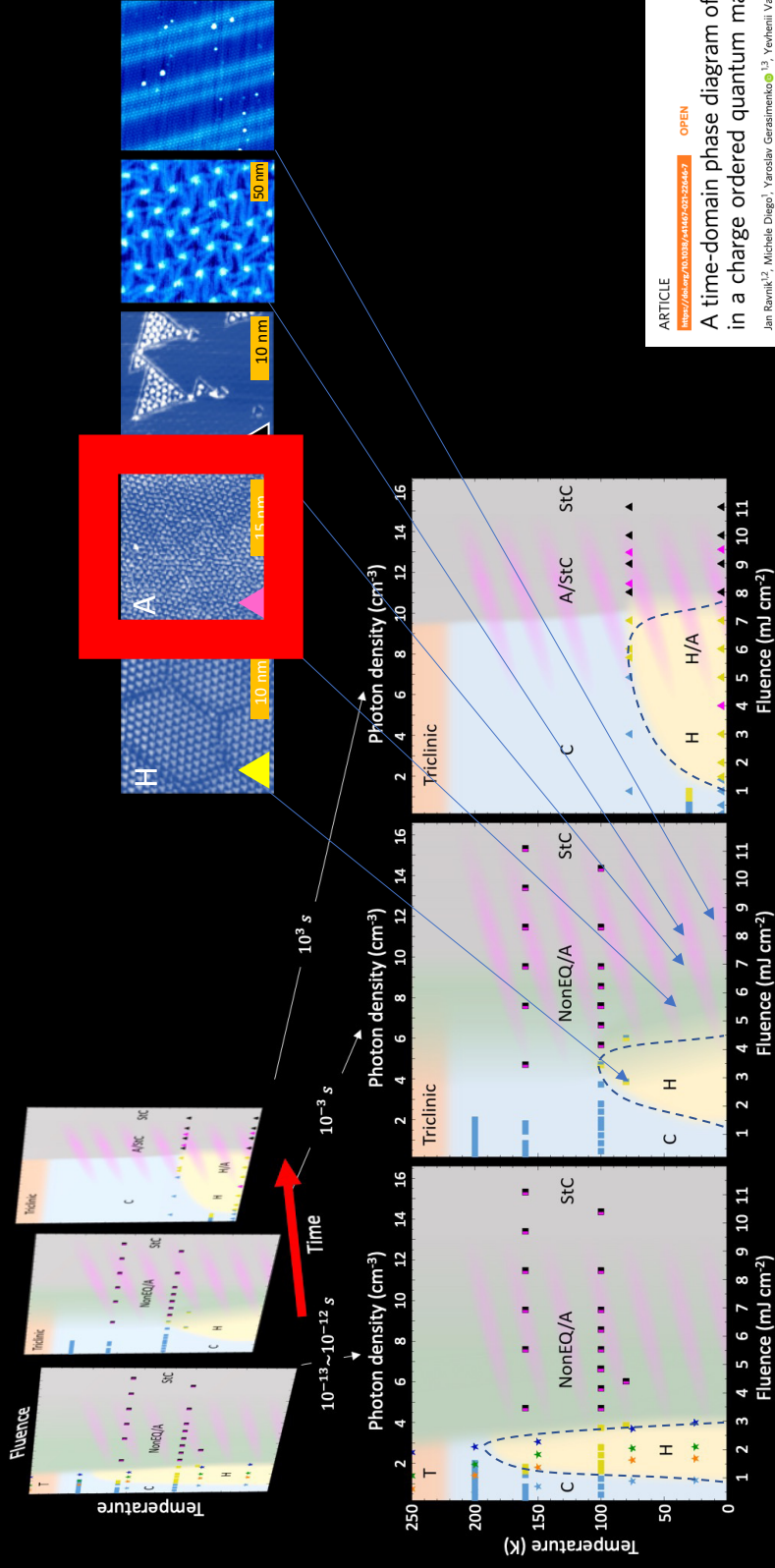
$$k_B T = 1.38 \pm 0.01 \text{ } \mu\text{eV}$$

Initial state: all 1



J. Vodeb et al., unpub. (2022)

# A time-domain phase diagram in 1T-TaS<sub>2</sub>



ARTICLE

OPEN

<https://doi.org/10.1038/s41467-021-23223-7>

A time-domain phase diagram of metastable states in a charge ordered quantum material

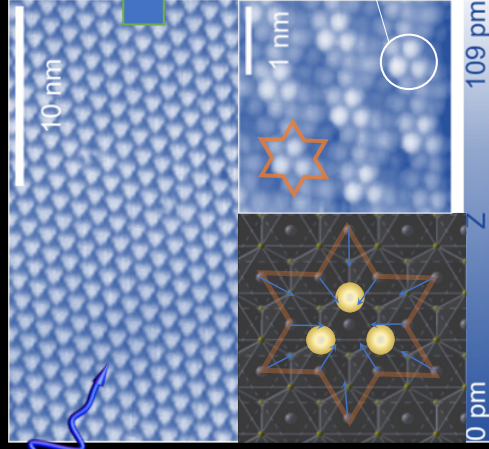
Jan Ravnik<sup>1,2</sup>, Michele Diogo<sup>1</sup>, Yaroslav Gerasimenko<sup>1,3</sup>, Yevhenii Vaskivskiy<sup>1</sup>, Igor Vaskivskiy<sup>1,3</sup>, Tomaz Mertelj<sup>1,3</sup>, Jaka Vodeb<sup>1</sup> & Dragan Mihailovic<sup>1,3,4</sup>

NATURE COMMUNICATIONS | (2021)12:23223 |

# Jamming transition to an amorphous Wigner glass

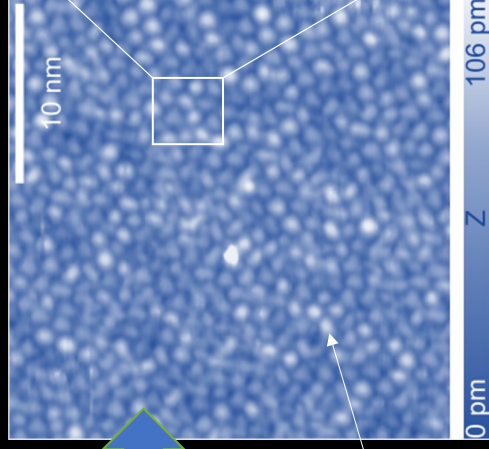
$$2.5 \sim 3 \text{ mJ}/\text{cm}^2$$

Initial C state



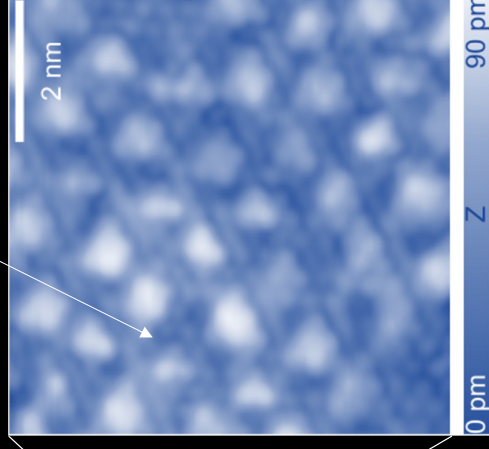
4K

Amorphous (jammed) Wigner state



Low resolution image

Atomic lattice

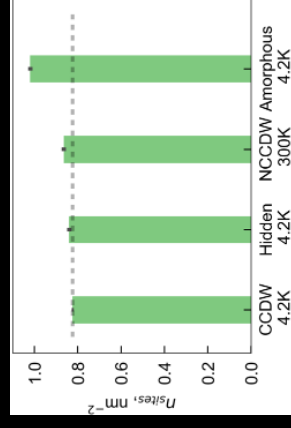


High resolution image



Gerashimko, et al.  
*Nature Materials* (2019)

Localized electron density ( $\text{nm}^{-2}$ )



# Hyperuniformity and jamming transitions

Classical jamming

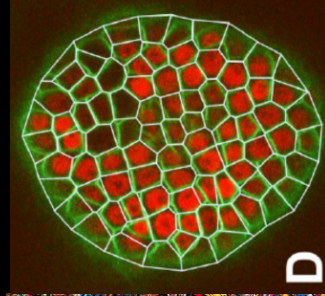
Pebbles



Kayak jam



Plant cells



Number variance in simple **random** systems:

$$\sigma_N^2(R) \sim R^d, \quad \text{where } d=\text{dimensionality}$$

Number variance in **hyperuniform** systems, for  $R \rightarrow \infty$ :

$$\sigma_N^2(R) \sim \begin{cases} R^{d-1}, & \alpha > 1, \\ R^{d-1} \ln R, & \alpha = 1, \\ R^{d-\alpha}, & 0 < \alpha < 1. \end{cases} \quad (R \rightarrow \infty).$$

Structure factor in hyperuniform systems :

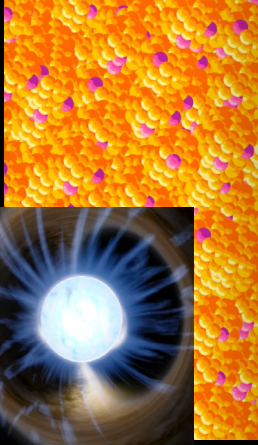
Definition of  $\alpha$  :  $\lim_{|k| \rightarrow 0} S(\mathbf{k}) = 0$

$$S(k) \sim |k|^\alpha$$

Traffic jams



Neutron stars?

