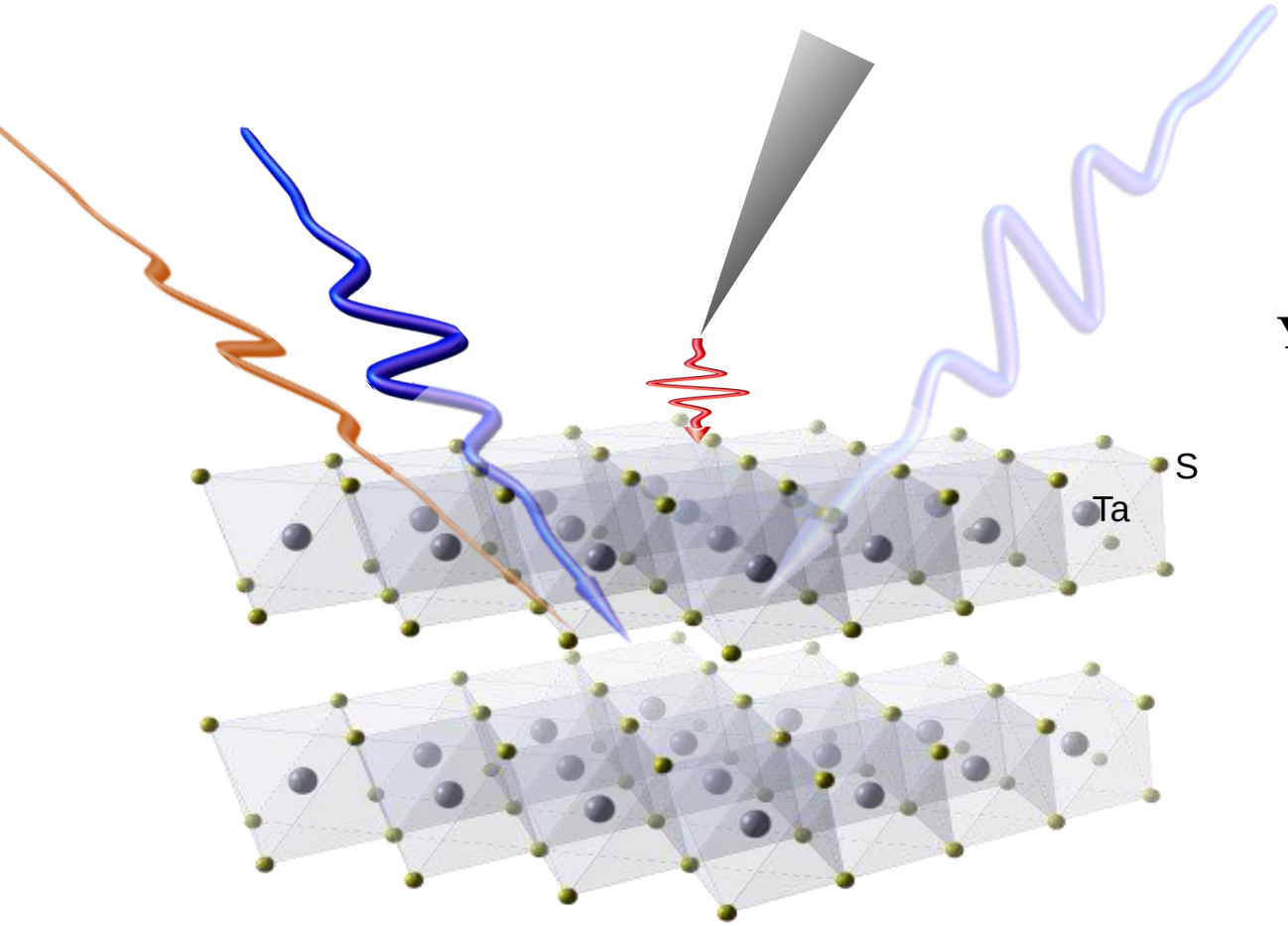
Exotic phenomena in a metastable polaronic Wigner crystal.



Y. Vaskivskyi[1], A.Mraz[1], J.Vodeb[1], E. Božin[2], I. Vaskivsyi[1] and D. Mihailovic[1,3,4]

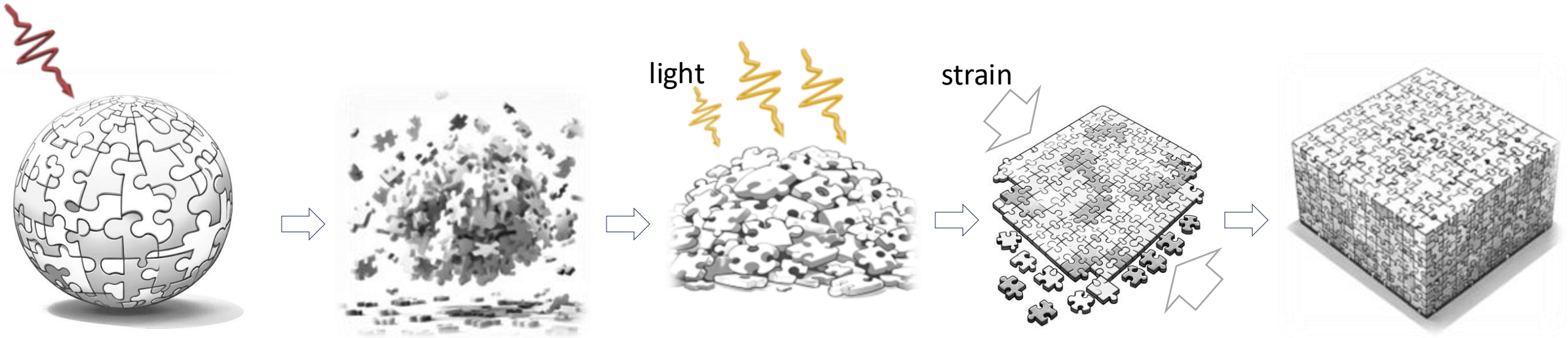
[1]Jožef Stefan Institute, Jamova 39, Ljubljana, Slovenia,

[2]Brookhaven National Laboratory, Upton, N.Y., USA

[3]Department. of Physics, Faculty of Mathematics and physics, University of Ljubljana, Slovenia

[4] CENN Nanocenter, Jamova 30, 1000 Ljubljana, Slovenia

Mesoscopic states and metastability in the aftermath of a phase transition



Conventional stroboscopic techniques

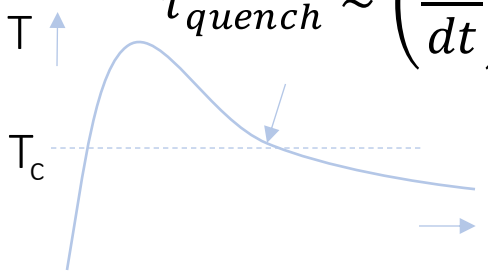
Unexplored, potentially useful

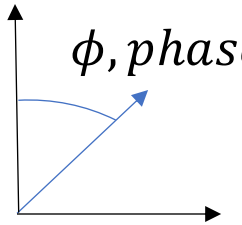
Conventional equilibrium property measurements

Creation of metastable states by a quench through a 2nd order transition

laser spot, universe, etc.

$$\tau_{quench} \sim \left(\frac{dT}{dt}\right)^{-1} T_c$$





$$\Psi = Ae^{i\phi}$$

If $\tau_{quench} < L/v$, multiple domains form (Kibble-Zurek mechanism)

whether as it expands and cools it might acquire a domain structure, as in a ferromagne cooled through its Curie point. Zel'dovich *et al* (1974; see also Kobzarev *et al* 1974 have discussed this question, and in particular pointed out the important gravitationa effects to be expected of domain walls. Everett (1974) has studied the propagation o waves across a domain boundary.

The aim of this paper is to discuss the topology and scale of the possible cosmi

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

Possible single 1st order transition outcomes

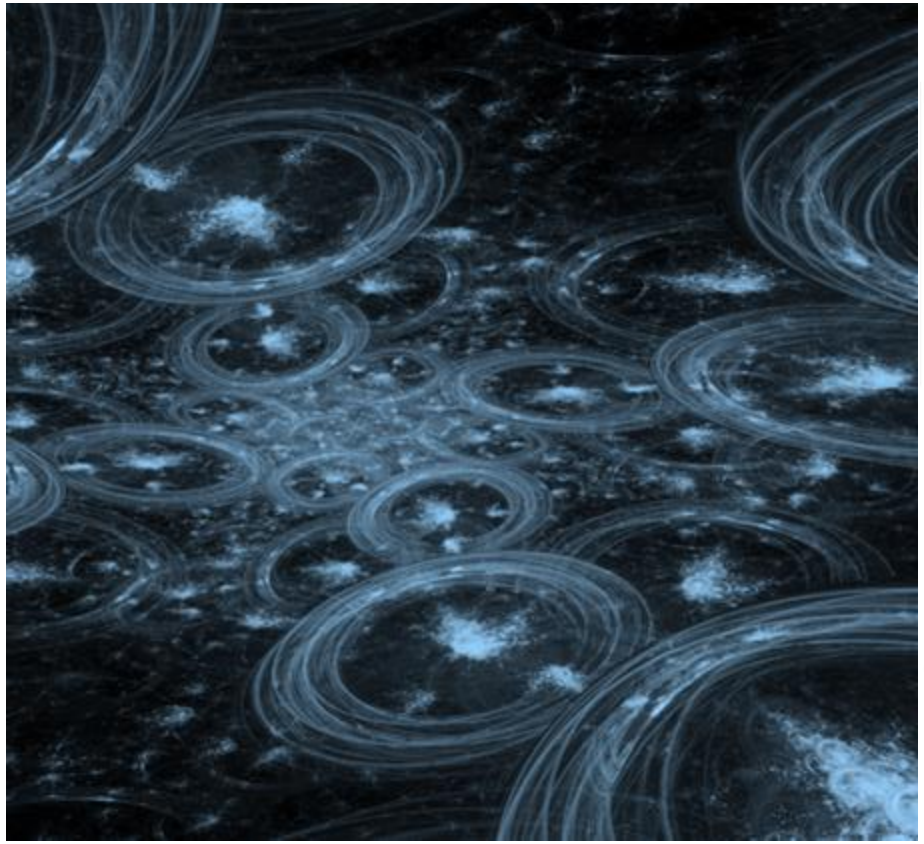
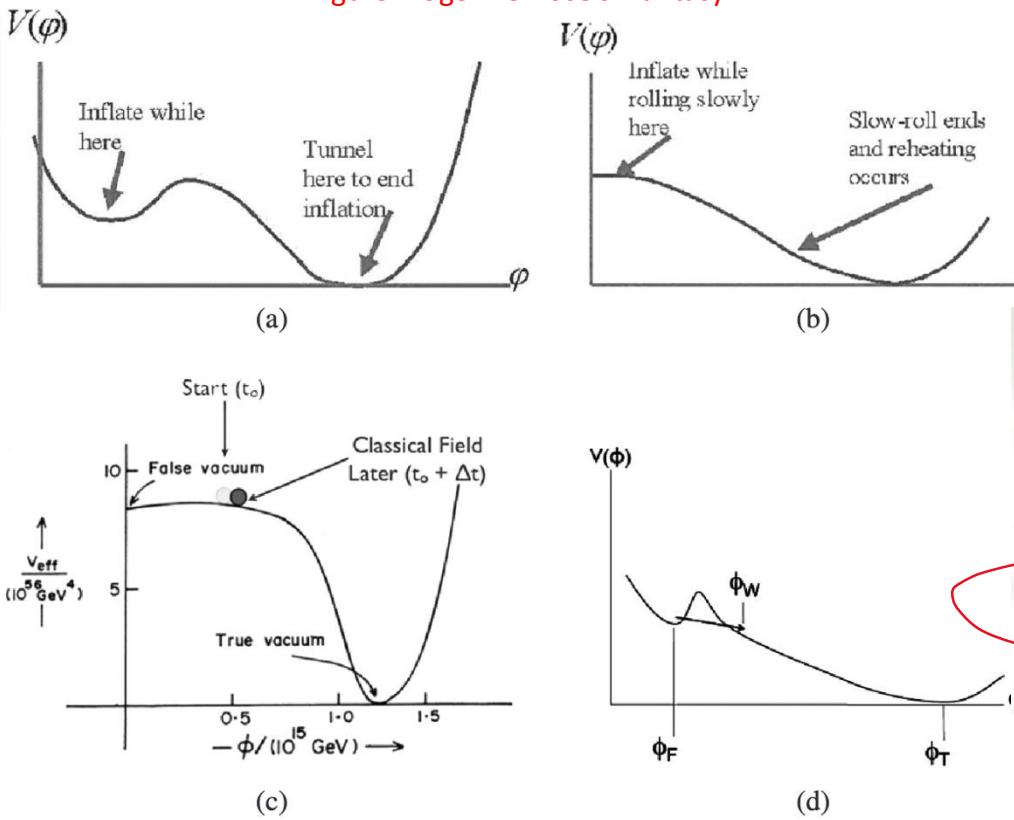
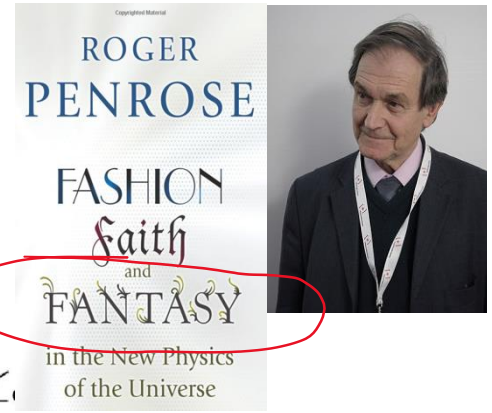


Figure: Roger Penrose's 'Fantasy'

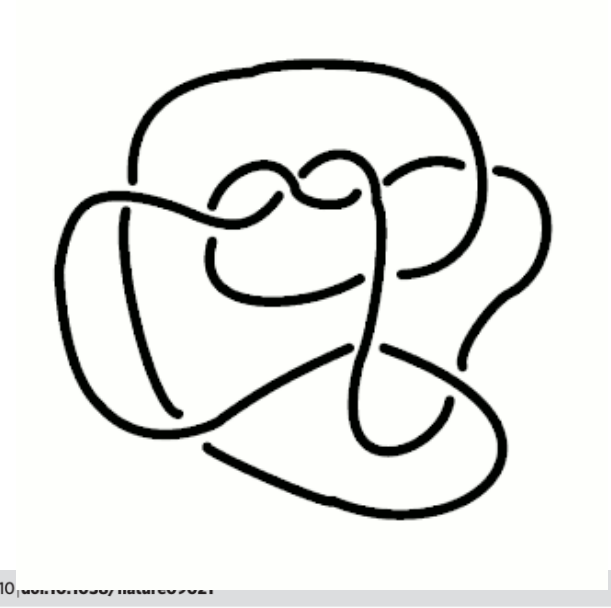


Starobinsky – Linde – Guth
Kibble, Zurek, Volovik



We have little data over a vast range of timescales!