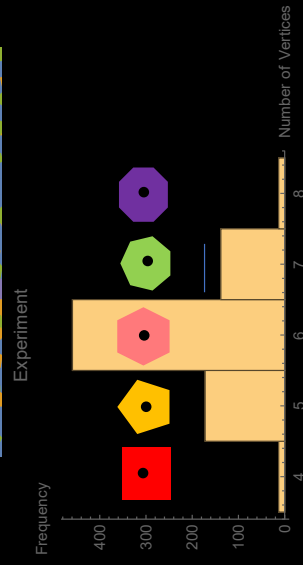
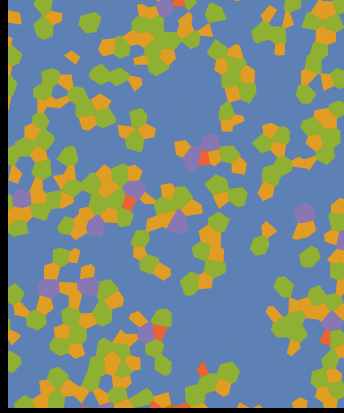


Torquato, S. Hyperuniformity and its generalizations.  
*Physical Review E* **94**, 022122 (2016).

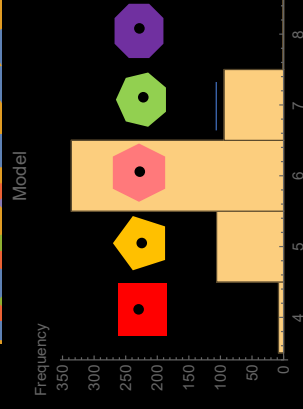
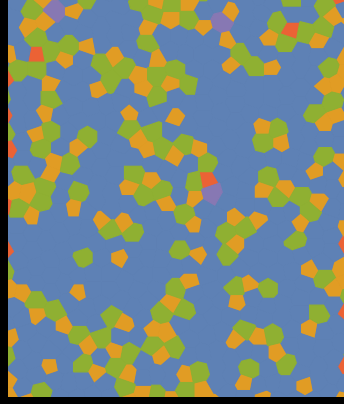


# CLG model prediction of the N-gon statistics in the amorphous (A) phase

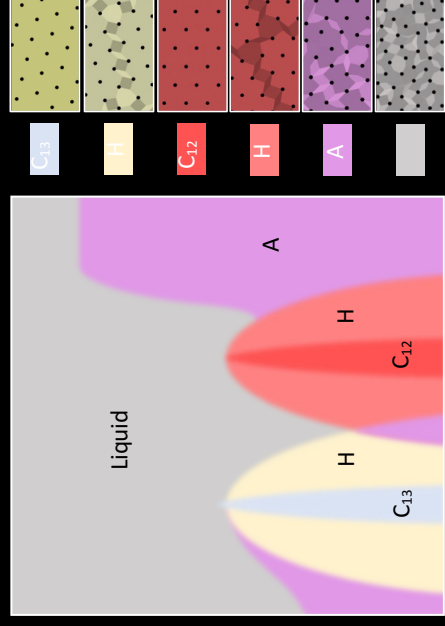
Experiment  
(STM, 4K,  
2 mJ/cm<sup>2</sup>)



CLG model  
calculation  
(MC  
simulation)



MC Simulations



Jaka Vodeb, unpub. work

# Can the *quantum* dynamics be described in terms of fractons?

PHYSICAL REVIEW LETTERS 120, 195301 (2018)

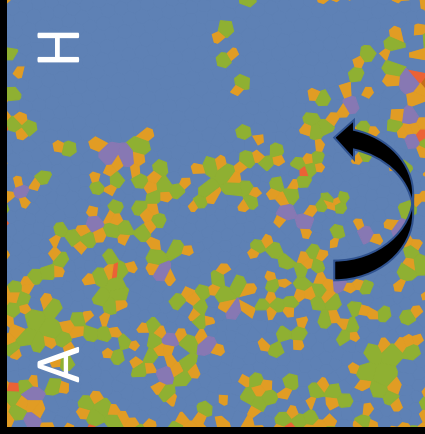
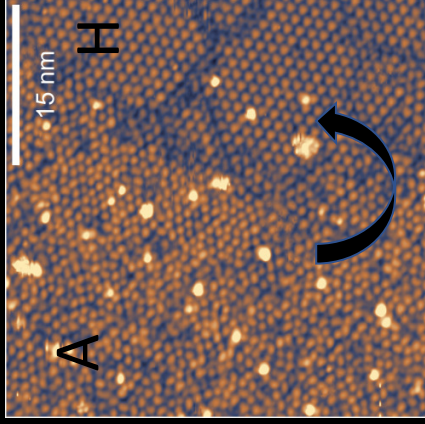
Editors' Suggestion

Featured in Physics

## Fracton-Elasticity Duality

Michael Pretko and Leo Radzihovsky  
 Department of Physics and Center for Theory of Quantum Matter, University of Colorado, Boulder, Colorado 80309, USA

“The conservation laws of fracton gauge theories provide a convenient and systematic tool for encoding and analyzing the dynamics of crystal defects.”

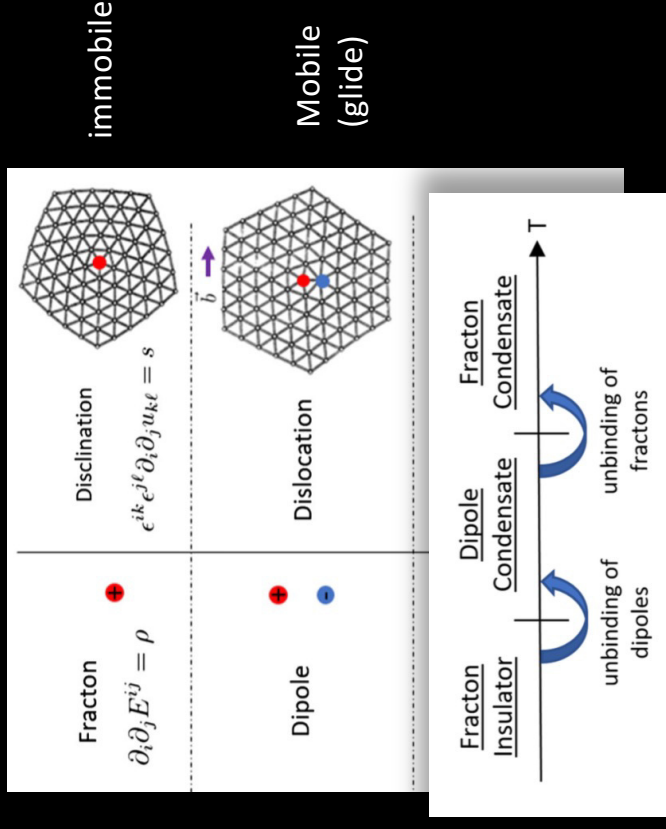


PHYSICAL REVIEW B 92, 235136 (2015)

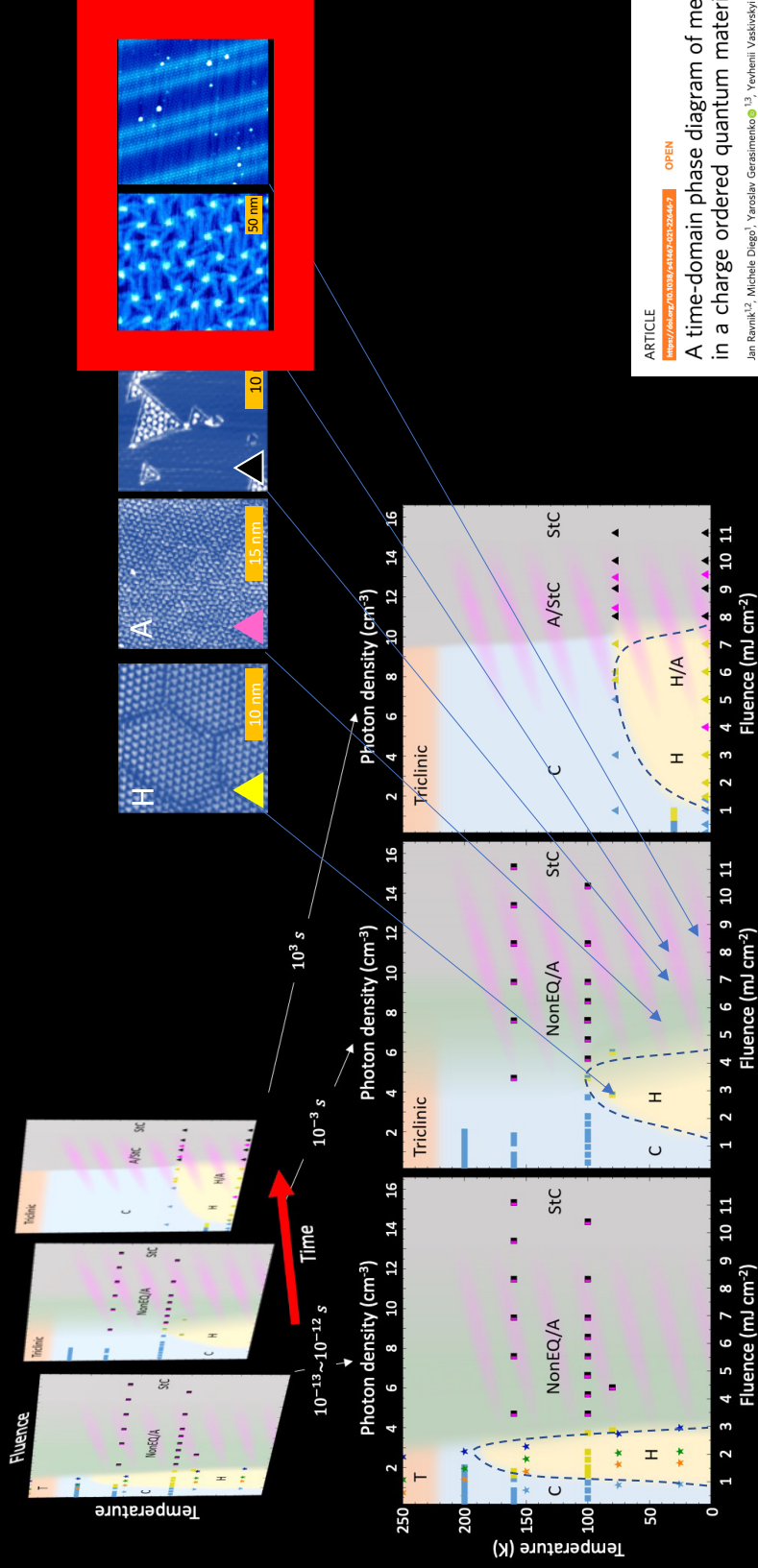


## A new kind of topological quantum order: A dimensional hierarchy of quasiparticles built from stationary excitations

Sagar Vijay, Jeongwan Haah, and Liang Fu



# A time-domain phase diagram in 1T-TaS<sub>2</sub>



ARTICLE

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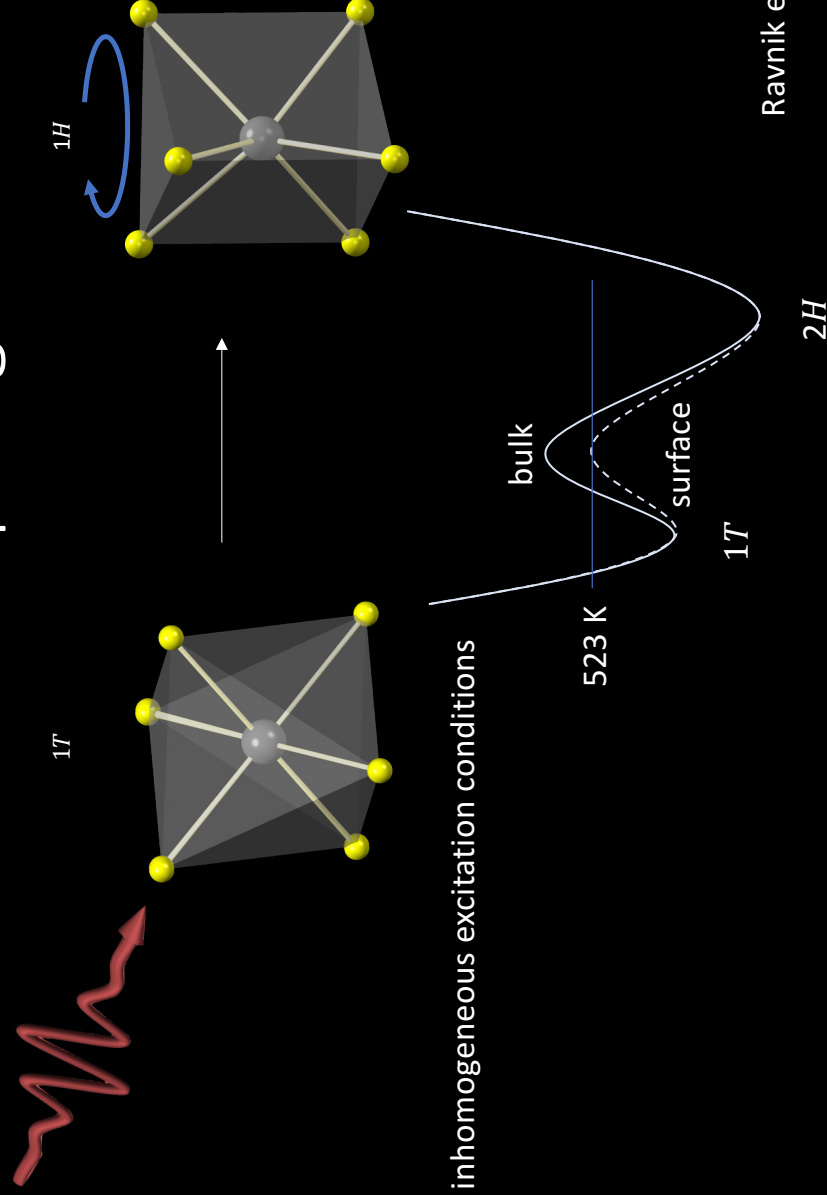
<https://doi.org/10.1038/s41467-021-23223-7>

A time-domain phase diagram of metastable states in a charge ordered quantum material

Jan Ravnik<sup>1,2</sup>, Michele Diago<sup>1</sup>, Yaroslav Gerasimenko<sup>1,3</sup>, Yevhenii Vaskivskiy<sup>1</sup>, Igor Vaskivskiy<sup>1,3</sup>, Tomaz Mertelj<sup>1,3</sup>, Jaka Vodeb<sup>1</sup> & Dragan Mihailovic<sup>1,3,4</sup>

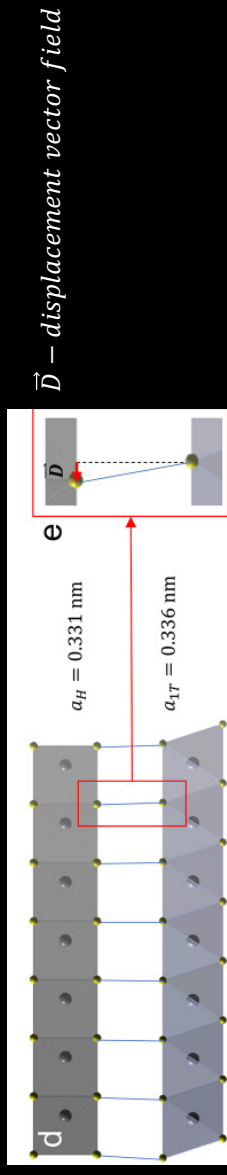
NATURE COMMUNICATIONS | (2021)12:23223 |

# Light-induced single-layer polytype transformation – topological CDWs



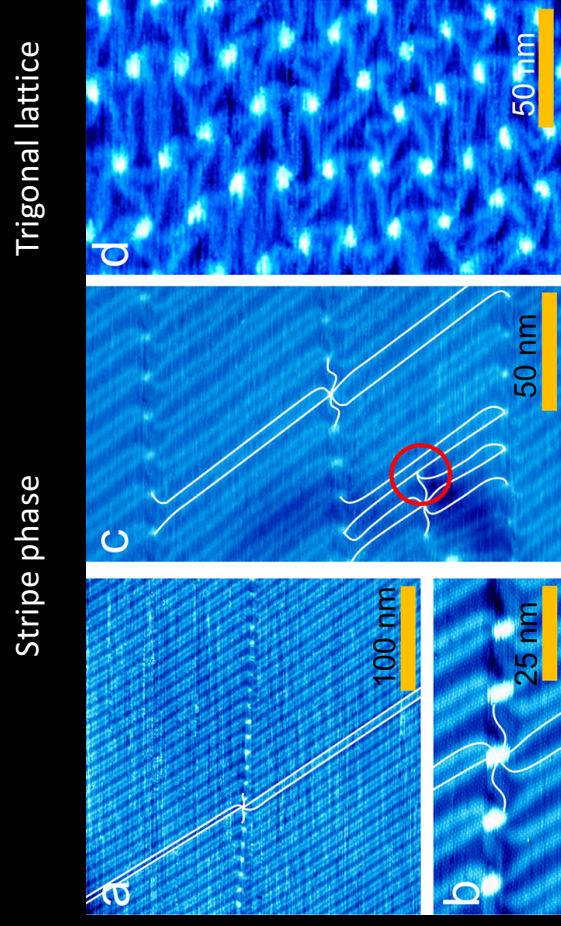
Ravnik et al., ACS Nano materials (2019)

# Light-induced 1H-1T heterostructure of TaS<sub>2</sub>



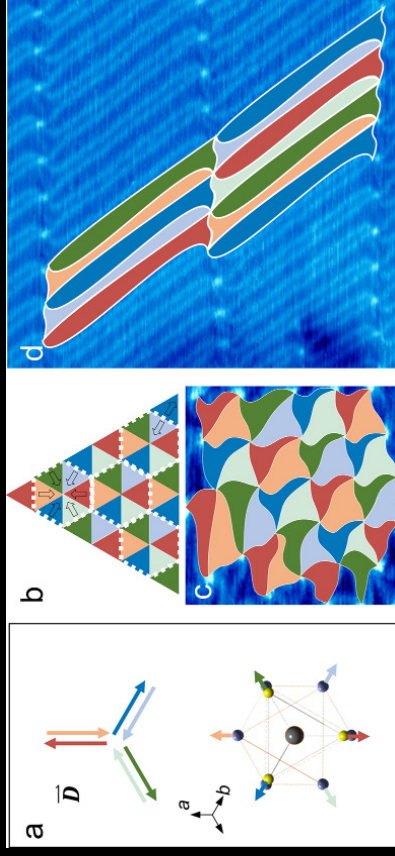
We may expect the charge density wave to adapt to the Moiré pattern (or discommensurations)