An example of multiple outcomes: Protein folding

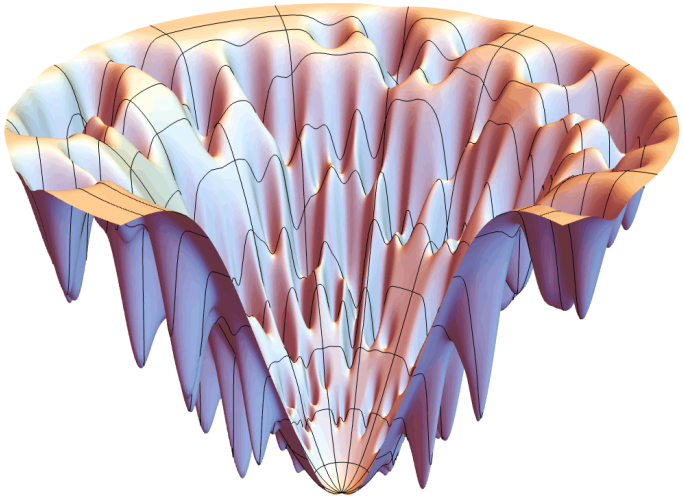


Vol 465|3 June 2010 nature

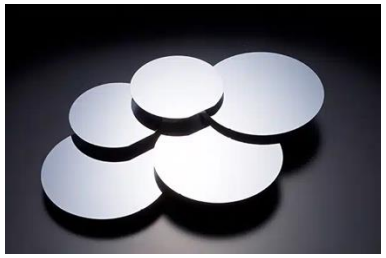
LETTERS

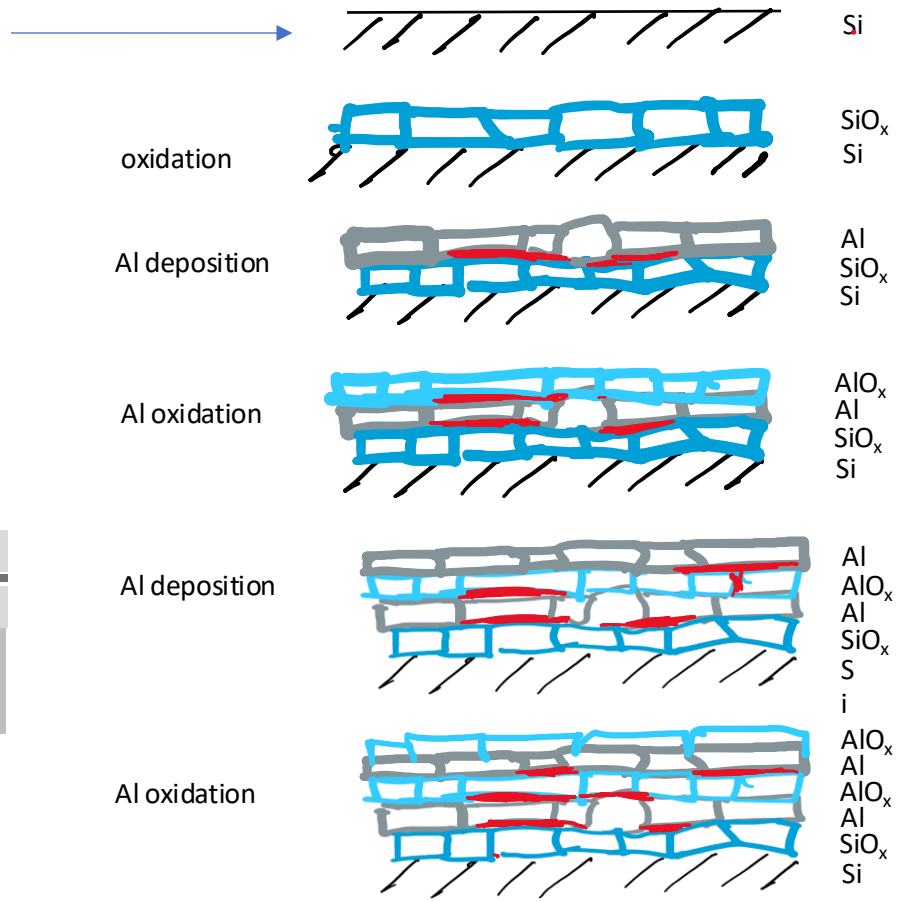
The folding cooperativity of a protein is controlled by its chain topology

Elizabeth A. Shank[1,2]*†, Ciro Cecconi[1,2]*†, Jesse W. Dill[2,3]*, Susan Marqusee[1,2] & Carlos Bustamante[1,2,4,5,6]



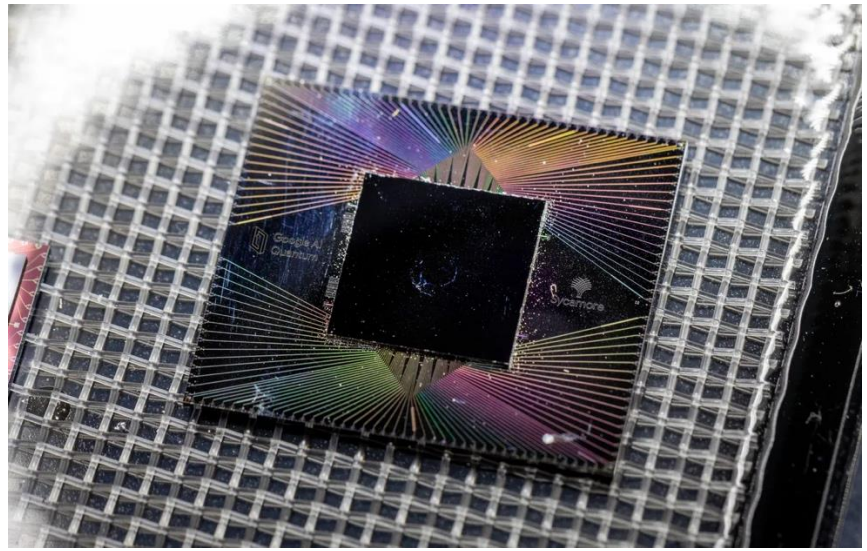
Superconducting QPU fabrication





Ideal engineering view:

The fabrication of a QPU typically requires ~40 steps



Journal of Applied Physics ARTICLE scitation.org/journal/jap

Optimization of Al/AlO$_x$/Al-layer systems for Josephson junctions from a microstructure point of view

Cite as: J. Appl. Phys. 125, 165301 (2019); doi: 10.1063/1.5089871
Submitted: 23 January
Published Online: 22 Ap

S. Fritz,[1,a)] L. Radtke,[2] R.

Al/Alx/A
junctior
differer
conditic

ibm_fez OpenQASM 3

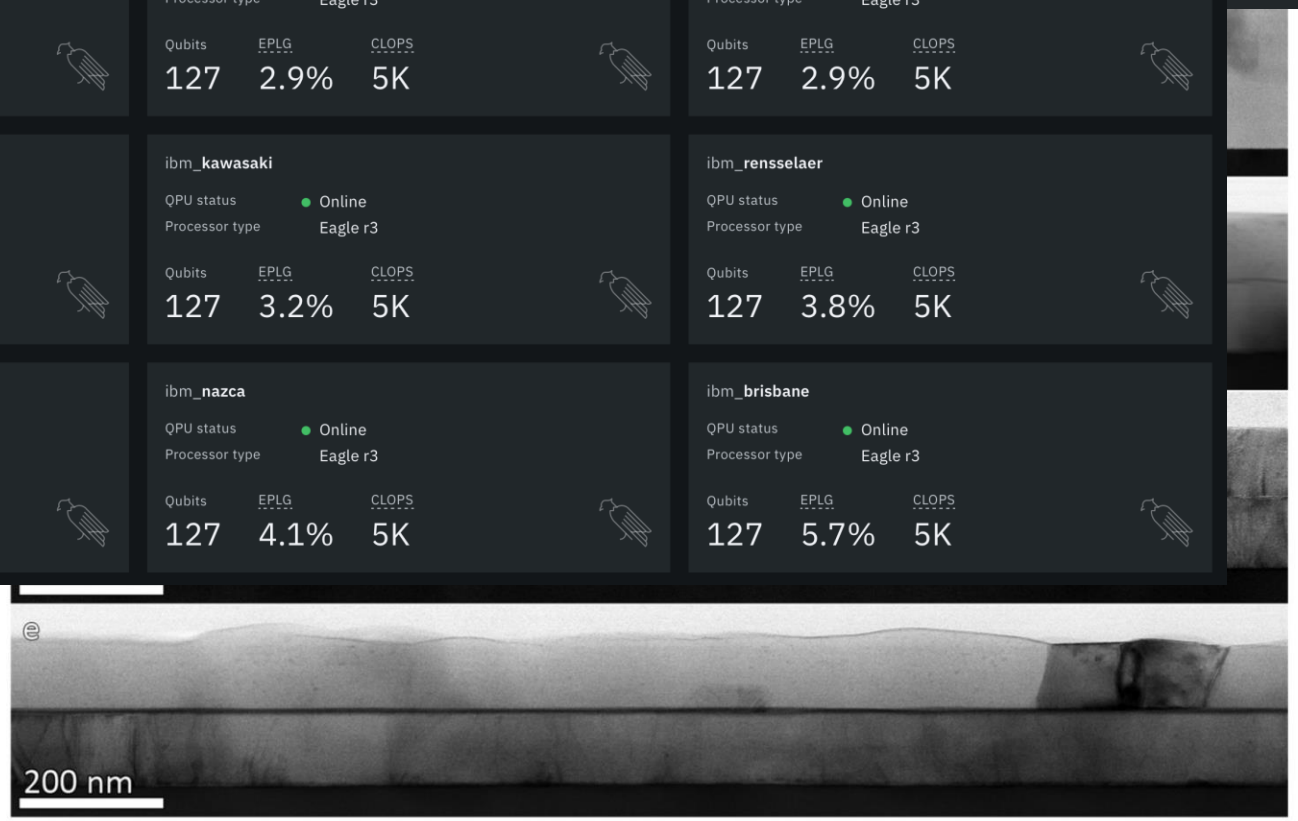
156

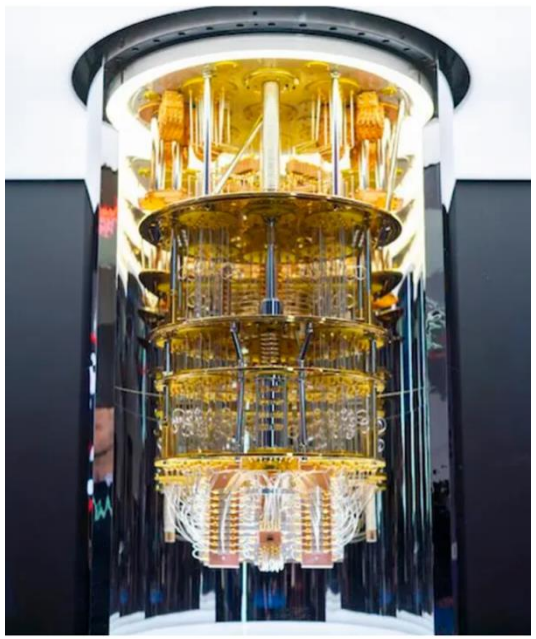
Status: Online

Median CZ error: 2.933e-3
Median SX error: 2.684e-4
Median readout error: 1.690e-2
Median T1: 116.16 us
Median T2: 94.94 us

2 jobs
n r2
SX, X

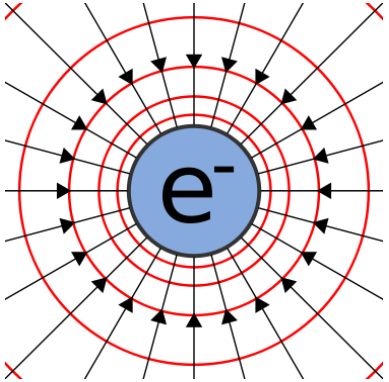
	QPU status	Processor type	Qubits	EPLG	CLOPS
ibm_fez	Online	Heron r2	156	0.5%	3.8K
ibm_torino	Online	Heron r1	133	0.7%	3.8K
ibm_kyiv	Online	Eagle r3	127	1.9%	5K
ibm_quebec	Online	Eagle r3	127	2.6%	5K
ibm_sherbrooke	Online	Eagle r3	127	2.9%	5K
ibm_kyoto	Online	Eagle r3	127	2.9%	5K
ibm_brussels	Online	Eagle r3	127	3%	5K
ibm_kawasaki	Online	Eagle r3	127	3.2%	5K
ibm_rensselaer	Online	Eagle r3	127	3.8%	5K
ibm_strasbourg	Online	Eagle r3	127	3.9%	5K
ibm_nazca	Online	Eagle r3	127	4.1%	5K
ibm_brisbane	Online	Eagle r3	127	5.7%	5K



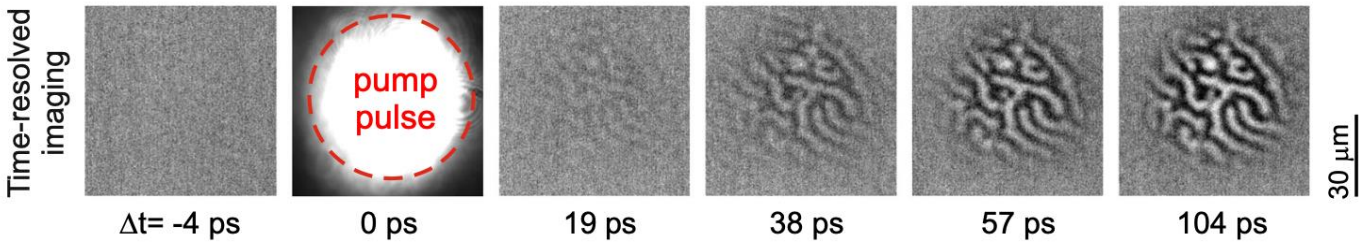


IBM Q1

Domains store information (spin and charge)

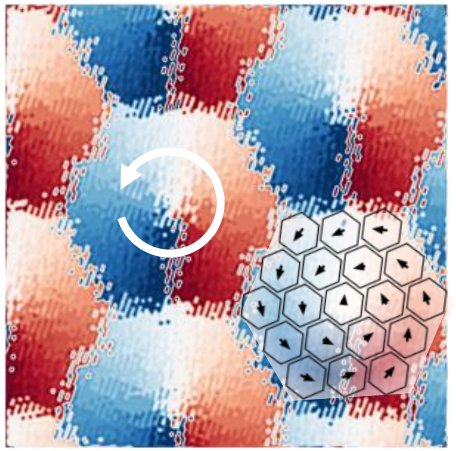


Spins are weakly coupled to the environment, whence they hold information better than charge, but information is encoded in the domain structure



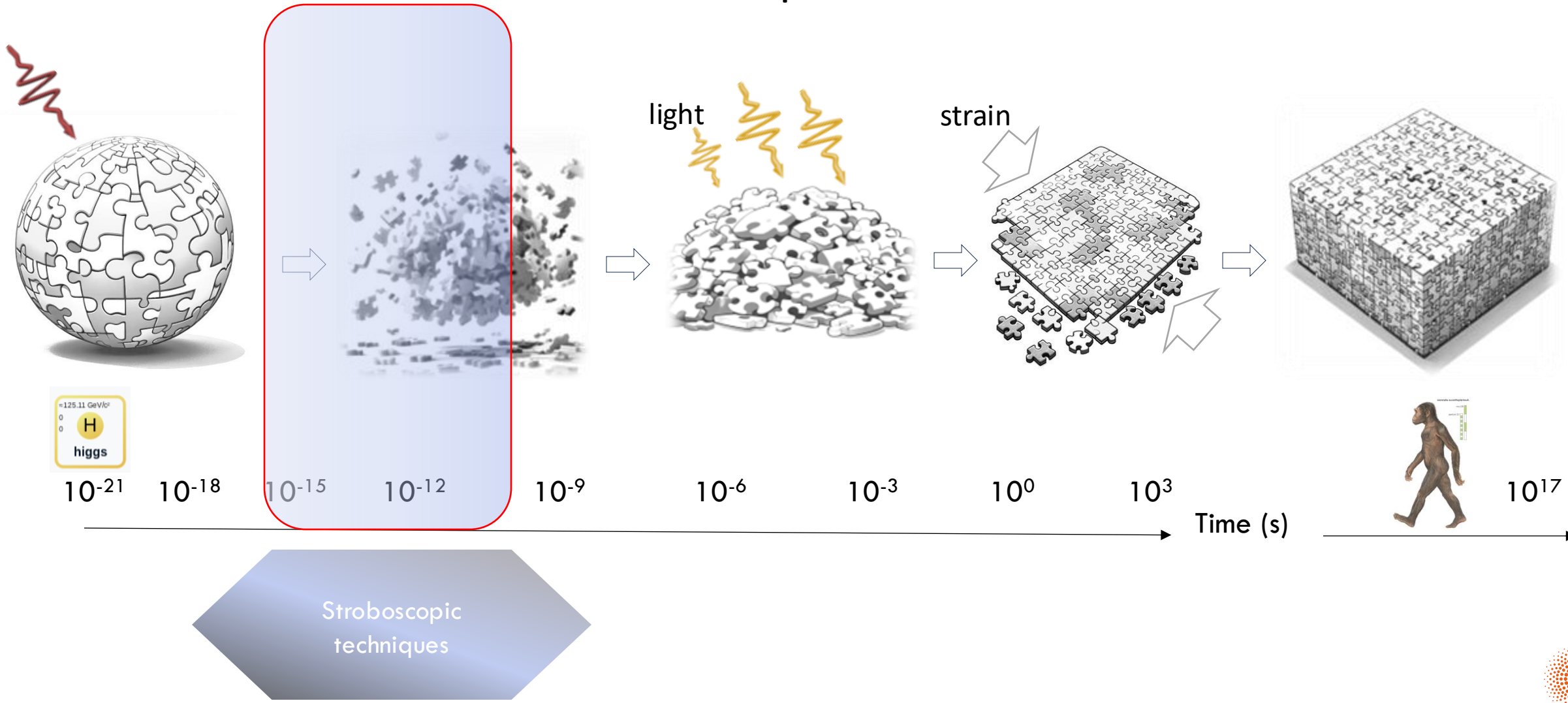
de Jong *et al.* PRL**108,** (2012).
Nature Communications | (2024) 15:4451

Charge is strongly coupled to the lattice, whence any information is rapidly dissipated.
But, information can be encoded in the domain structure.