# Topological charge density wave patterns of a 1H/1T-TaS<sub>2</sub> bilayer



Ravnik et al., *ACS Applied Nano materials* 2, 3743 (2019)

# Topology of the Moiré electron density map of a 1H/1T-TaS<sub>2</sub> bilayer.



The topology of the CDW is described by the cyclic group  $Z_k$ :

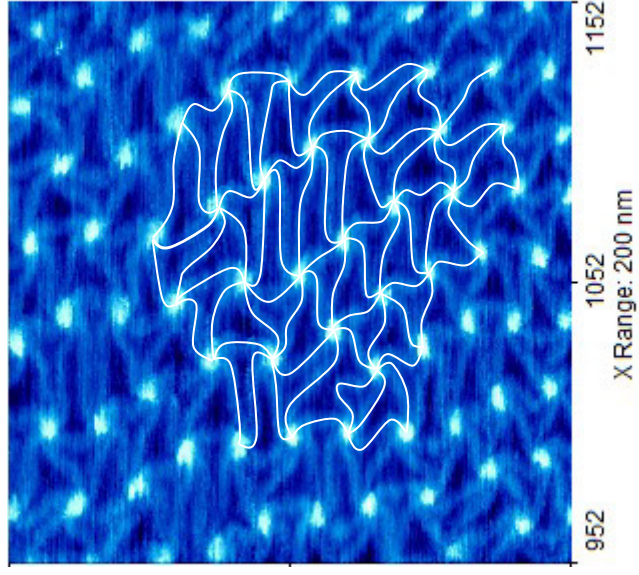
$$Z_6 = Z_3 \times Z_2$$

$Z_n = 2$  the number of possible antiphase domains (colour map)

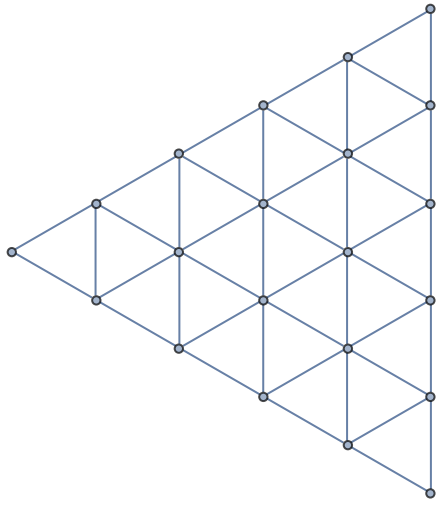
----- Antiphase domain boundaries

$Z_m = 3$  the number  $m$  of directional variants of  $\vec{D}$  (arrows)

# Topology: a triangular density wave network

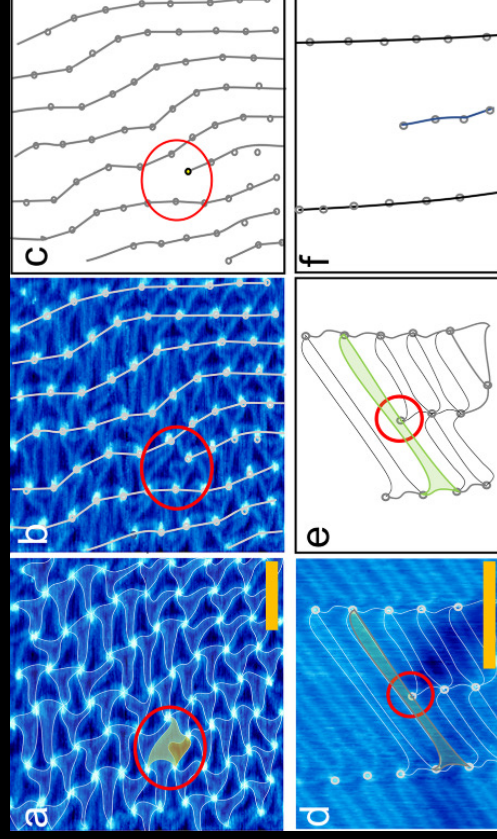


No visible symmetry





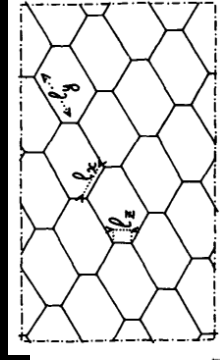
# Topological defects: dislocations in electron density maps of a 1H/1T-TaS<sub>2</sub> bilayer.



Dislocations in the electronic density wave pattern

Ravnik et al., *ACS Applied Nano materials* 2, 3743 (2019)

# Phase diagram of a discommensurate 2D honeycomb network



Surface Science 97 (1980) 219–242  
 © North-Holland Publishing Company

## COMMENSURATE–INCOMMENSURATE TRANSITION OF KRYPTON MONOLAYERS ON GRAPHITE: A LOW TEMPERATURE THEORY

Jacques VILLAIN

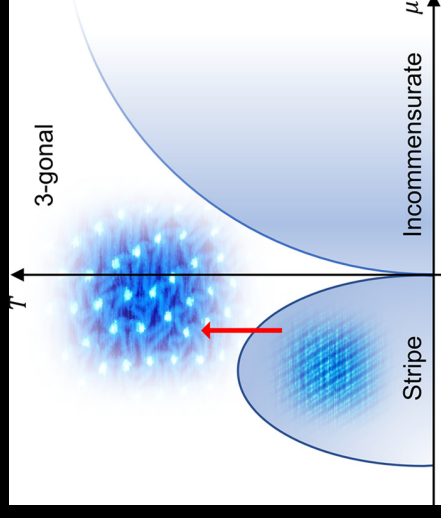
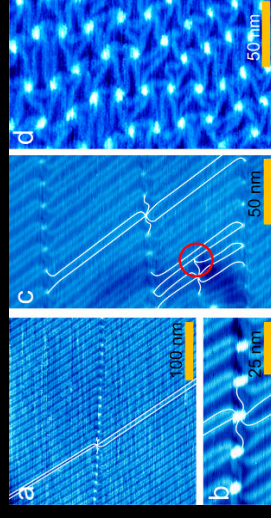
Département de Recherche Fondamentale, Laboratoire de Diffraction Neutronique, Centre d'Etudes Nucléaires de Grenoble, 85 X, F-38041 Grenoble Cédex, France

Free energy of a discommensured 2D honeycomb network:

$$F = 2\Lambda v + \underbrace{\mu L}_{\text{vertices segment length}} - T \underbrace{\log G(g, L)}_{\text{entropy}}$$

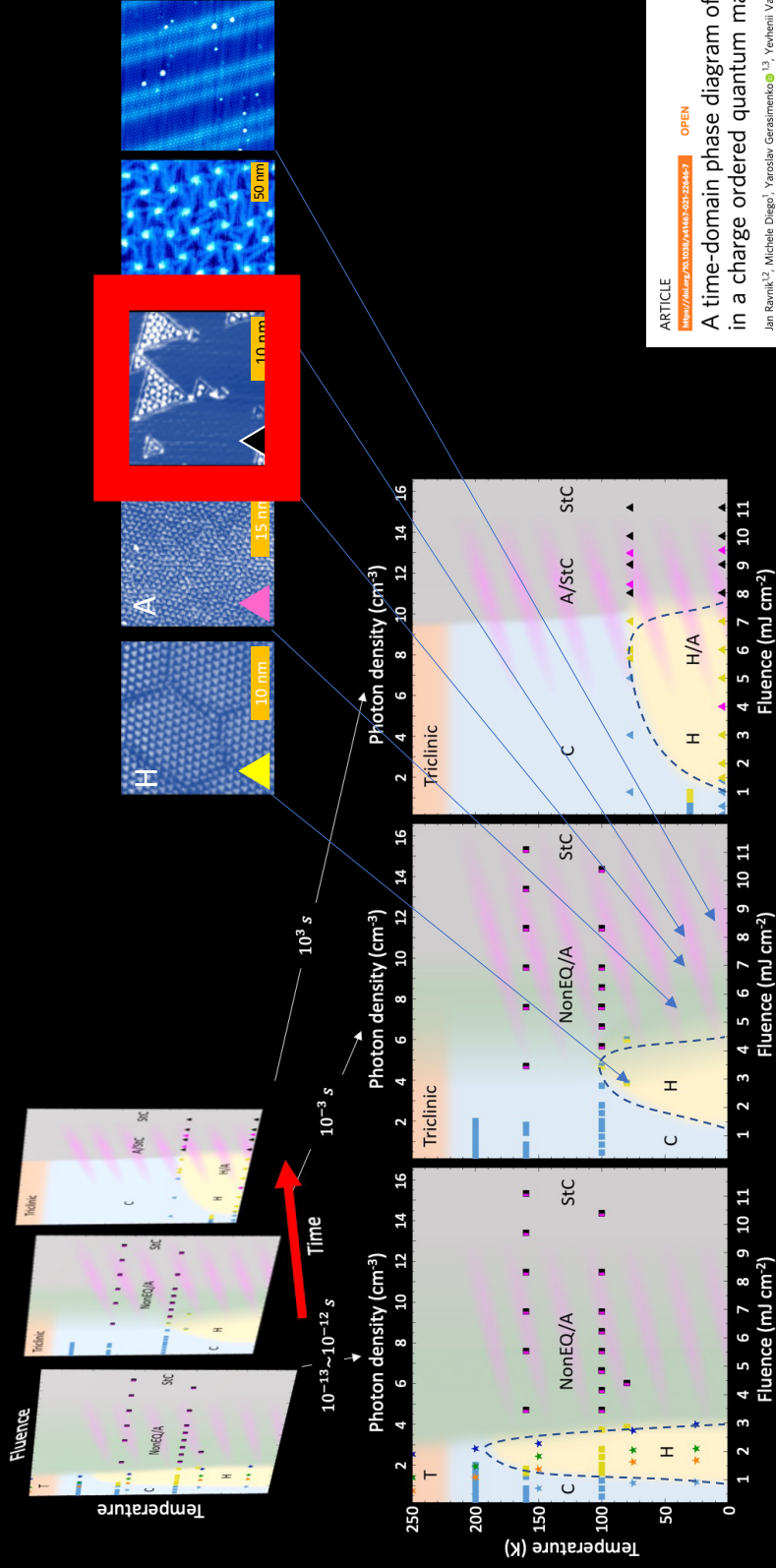
This approximation can only be used for positive values of  $\mu$ . For negative  $\mu$  indeed, the minimum of  $F$  is  $-\infty$  for  $l_x = \infty$  and  $l_y = l_z = 0$ . This result is complete nonsense. Thus, the model can only be used near the C–I transition, and for positive  $\Lambda$ .