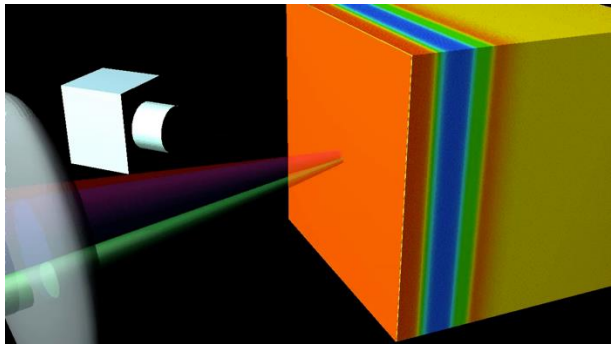
e.g. 1T-TaS2 memory (Mraz et al., *Nanolett*. 2022)

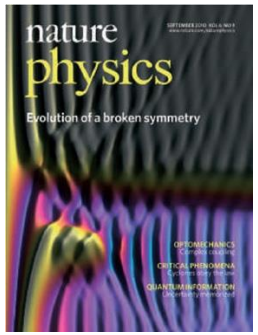
Mesoscopic states and metastability in the aftermath of a phase transition

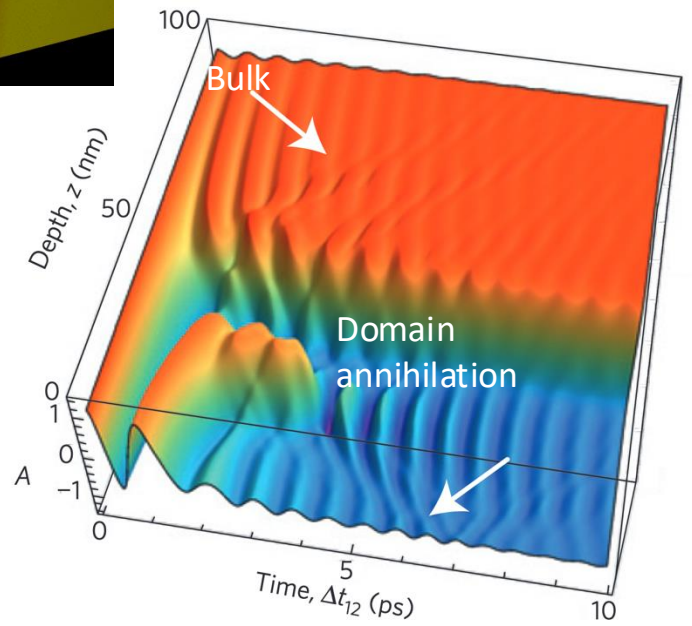


Coherent domain dynamics in $TbTe_3$

Domains form due to inhomogeneous excitation

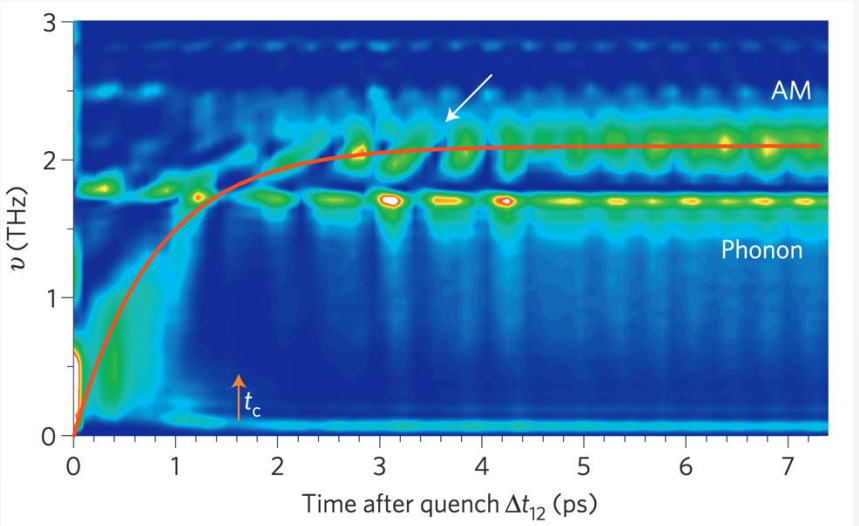




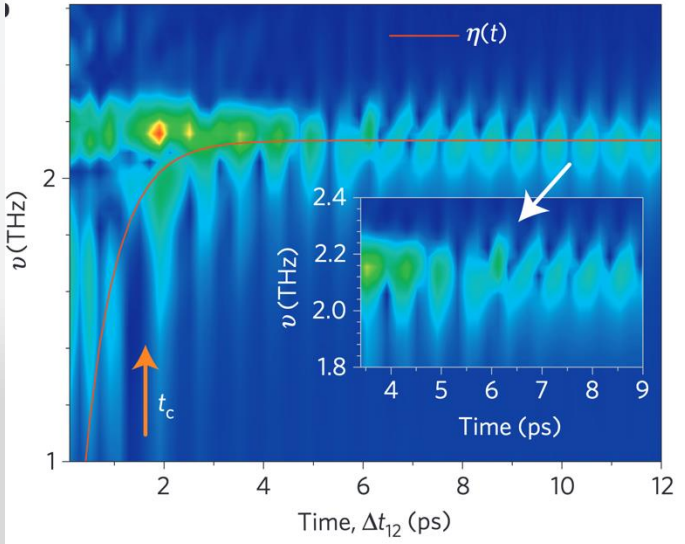


Yusupov, R. *et al.* Coherent dynamics of macroscopic electronic order through a symmetry breaking transition. *Nat Phys* **6**, 681–684 (2010).

Experiment



Theory



Incoherent Topological Defect Recombination Dynamics in $TbTe_3$

T. Mertelj,[1] P. Kusar,[1] V. V. Kabanov,[1] P. Giraldo-Gallo,[2] I. R. Fisher,[2,3] and D. Mihailovic[1,4]

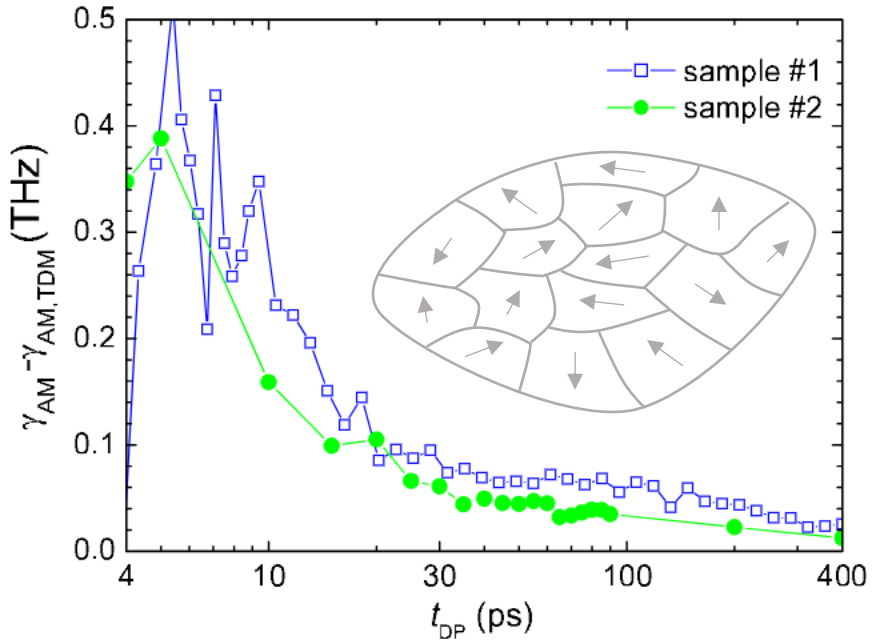
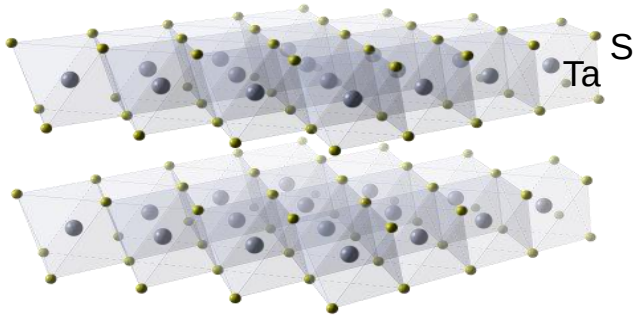


FIG. 4 (color online). The time dependence of the excess γ_{AM} due to topological defect annihilation. Data for two different samples show a difference primarily in the long time behavior beyond 30 ps, which appears as an offset.

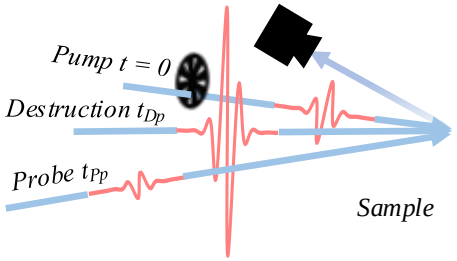
See also Trigo et al (e.g. TR-XRD)

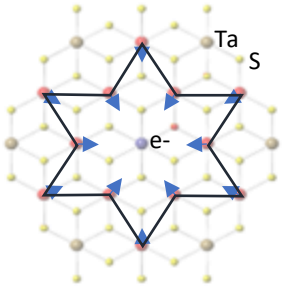
Ultrafast Switching to a Stable Hidden Quantum State in an Electronic Crystal

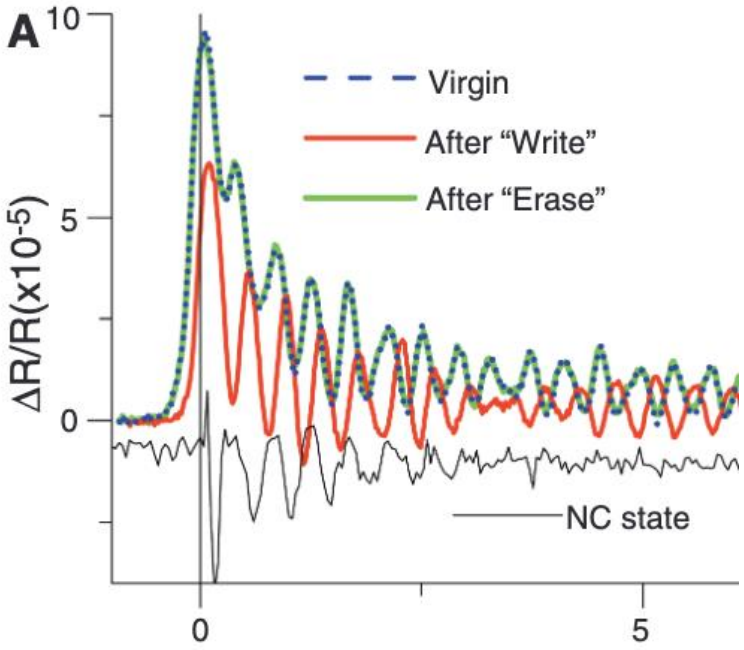
L. Stojchevska,[1,2] I. Vaskivskyi,[1] T. Mertelj,[1] P. Kusar,[1] D. Svetin,[1] S. Brazovskii,[3,4] D. Mihailovic[1,2,5]*



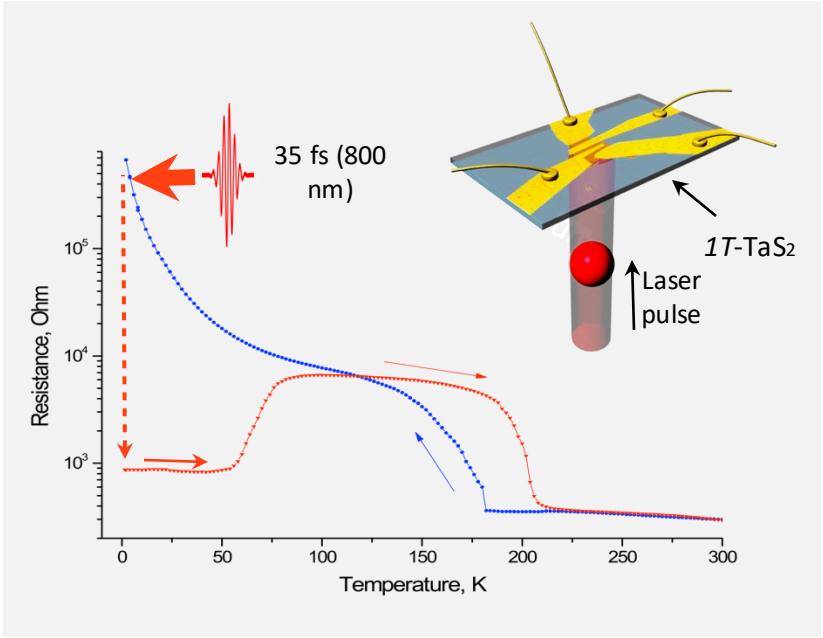
Collective mode frequency switching in 1T-TaS_2





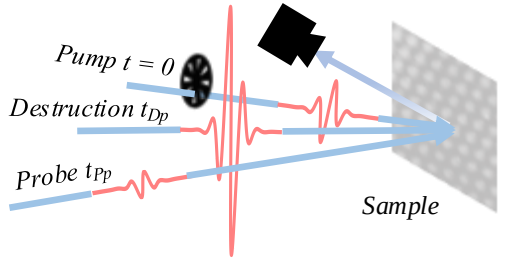


Resistance switching to a 'hidden' state



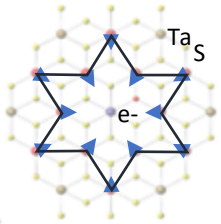
Demsar et al, Phys. Rev B (2002); Demsar et al, Phys. Rev. Lett (1999); Stojchevska et al. Science (2014)

Coherent switching control



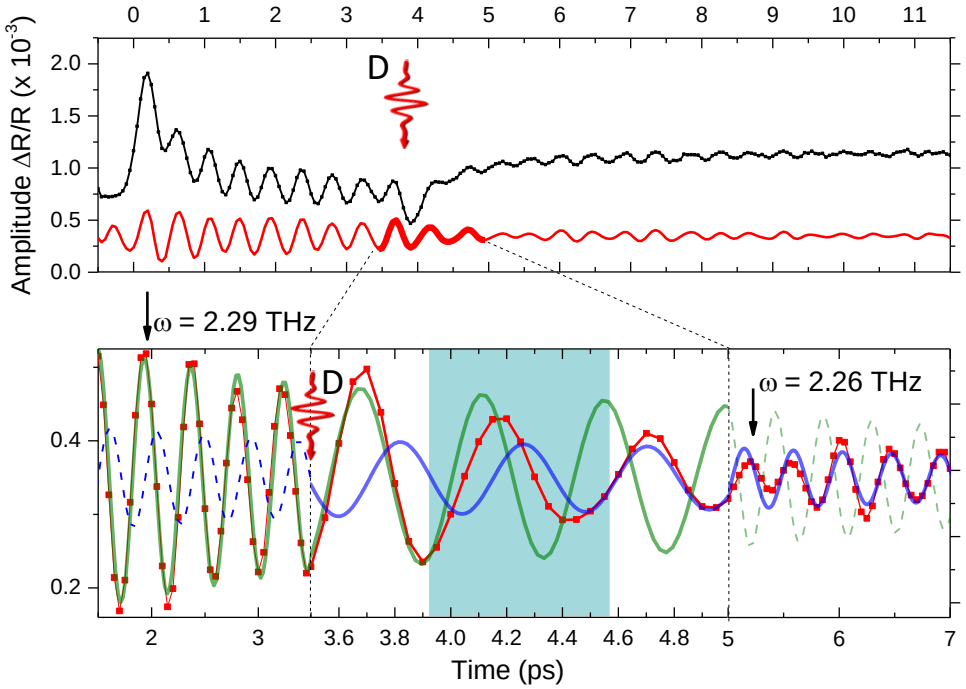
Multipulse optical coherent control

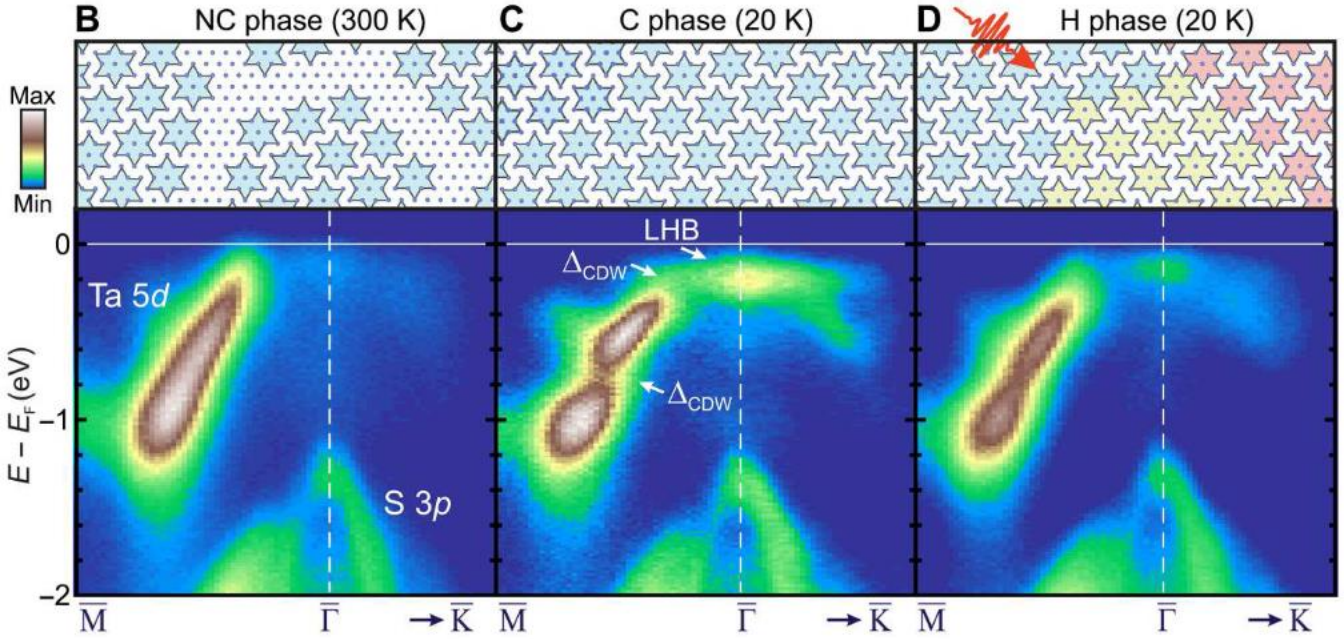
Ravnik, et al., *Phys Rev B* **97**, e1400173 (2018).



Multipulse ARPES coherent control

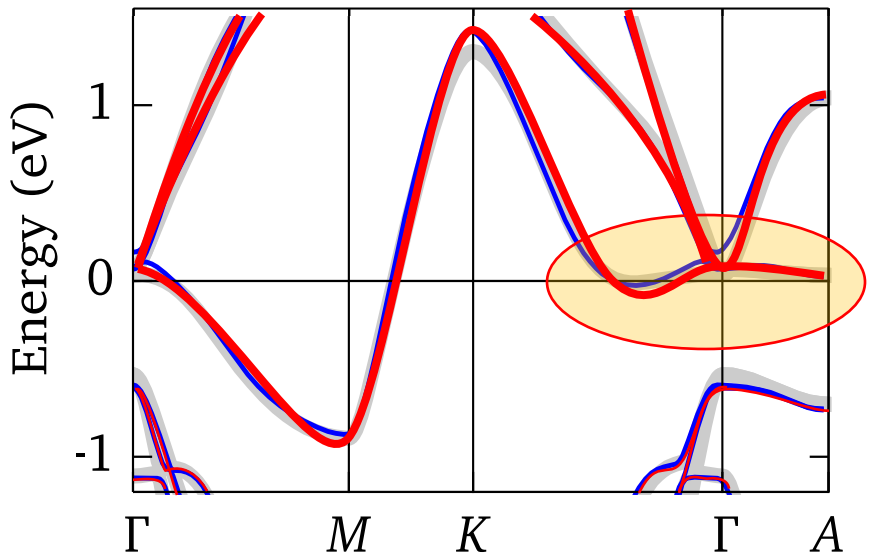
Maklar et al, *Science advances* 9, eadi4661 (2023)





The C-H transition takes place in < 400fs.

Undistorted 1T-TaS_2 exhibits a flat band at E_F along $\Gamma - K$.



Carriers are prone to localisation (formation of polarons):

The threshold for localization is defined by the dimensionless parameter, the Wigner-Seitz radius $r_s = \frac{a}{a_{Bohr}}$

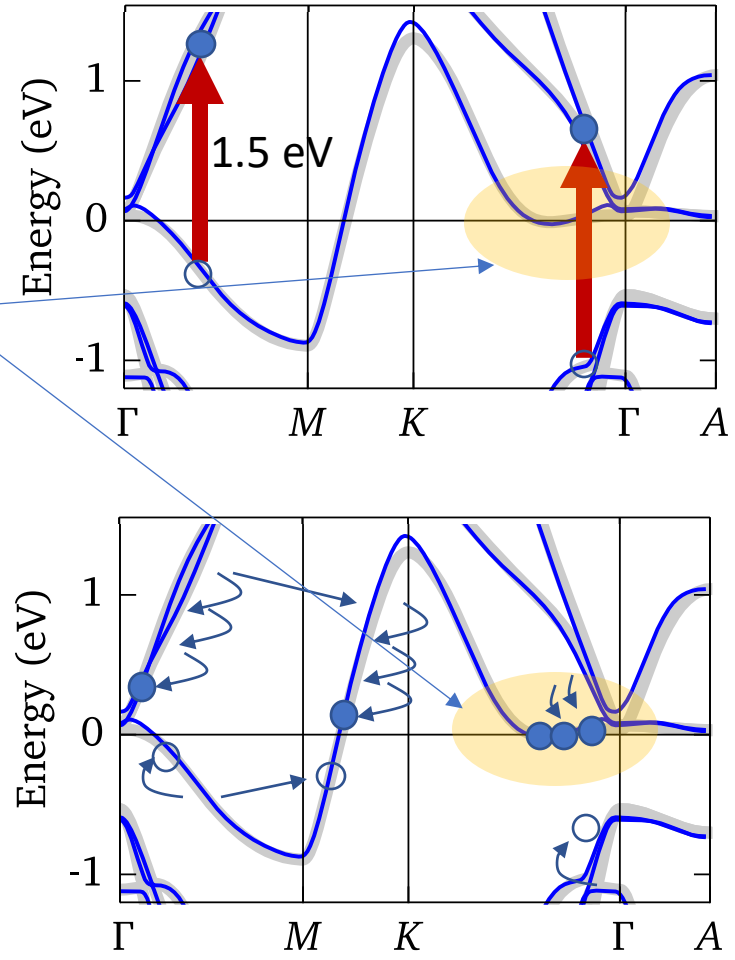
In 2D, $r_s = \frac{V}{t} = \frac{e^2 m^*}{\hbar^2 \sqrt{n}} = 31\sim38^{\dagger}$

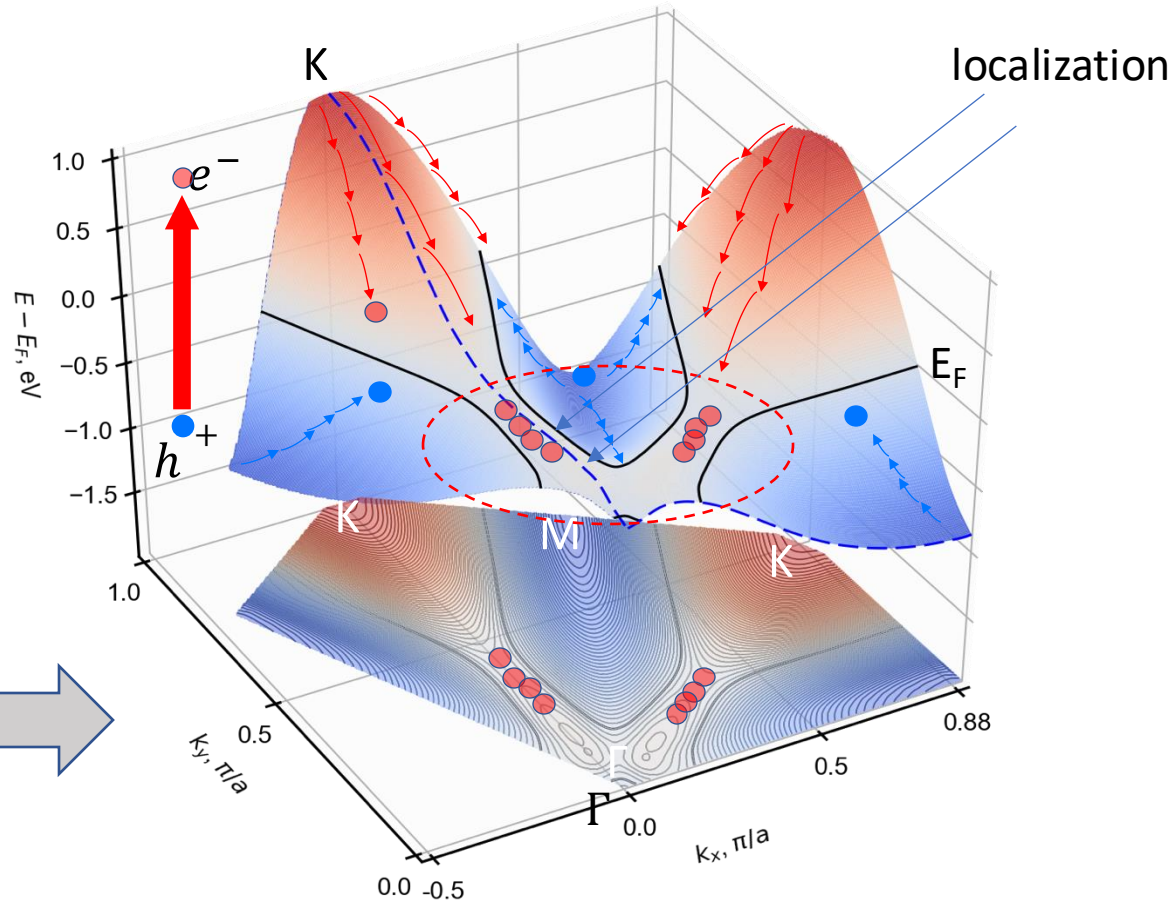
1T-TaS_2: f=1/13, $m^* \sim 3 - 5m_e \rightarrow r_s = \frac{V}{t} = 70\sim100$

Photodoping in 1T-TaS_2 : carrier localization and jamming

Band structure has a single Ta band within +/-1 eV, with a flat band near the Γ point.

e^- and h^+ thermalization via phonons shows an imbalance, leading to electron condensation