Experiment:



Villain 1982, Ravnik et al., ACS Applied Nano materials 2, 3743 (2019)

# A time-domain phase diagram in 1T-TaS<sub>2</sub>



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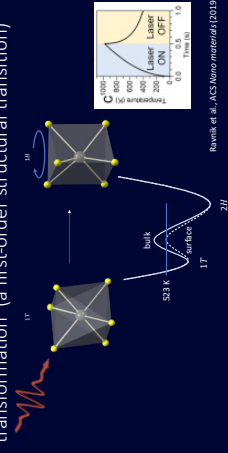
<https://doi.org/10.1038/s41467-021-23223-7>

A time-domain phase diagram of metastable states in a charge ordered quantum material

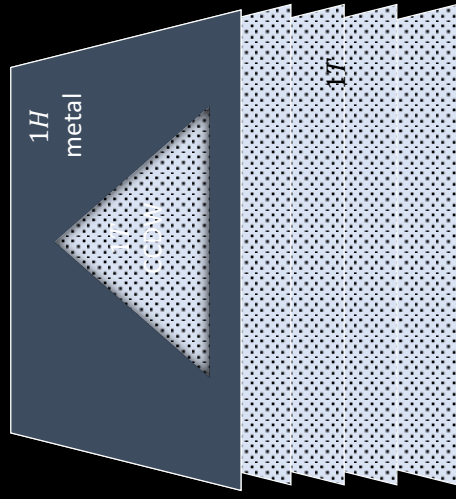
Jan Ravnik<sup>1,2</sup>, Michele Diogo<sup>1</sup>, Yaroslav Gerasimenko<sup>1,3</sup>, Yevhenii Vaskivskiy<sup>1</sup>, Igor Vaskivskiy<sup>1,3</sup>, Tomaz Mertelj<sup>1,3</sup>, Jaka Vodeb<sup>1</sup> & Dragan Mihailovic<sup>1,3,4</sup>

NATURE COMMUNICATIONS | (2021)12:23223 |

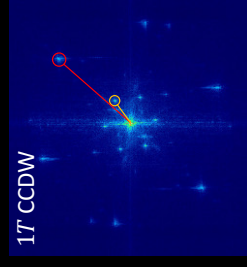
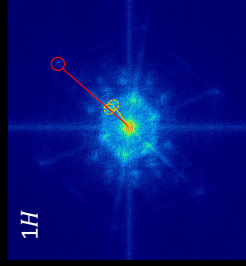
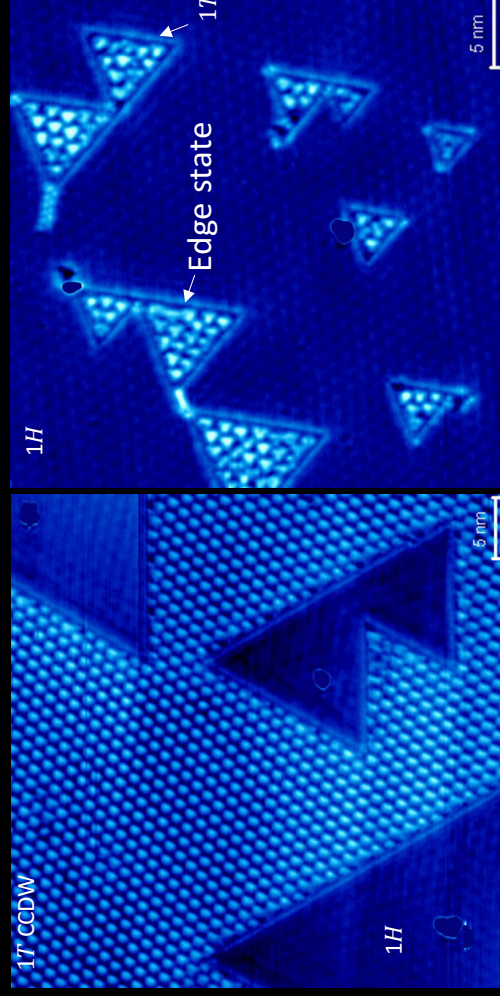
Laser-induced single-layer polytype transformation (a first-order structural transition)



Ravnik et al., ACS Nano materials, (2019)

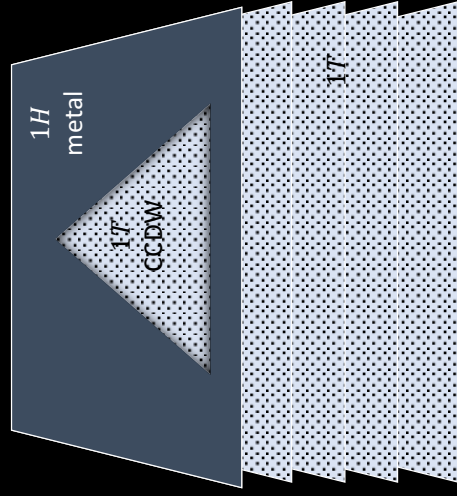


# Laser-induced 1T-1H polytype separation

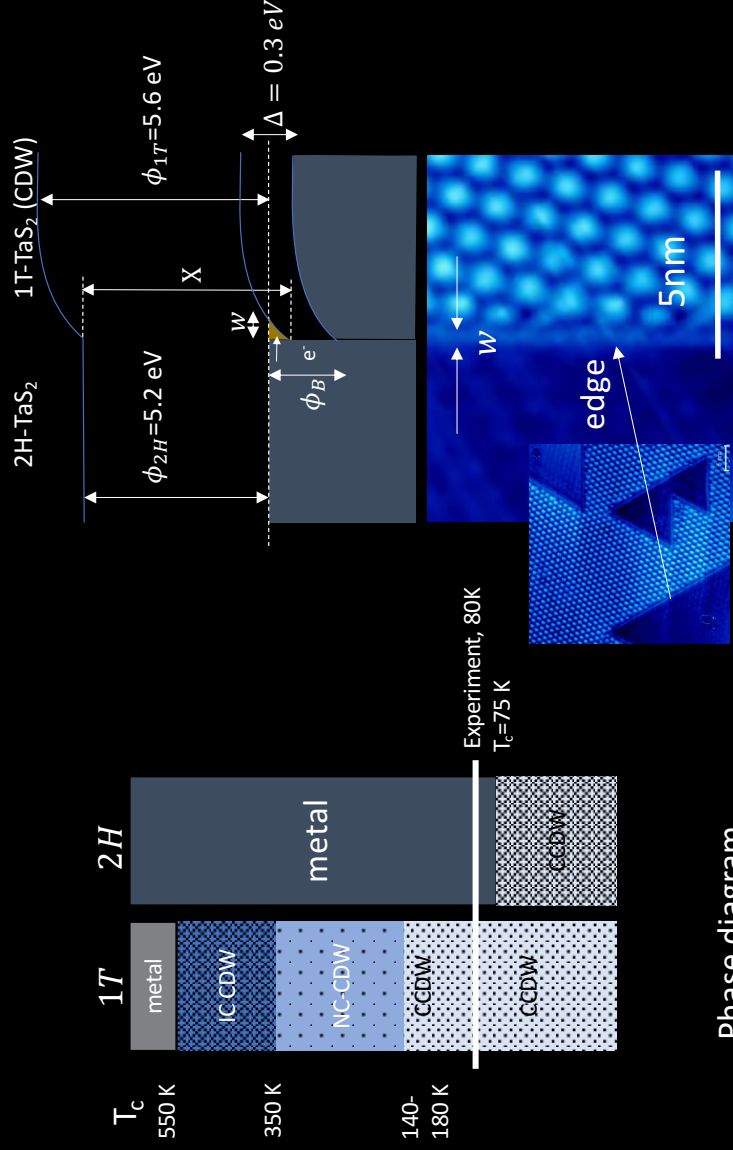


Ravnik et al., ACS Applied Nano materials 2, 3743 (2019)