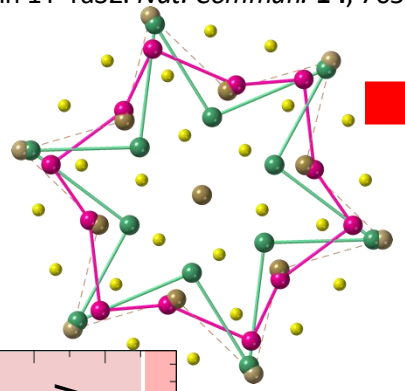


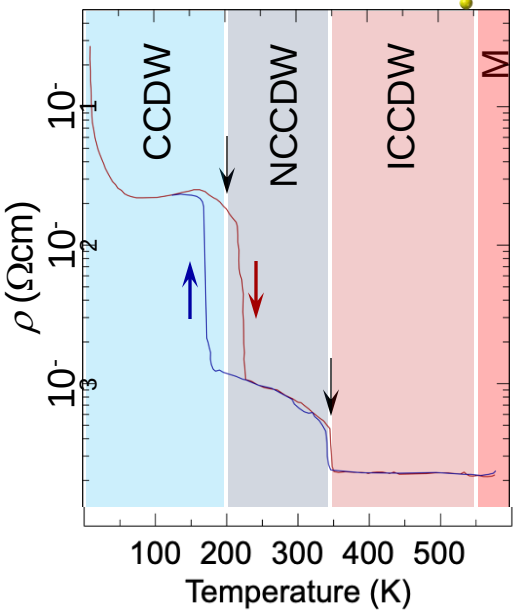


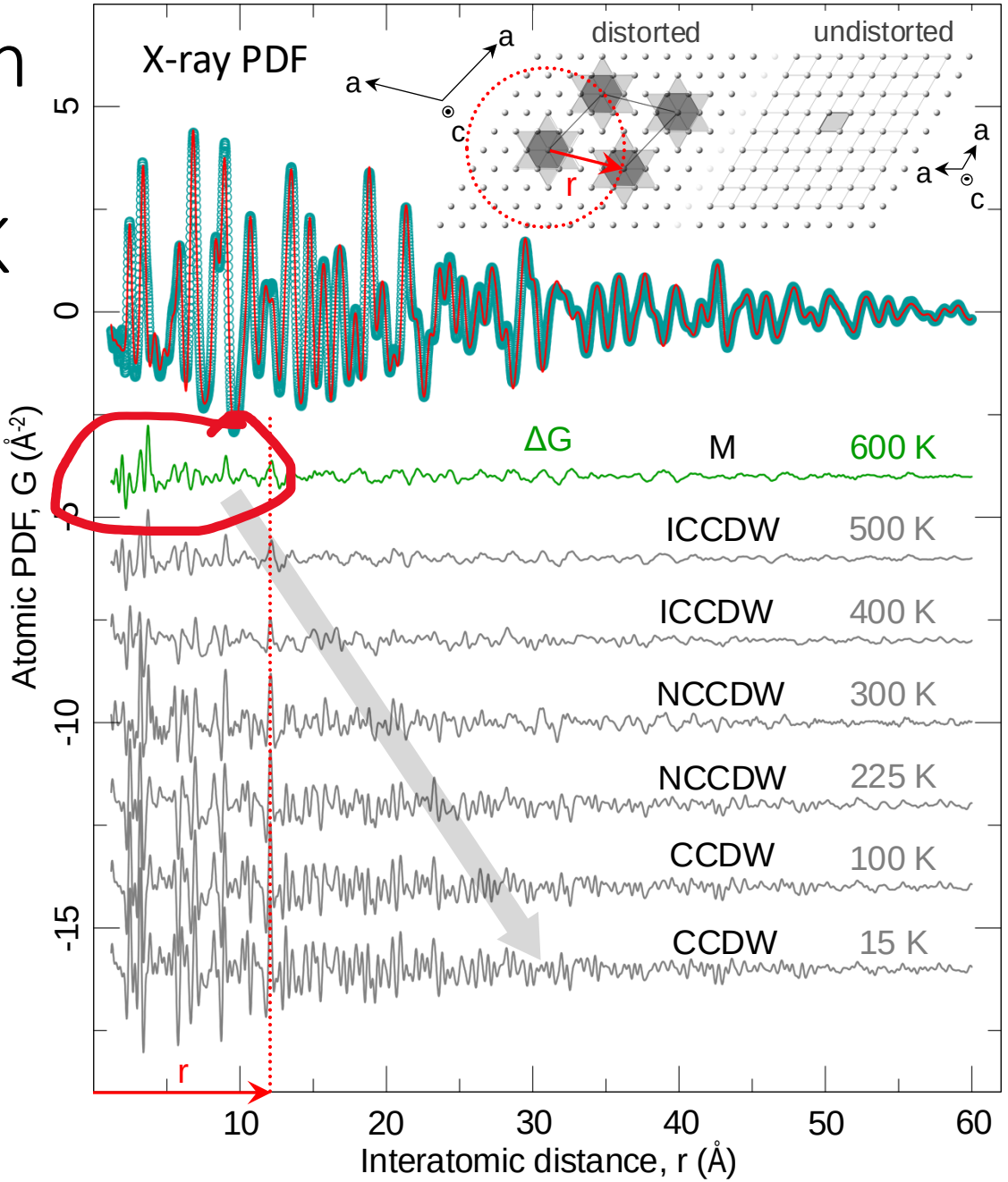
1T-TaS_2 band structure from Ritschel, Nat. Phys. 2014

Polaron signatures in the local structure from 15 K to > 600 K

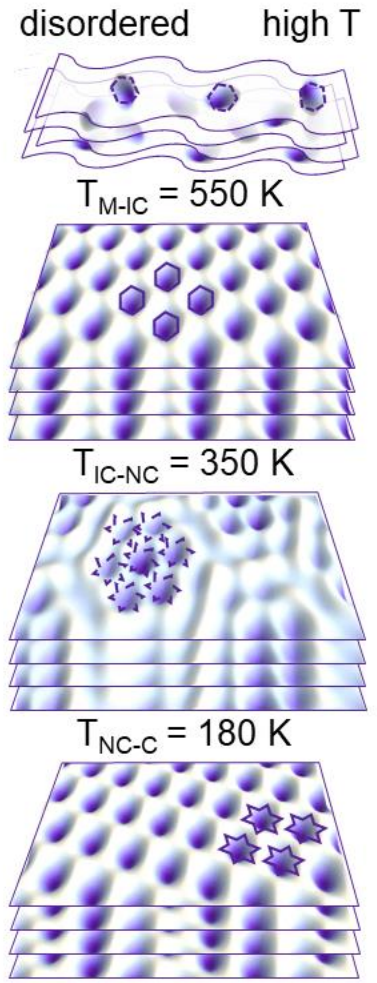
Bozin, E. S. *et al.* Crystallization of polarons through charge and spin ordering transitions in 1T-TaS2. *Nat. Commun.* **14**, 7055 (2023).







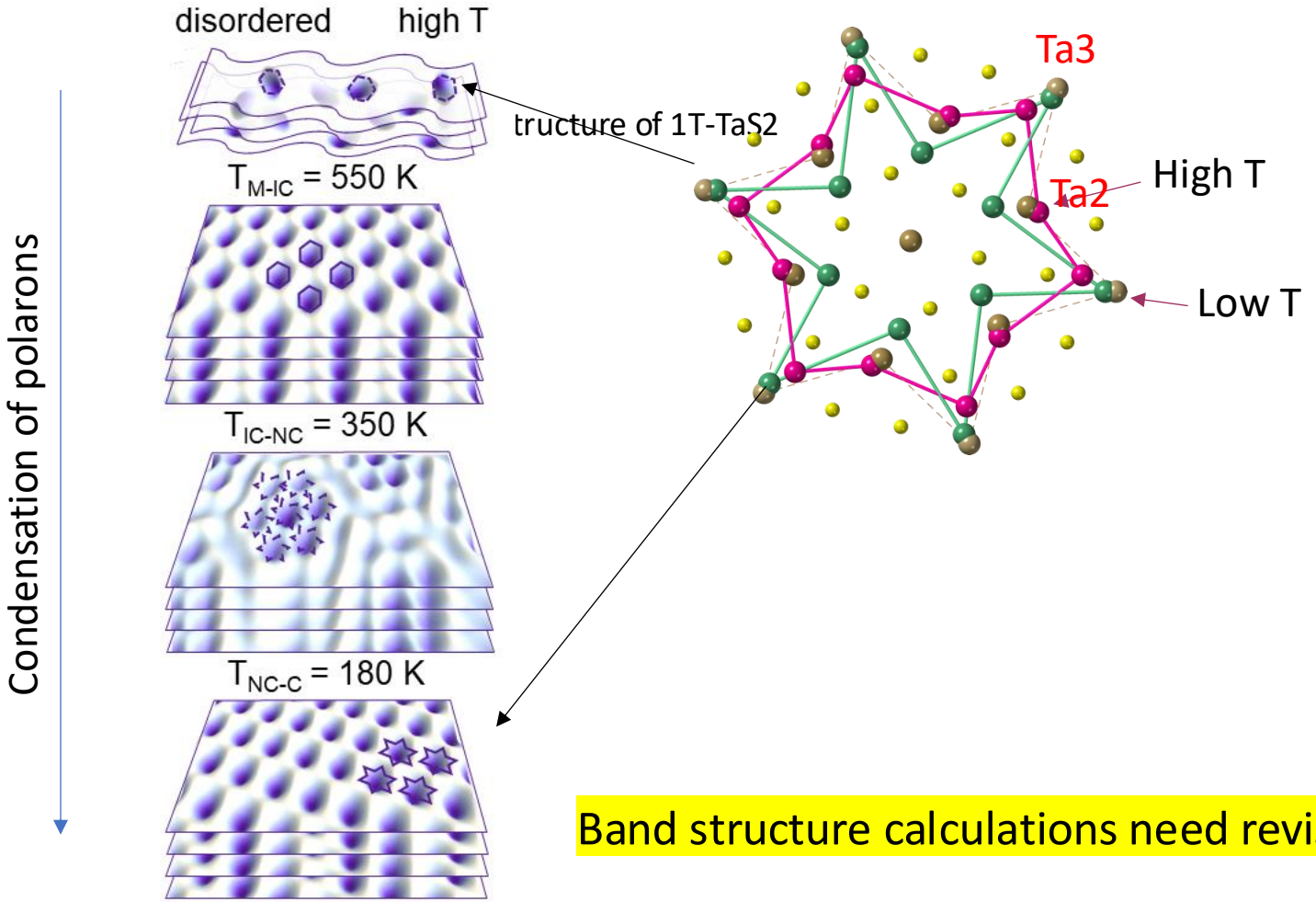
Emil Bozin,



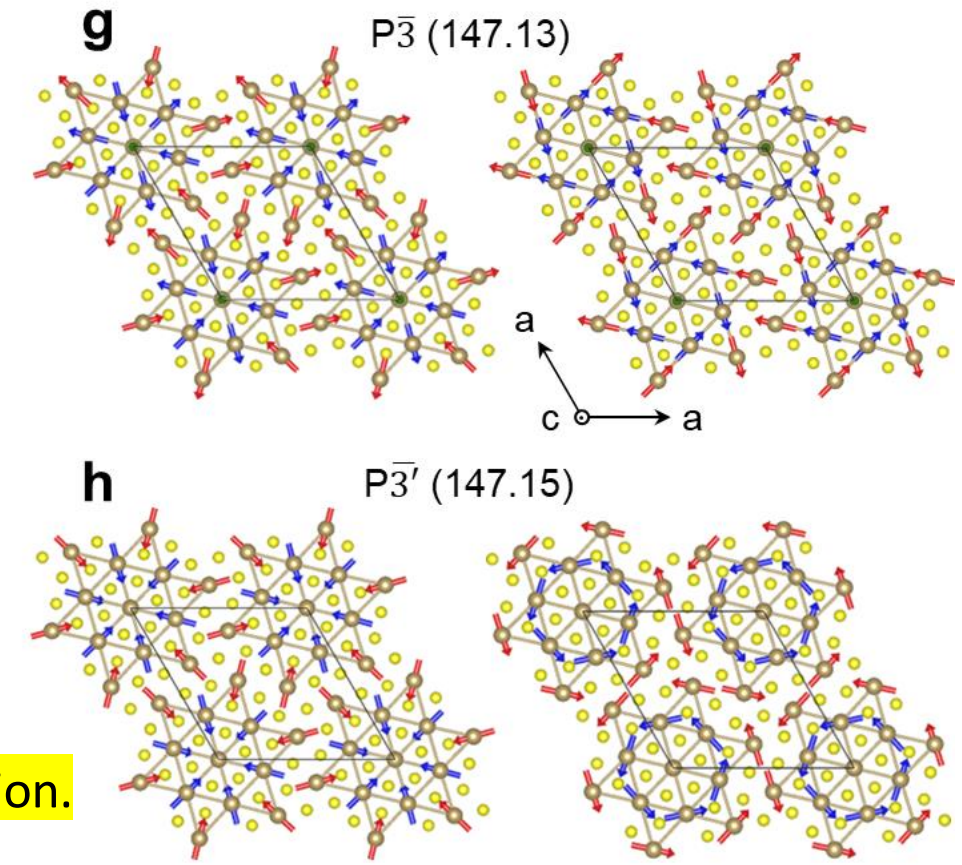
Condensation of polarons

Symmetry-breaking polaron fluctuations at high temperature (X-ray PDF) and a sequence of orders on reducing T

Emil Bozin, 2022



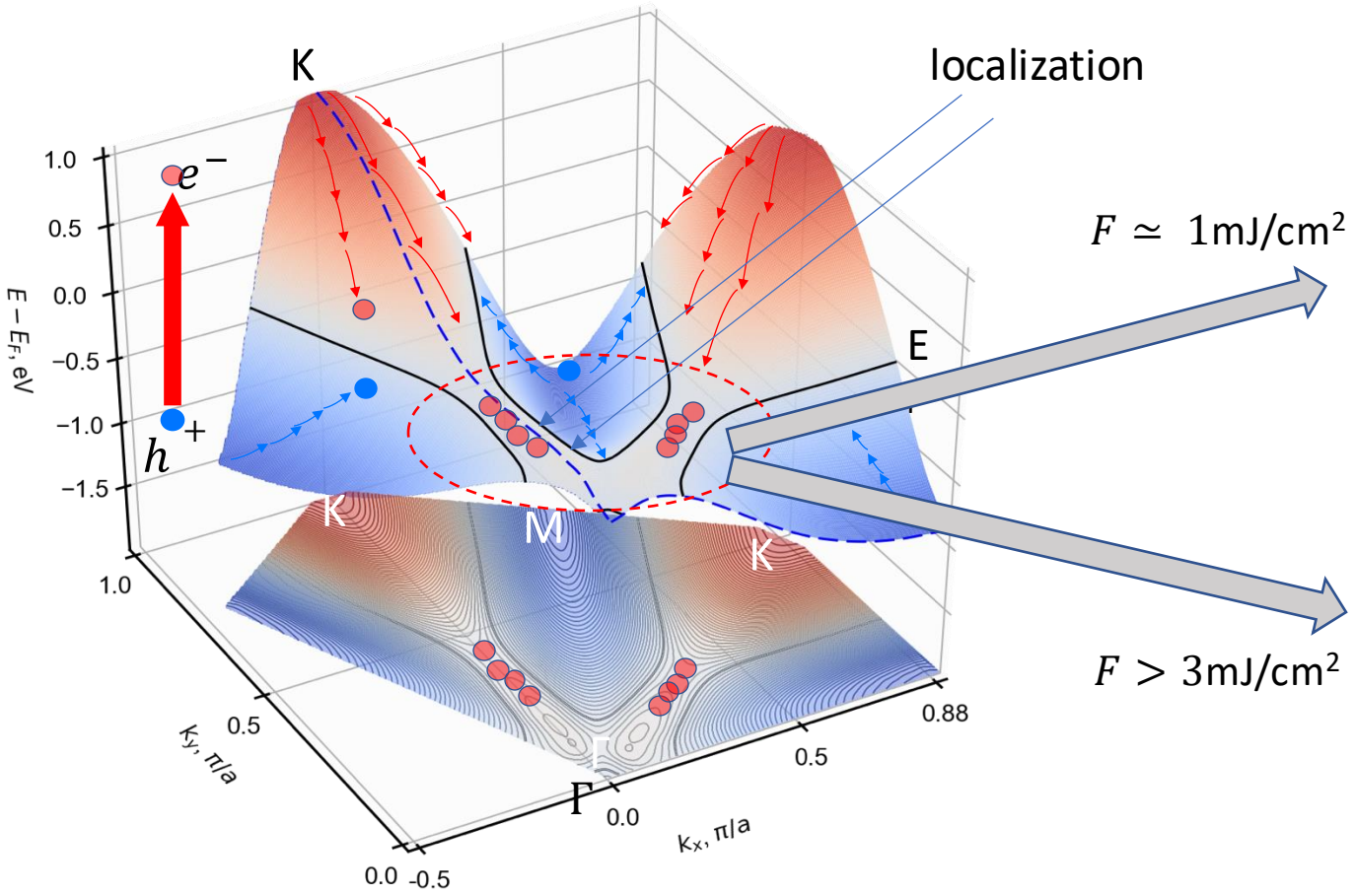
Possible spin structures



Band structure calculations need revision.

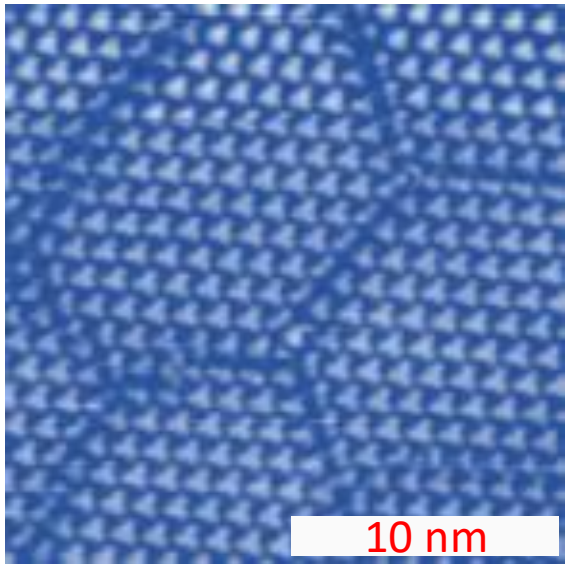
Bozin, E. S. *et al.* Crystallization of polarons through charge and spin ordering transitions in 1T-TaS2. *Nat. Commun.* **14**, 7055 (2023).

Different hidden states reached by varying the excitation conditions



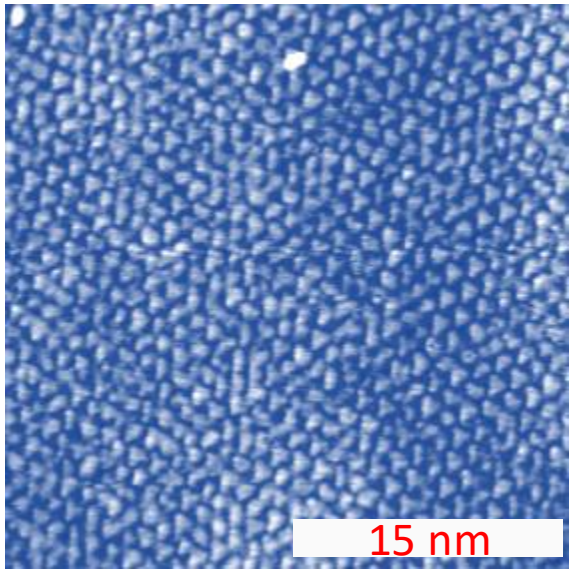
$F \simeq 1\text{mJ/cm}^2$

$F > 3\text{mJ/cm}^2$



'Hidden domain state'

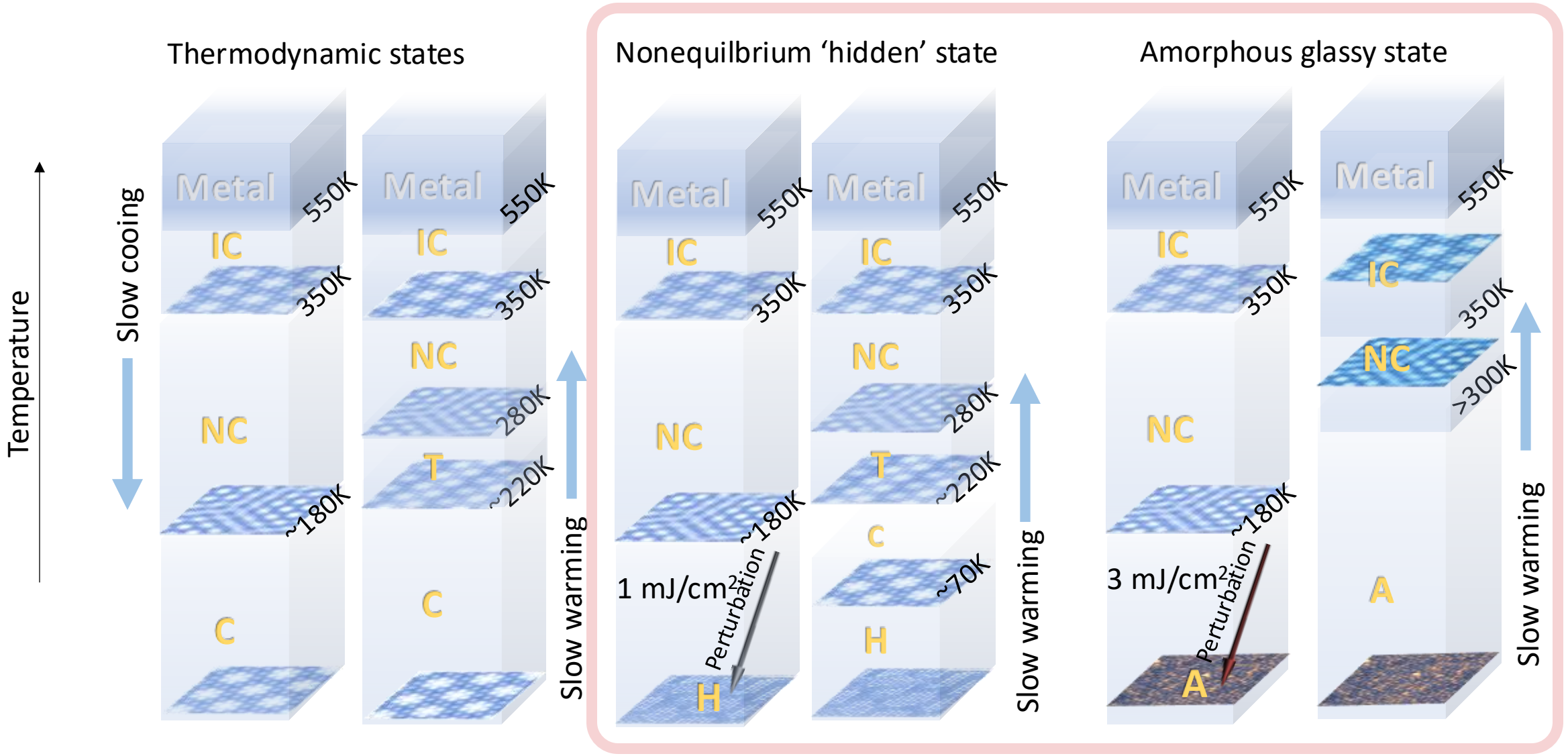
Stojchevska et al ***Science*** 2014



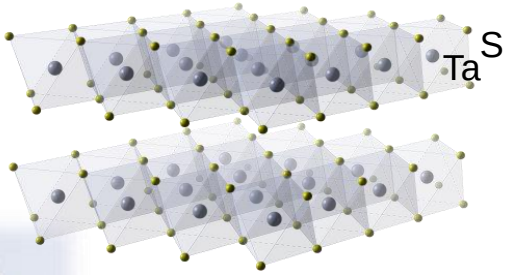
Amorphous electronic state

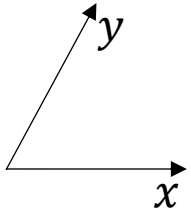
Gerasimenko et al ***Nat Mat*** 2019

Metastable and thermodynamic phases of 1T-TaS_2

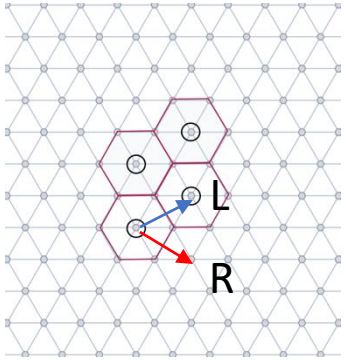


Magic superlattices and Wigner crystals



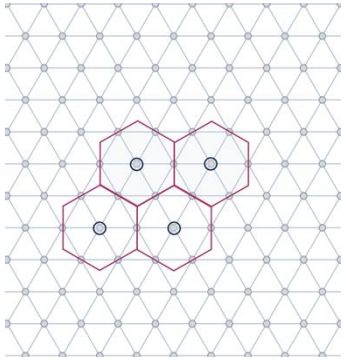


$$\frac{1}{f} = x^2 + y^2 + xy, \text{where } x, y \text{ are integers}$$



$\frac{1}{f} = 3$
$(x = 1, y = 1)$

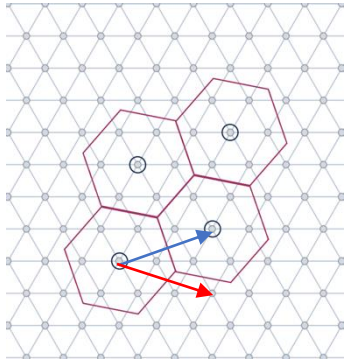
2H-$Fe_{0.33}TaS_2$



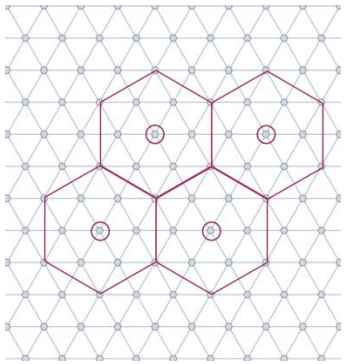
$\frac{1}{f} = 4$
$(x = 2, y = 0)$

1T-$TiSe_2$,
2H-$Fe_{0.33}TaSe_2$,
2H-$Fe_{0.33}NbSe_2$

1T-$Cu_{0.08}TiSe_2$

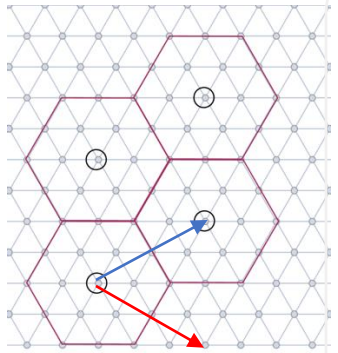


$\frac{1}{f} = 7$
$(x = 2, y = 1)$



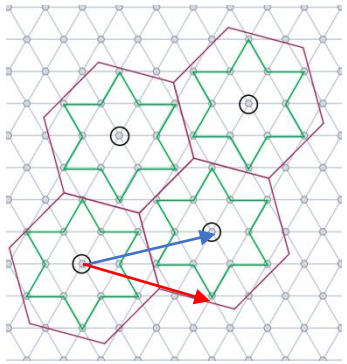
$\frac{1}{f} = 9$
$(x = 3, y = 0)$

2H-TaS_2
2H-$TaSe_2$



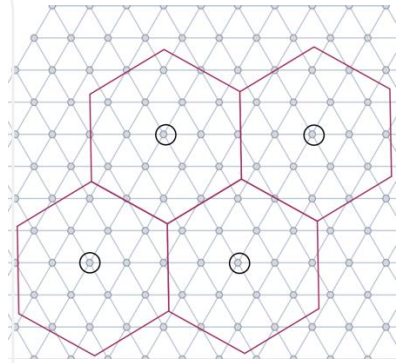
$\frac{1}{f} = 12$
$(x = 2, y = 2)$

H-1T-TaS_2
1T-$Ti_{0.07}Ta_{0.93}Se_2$
1T-TaSeS
1T-$Ta_{0.99}Fe_{0.01}S_2$



$\frac{1}{f} = 13$
$(x = 3, y = 1)$

1T-TaS_2,
1T-$Ti_{0.07}Ta_{0.93}Se_2$
1T-TaSeS
1T-$Ta_{0.99}Fe_{0.01}S_2$



$\frac{1}{f} = 16$
$(x = 4, y = 0)$

1T-VSe_2

Modelling of Wigner crystal superlattices

Jaka Vodeb

Classical charged lattice gas model with screened coulomb interaction:

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

where

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

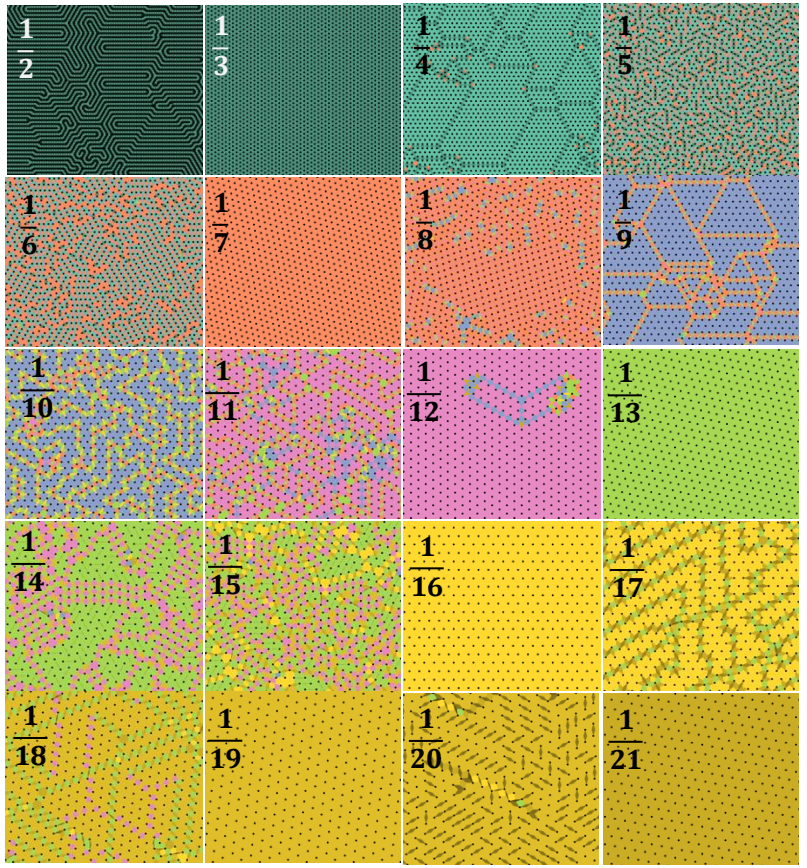
Valid when $r_s = \frac{V}{T} \gg 1$

T is the kinetic energy

Commensurate structures satisfy:

$$\frac{1}{f} = x^2 + y^2 + xy\,,$$

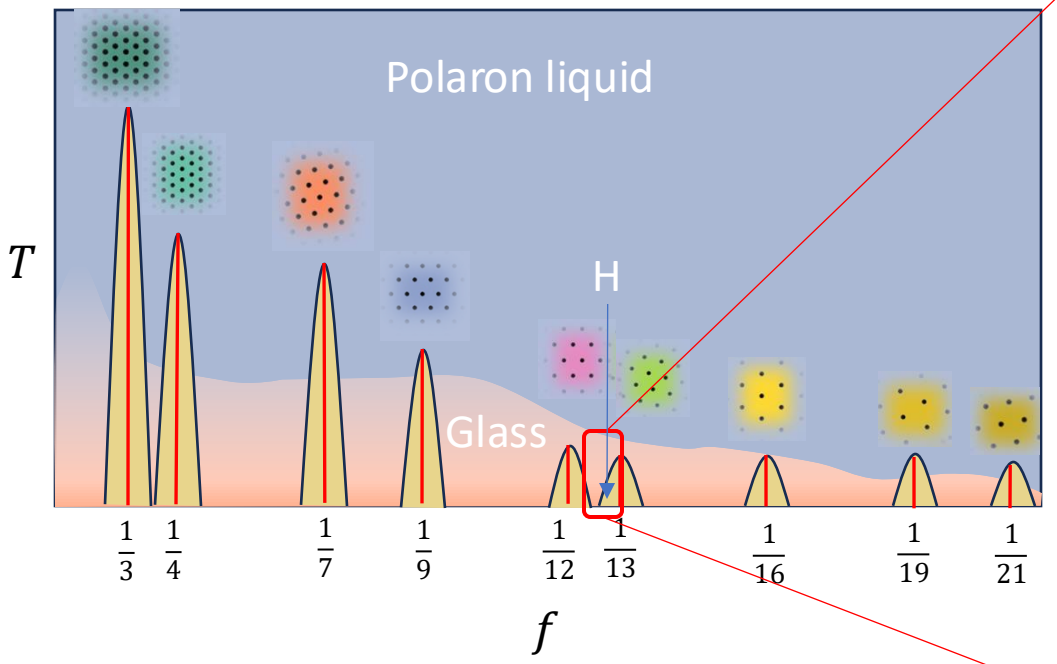
where x and y are integers



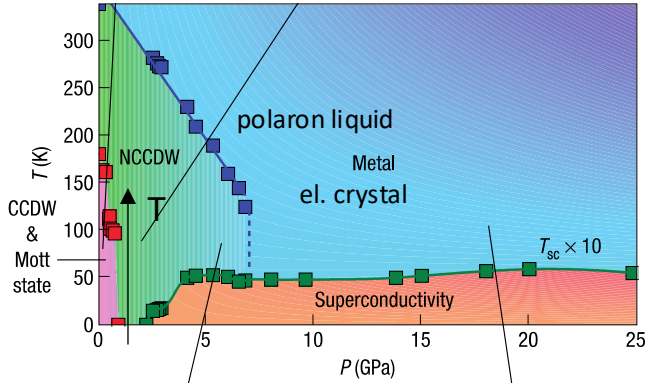
System	f	Phase
2H-$Fe_{0.33}TaS_2$	1/3	crystal
1T-$TiSe_2$	1/4	crystal
1T-$Cu_{0.08}TiSe_2$	1/4.2	domain state
2H-$Fe_{0.33}TaSe_2$	1/4	crystal
2H-$Fe_{0.33}NbSe_2$	1/4	crystal
2H-TaS_2	1/9	crystal
2H-$TaSe_2$	1/9	crystal
2H-$NbSe_2$	$\sim$ 1/9	domain state
1T-TaS_2	1/13	crystal
PD 1T-TaS_2	1/12.6	domain state
1T-TaSeS	1/12.6	domain state
1T-$Ta_{0.99}Fe_{0.01}S_2$	1/12.6	domain state
1T-$Nb_{0.04}TaS_2$	$\sim$ 1/13	domain state
1T-$Nb_{0.07}TaS_2$	$\sim$ 1/13	domain state
PD 1T-TaS_2	1/11	amorphous state
1T-$Nb_{0.1}TaS_2$	$\sim$ 1/11	possible amorphous state
4Hb-TaS_2	1/13	crystal
1T-$TaSe_2$	1/13	crystal
1T-$Ti_{0.07}Ta_{0.93}Se_2$	1/12.6	domain state
4Hb-$TaSe_2$	1/13	crystal
1T-$NbSe_2$	1/13	crystal
1T-VSe_2	1/16	crystal

Karpov, P. & Brazovskii, S. Sci Rep **8**, 1–7 (2018).
Vodeb, J. *et al. New J Phys* **21**, 083001 (2019).