# Setting up the Quantum billiard for confined electrons by temperature tuning



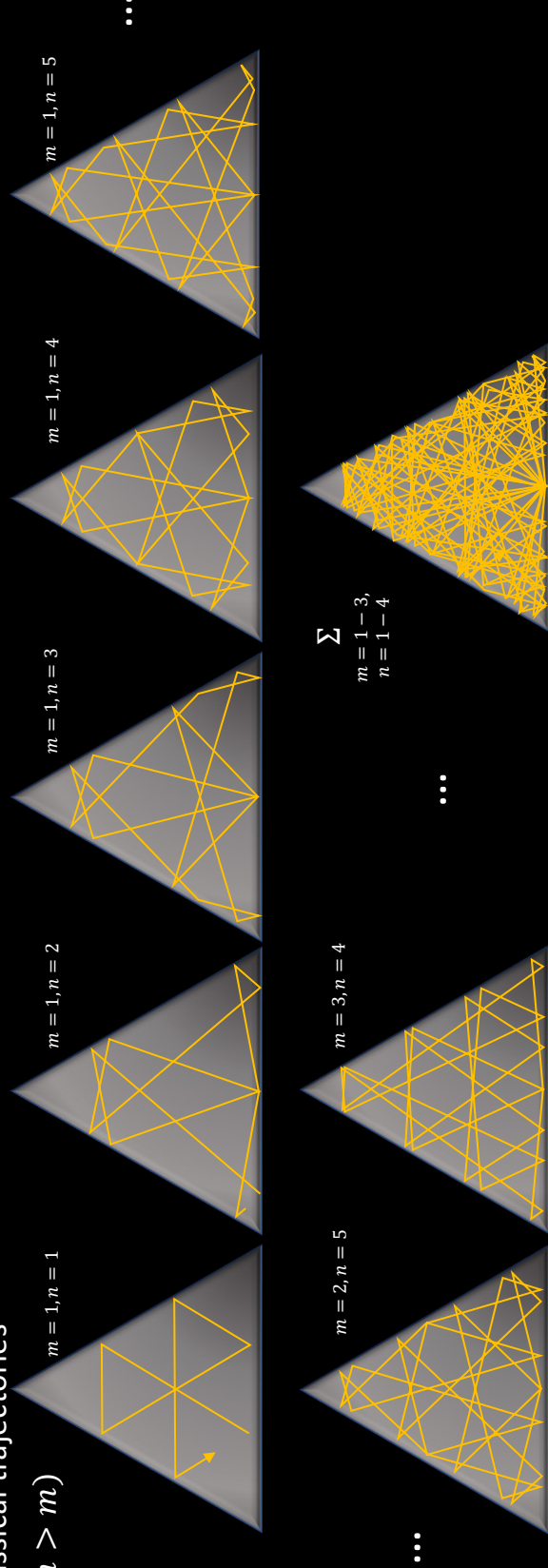
Superlattice structure



# Classical billiard in an equilateral triangle

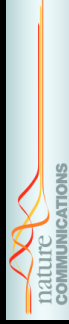
Classical trajectories

$(n > m)$



# Quantum billiards in a perfect equilateral triangle

(Eigenstates of the Schrödinger equation)



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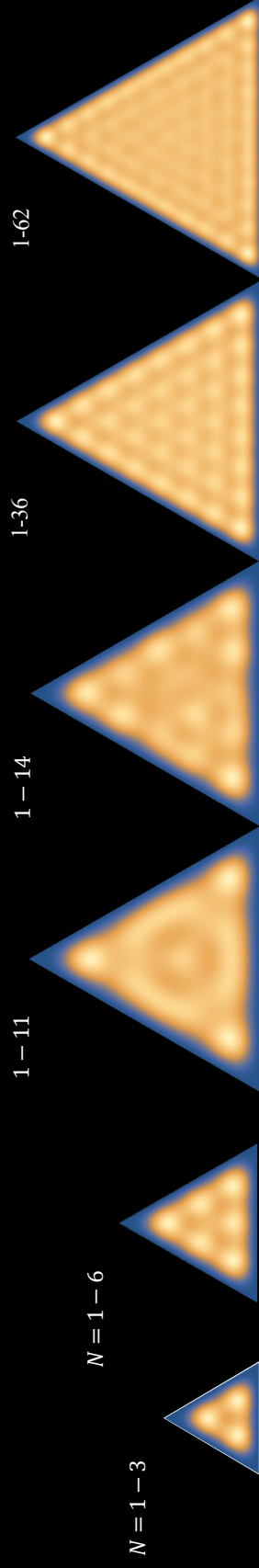
<https://doi.org/10.1038/s41467-021-24075-0>

OPEN



Quantum billiards with correlated electrons confined in triangular transition metal dichalcogenide monolayer nanostructures

Jan Ravnik<sup>1,2,3\*</sup>, Yevhenii Vaskivskyi<sup>1</sup>, Jaka Vodeb<sup>1,3</sup>, Polona Aupič<sup>1</sup>, Igor Vaskivskyi<sup>1,4</sup>, Denis Goloz<sup>2,5,6</sup>, Yaroslav Gerasimenko<sup>1,4</sup>, Viktor Kabanov<sup>4</sup> & Dragan Mihailovic<sup>1,4,8\*</sup>



Plot of  $\sum_N |\psi_i|^2$

# Departure from a perfect equilateral triangle → Quantum chaos

VOLUME 83, NUMBER 23

PHYSICAL REVIEW LETTERS

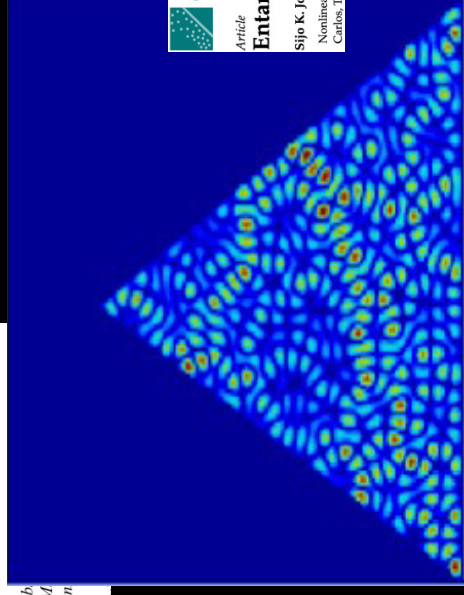
6 DECEMBER 1999

## Mixing Property of Triangular Billiards

Giulio Casati<sup>1</sup> and Tomaž Prosen<sup>2</sup>

<sup>1</sup>International Center for the Study of Dynamical Systems, Università degli Studi dell'Insubria and Istituto Nazionale di Fisica della Materia and INFN, Unità di Milano

<sup>2</sup>Physics Department, Faculty of Mathematics and Physics, University of Ljubljana, Jadranska (Received 24 June 1999)



entropy



Article

## Entanglement Entropy in a Triangular Billiard

Sijo K. Joseph<sup>\*</sup> and Miguel A. F. Sanjuán

Nonlinear Dynamics, Chaos and Complex Systems Group, Departamento de Física, Universidad Rey Juan Carlos, Tulipán s/n, Mostoles, Madrid 28933, Spain; miguel.sanjuan@urjc.es



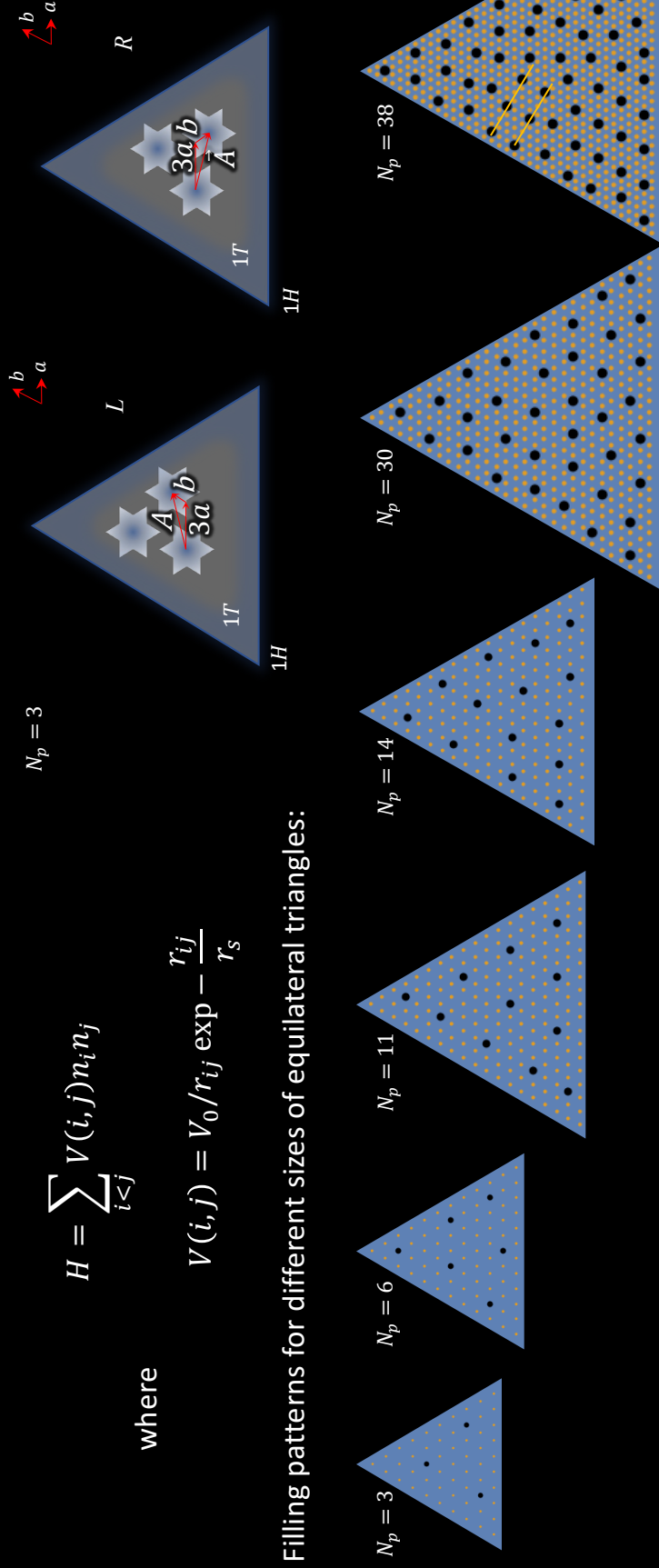
# Wigner crystal confined within an E.T.