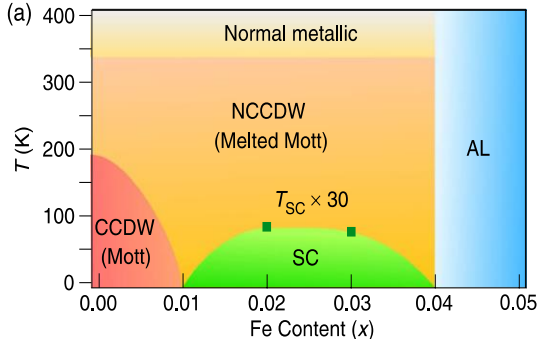
Phase diagram of magical fraction superlattices



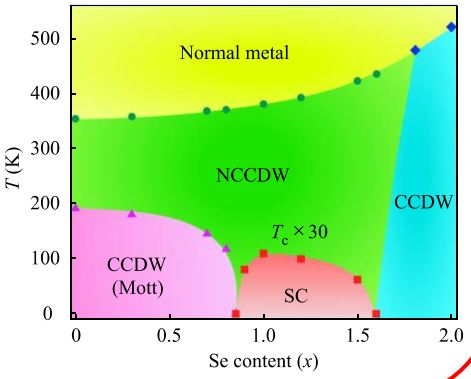
Hydrostatic pressure



Fe doping



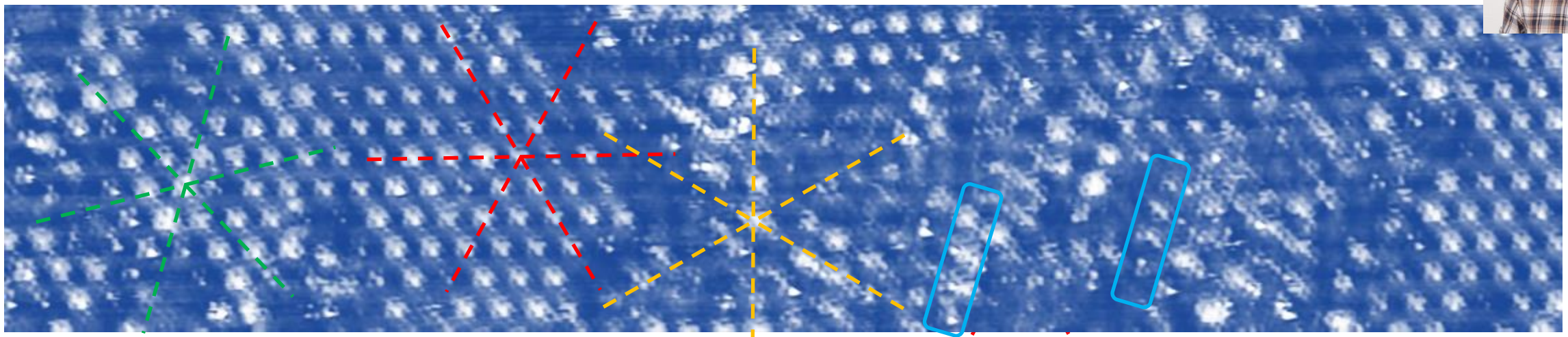
Se substitution



NB: WC physics is dominant for small t and large $r_s = V/t$

t is determined by the e-p coupling strength of conduction band electrons

Coexisting metastable superlattices after photoexcitation



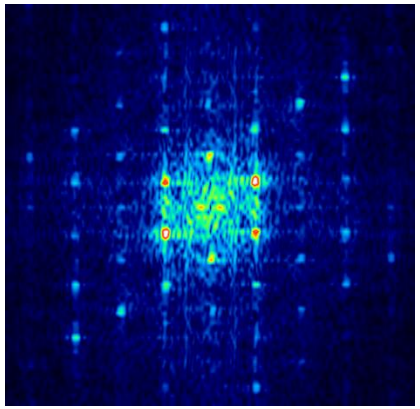
4 K

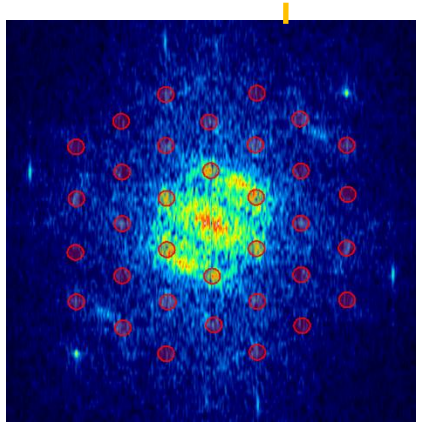
Crystal lattice

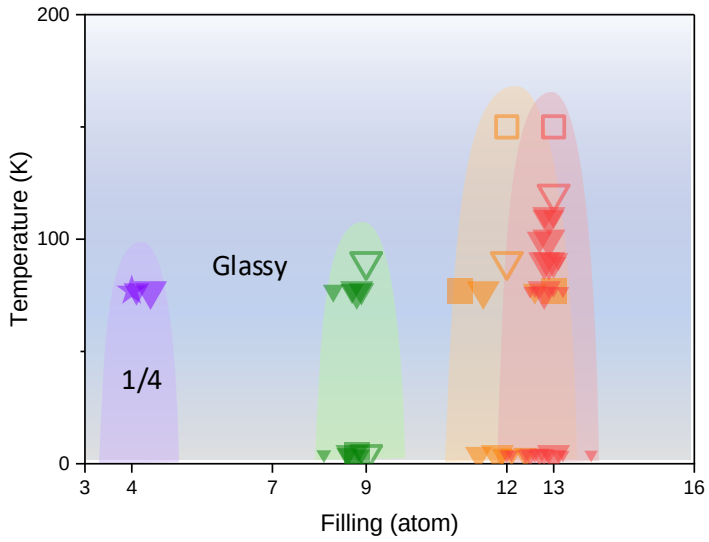
1/13 L

1/13 R

1/9

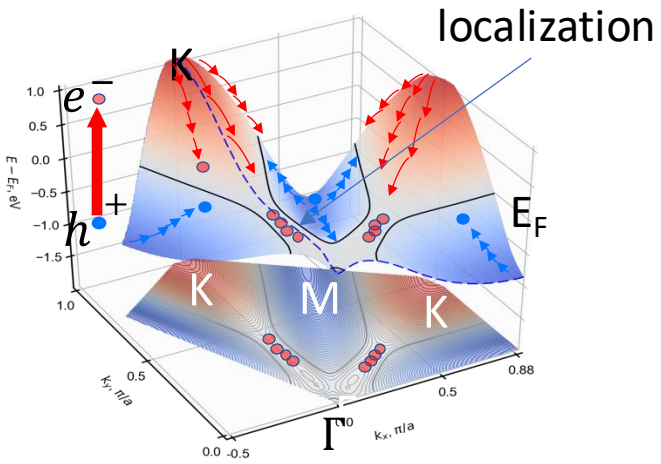


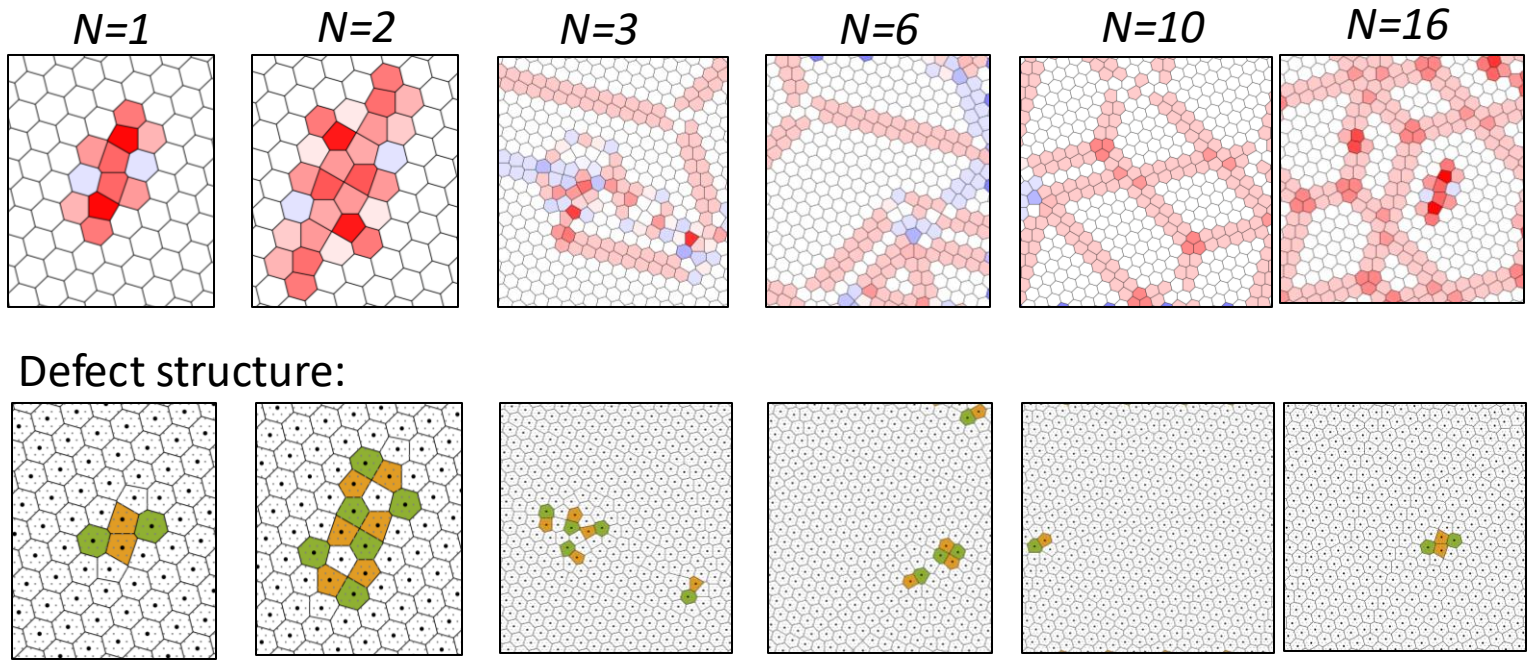




(Photo) doping of the C superlattice

MC simulations of a polaronic Wigner crystal

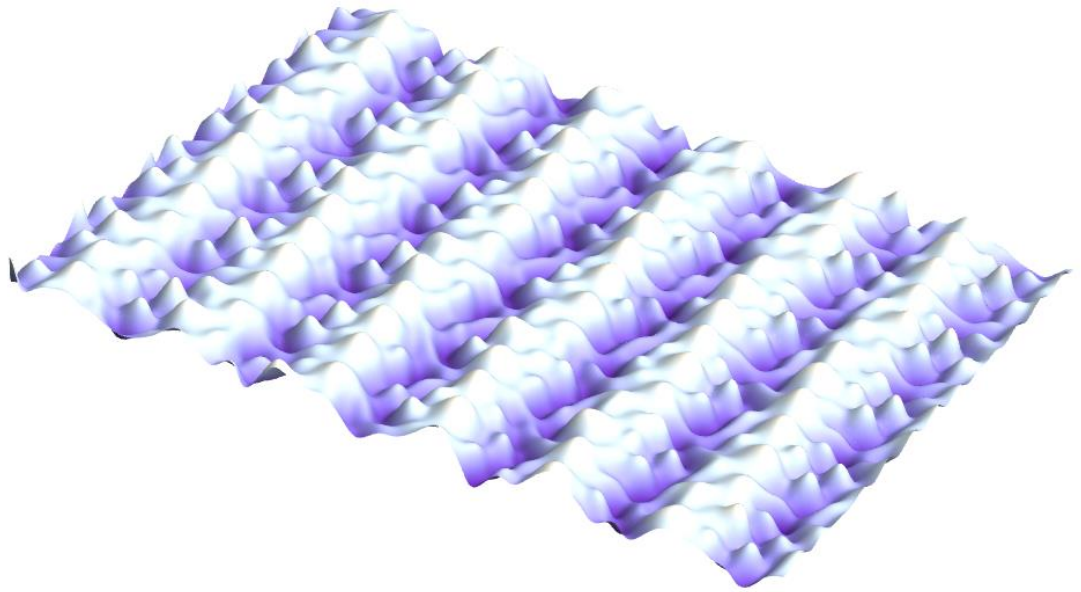


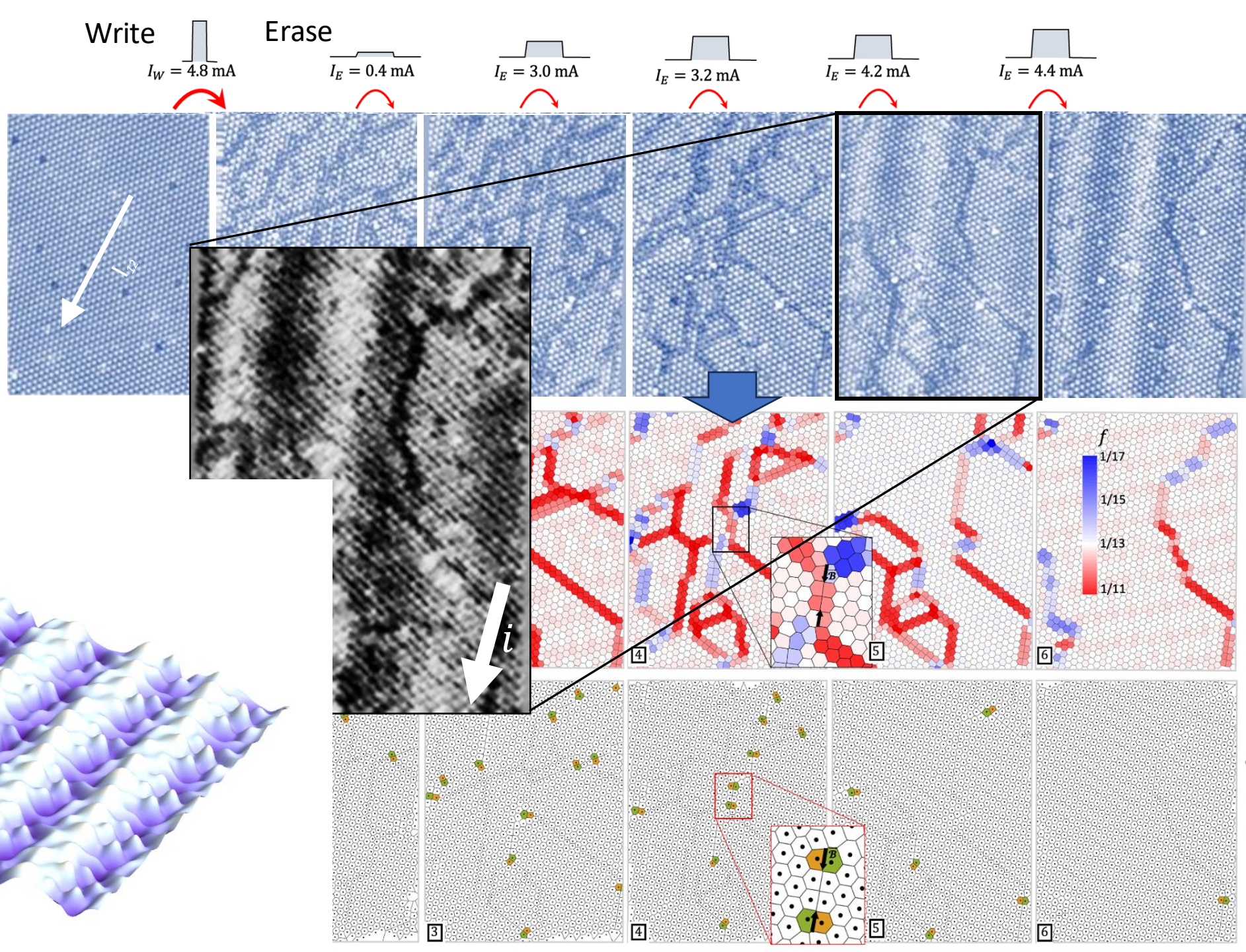


Mraz, A. *et al. Nat. Commun.* **14**, 8214 (2023).