Confined charged lattice gas model with screened coulomb interaction (Vodeb et al, 2019) :

$$H = \sum_{i < j}^{N_p} V(i, j) n_i n_j$$

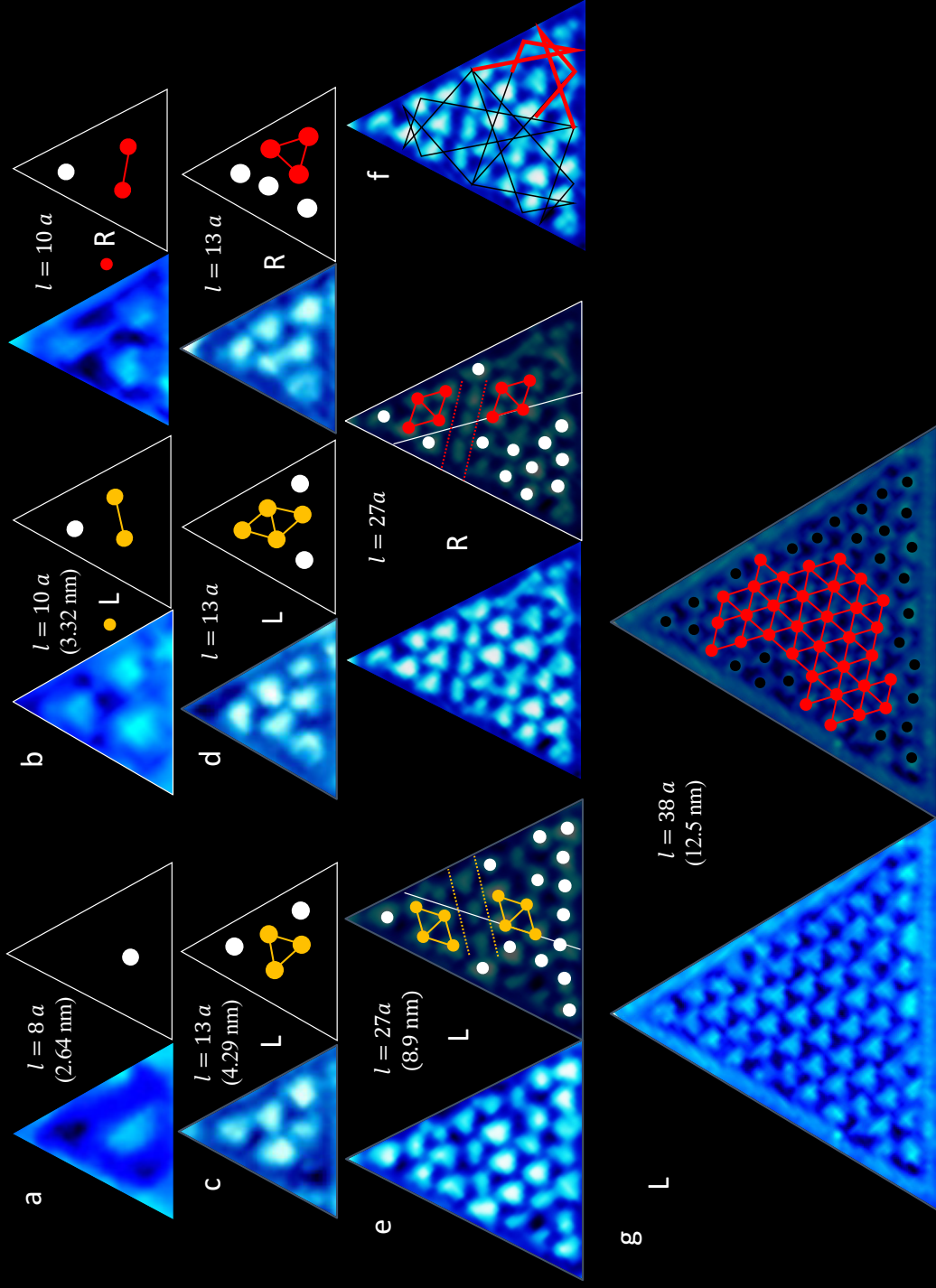
where

$$V(i, j) = V_0 / r_{ij} \exp - \frac{r_{ij}}{r_s}$$

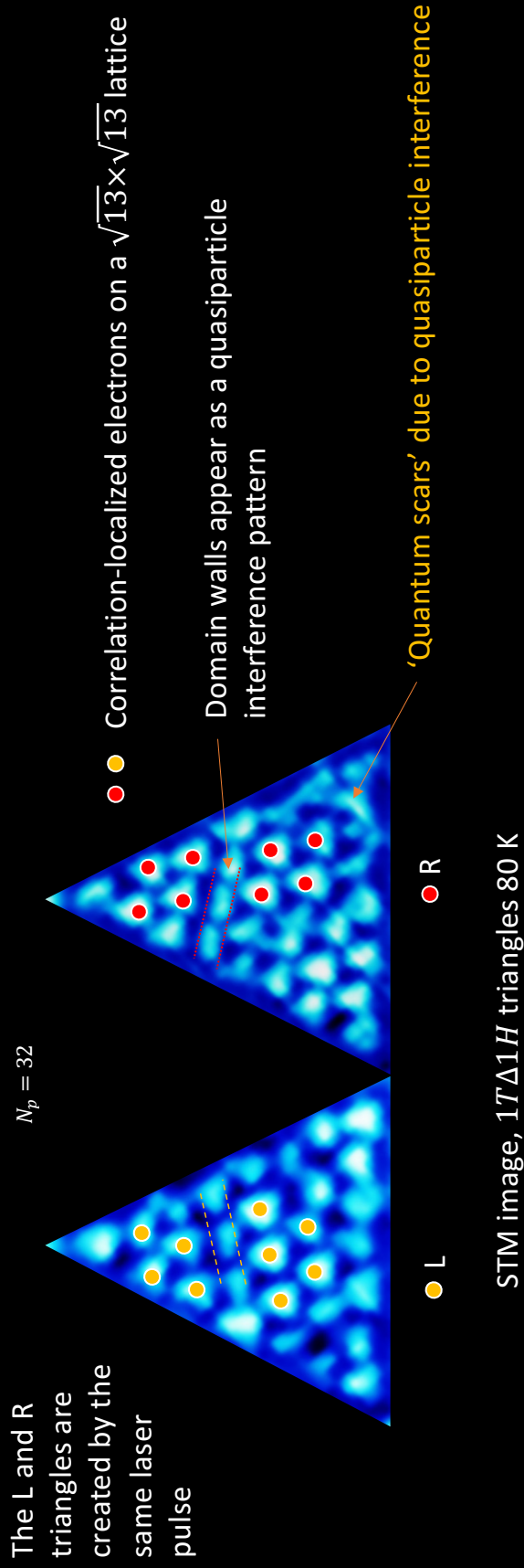


Filling patterns for different sizes of equilateral triangles:

A few observed  
1T@1H triangles  
after laser  
excitation

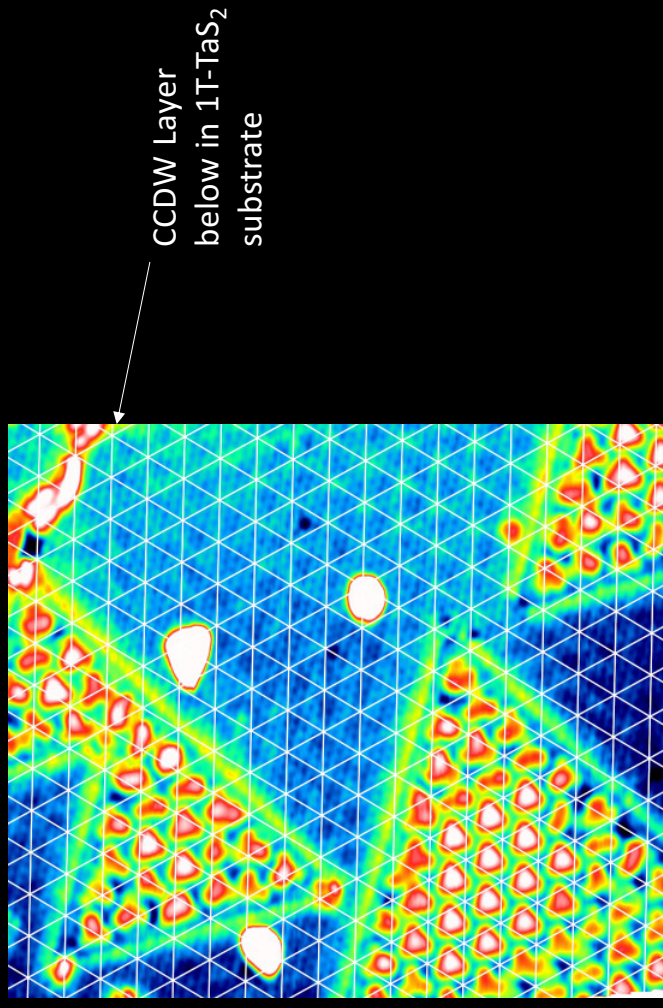


# Intertwined localized and itinerant electrons (a mixture of quantum billiards and CCDW)

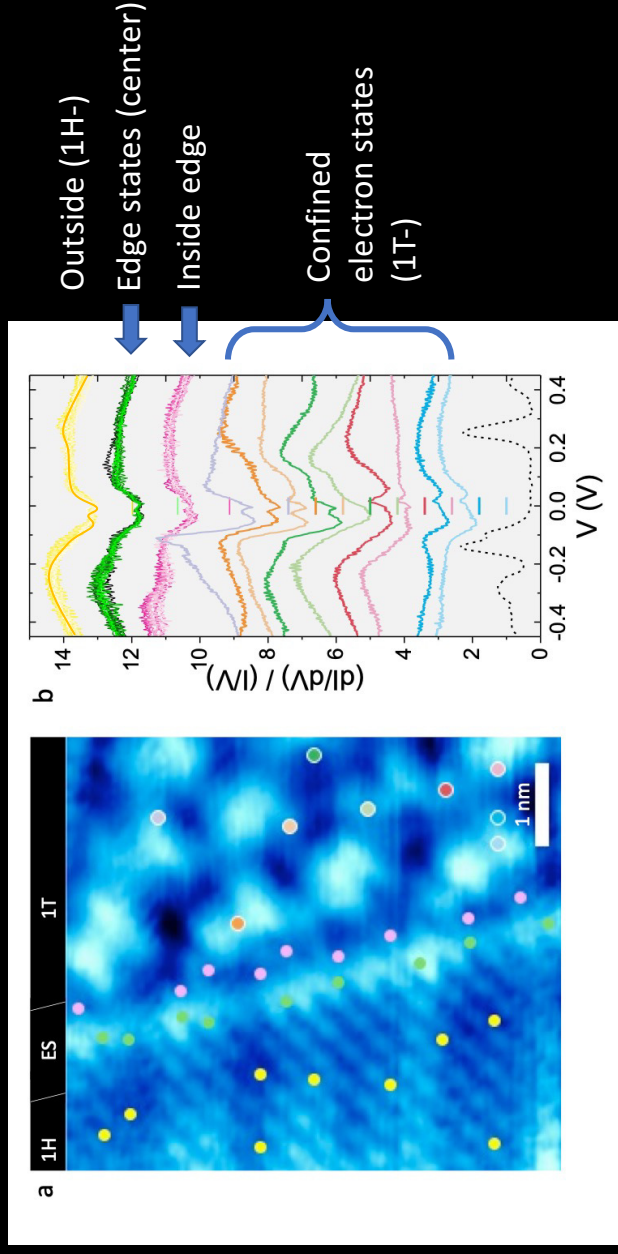
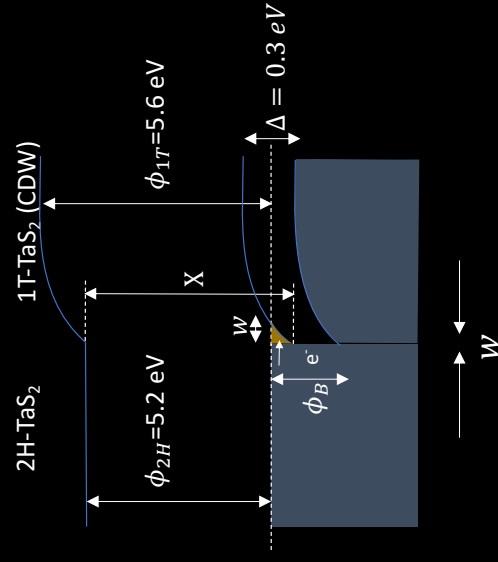


Note: the itinerant particles are directly observed by the Quasiparticle interference  
(in mixed systems usually only the localized electron density is observed)

Interlayer effects: There is no preferential stacking between layers.



# Edge effects, confined and unconfined electron states (STS measurements).



# Carrier delocalization at incommensurate filling

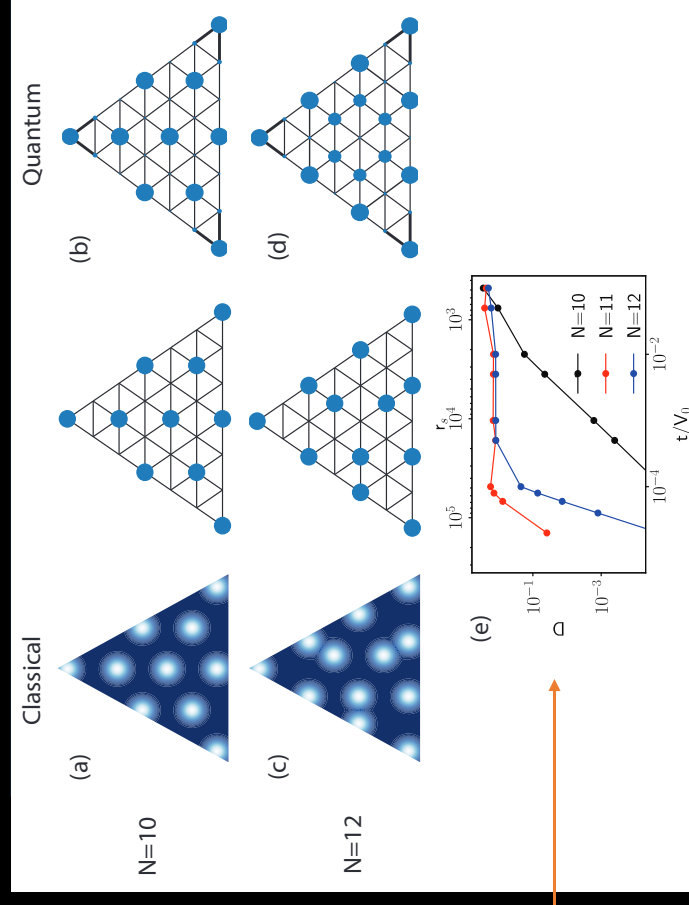
Exact diagonalization calculation of electron delocalization (fully quantum)

$$H = -t \sum_{\langle i,j \rangle} c_i^\dagger c_j + \sum_{i \neq j} V(|i-j|) [n_i - \bar{n}] [n_j - \bar{n}],$$

Delocalization parameter:

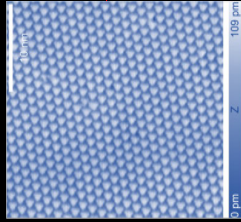
$$D = \sqrt{\sum_i [\langle n_i \rangle - \langle n_i \rangle_{t=0}]^2}$$

Incommensurate states ( $N \neq 10$ ) are orders of magnitude more susceptible to delocalization than commensurate ones

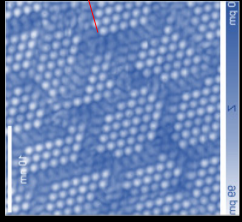


# The different photoinduced states have very different transport (itinerant, localized)

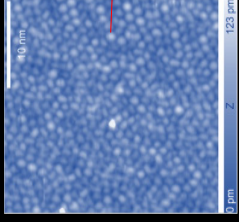
Classical systems:  
Kinematic constraints prevent lane change in a traffic jam



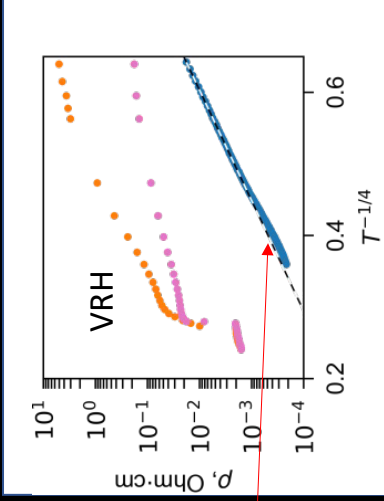
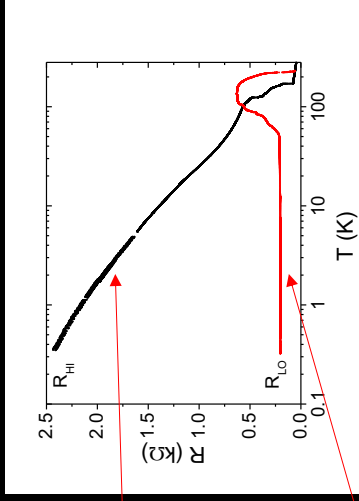
C state



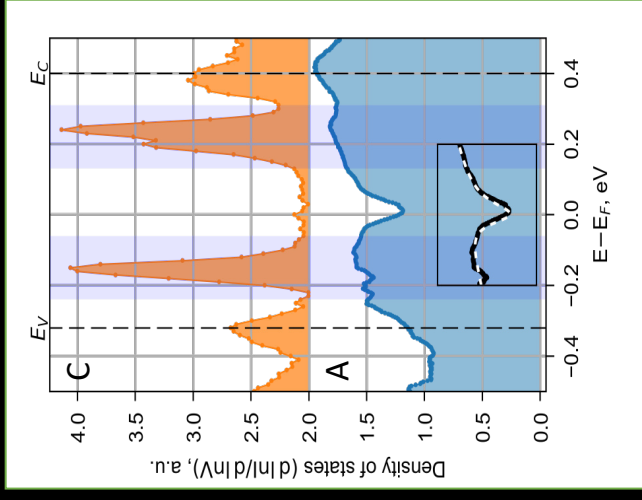
H state



A state



Tunnelling spectroscopy:





'Nature Morte Vivante '  
by Salvador Dalí, 1956