STM experiment: Wigner-Seitz tesselation and non-trivial defects

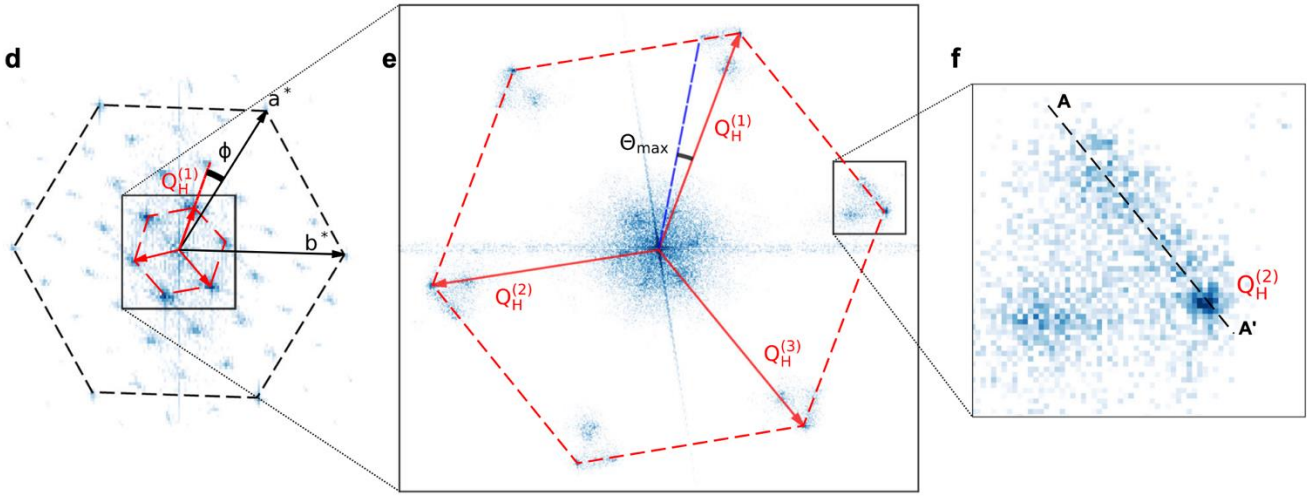
Raw STM images



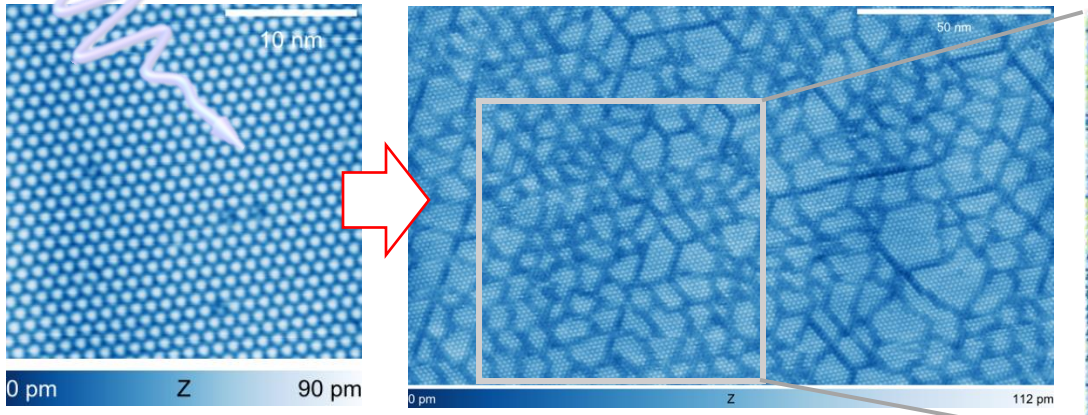


The hidden state shows emergent mesoscopic orders

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

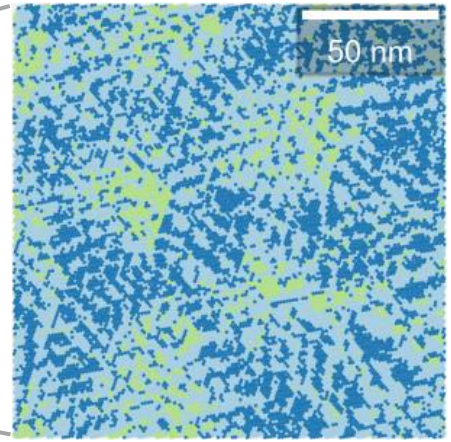


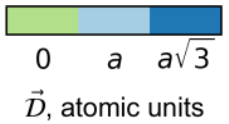
STM topography



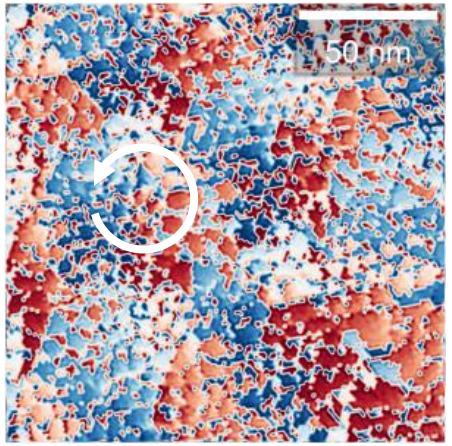
35 fs, 1 mJ/cm² laser pulse, or electrical pulse

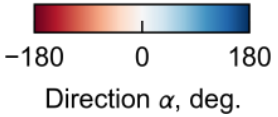
Displacement $|\vec{D}|$



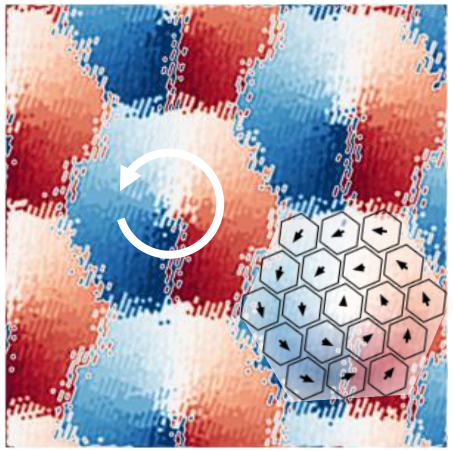


Displacement angle $\boldsymbol{\alpha}$





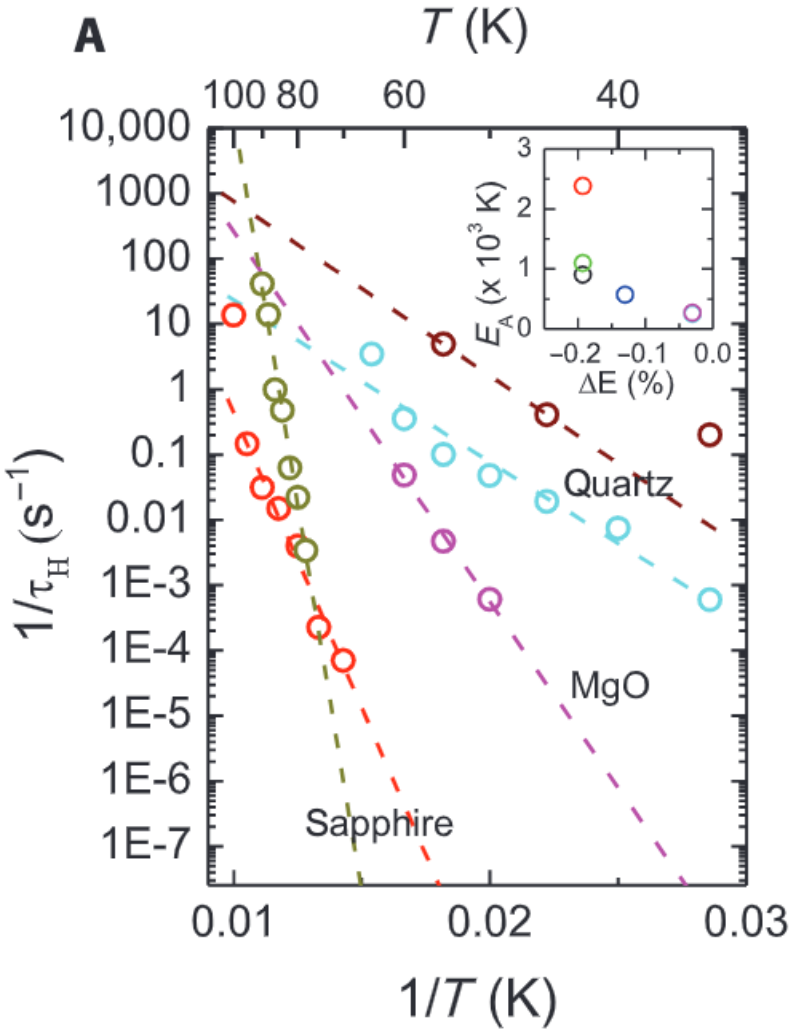
Simulation of $\boldsymbol{\alpha}$

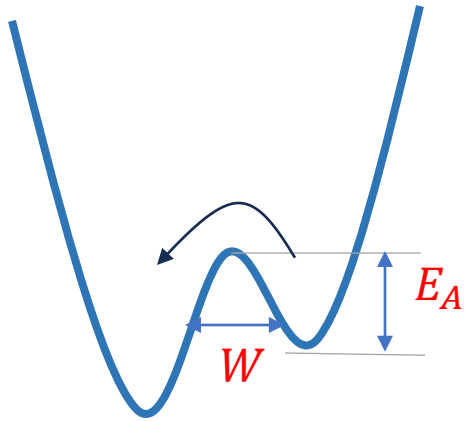


$\vec{D}$

Dynamics

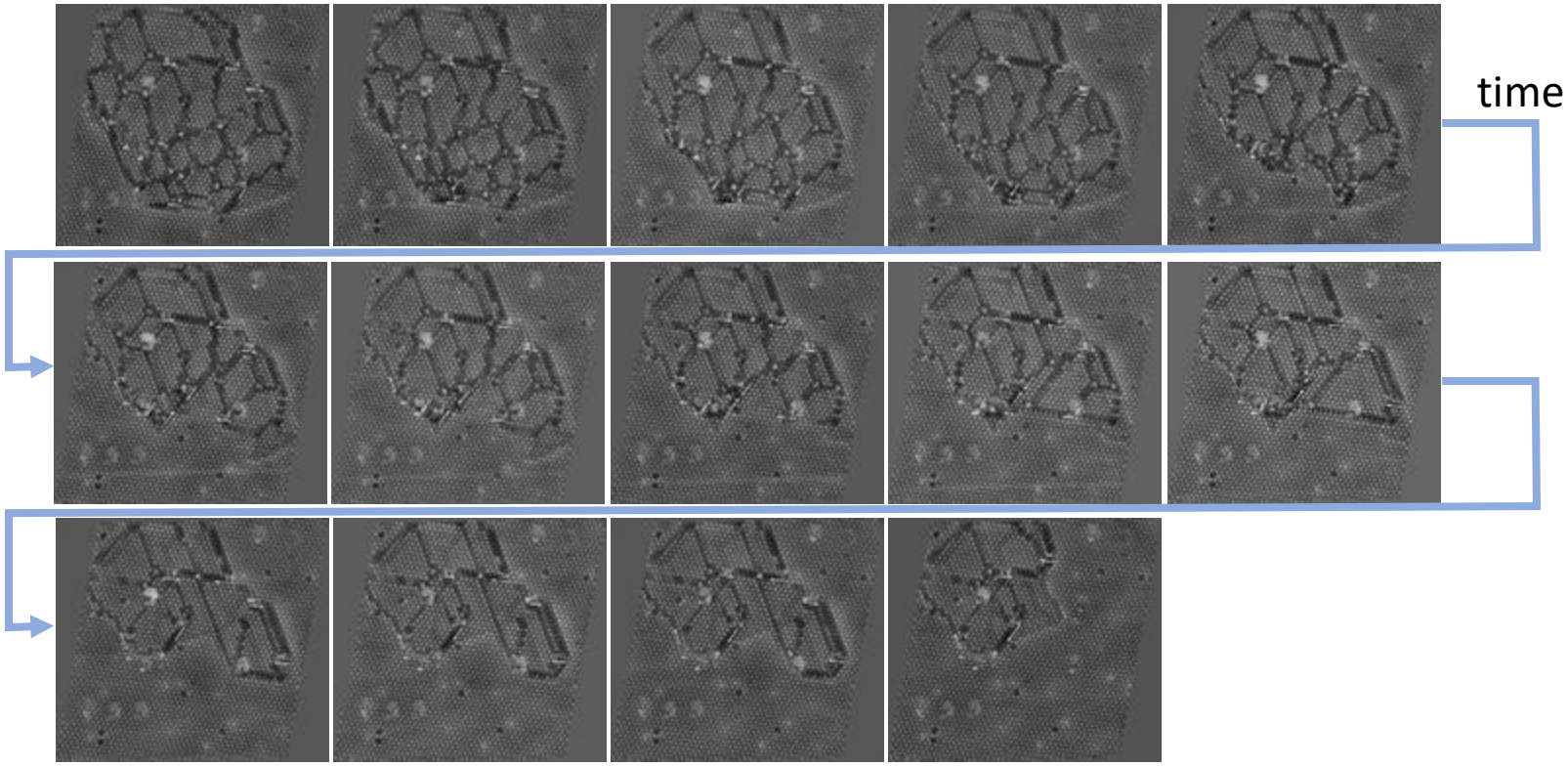
The Hidden state relaxation time depends on temperature and strain

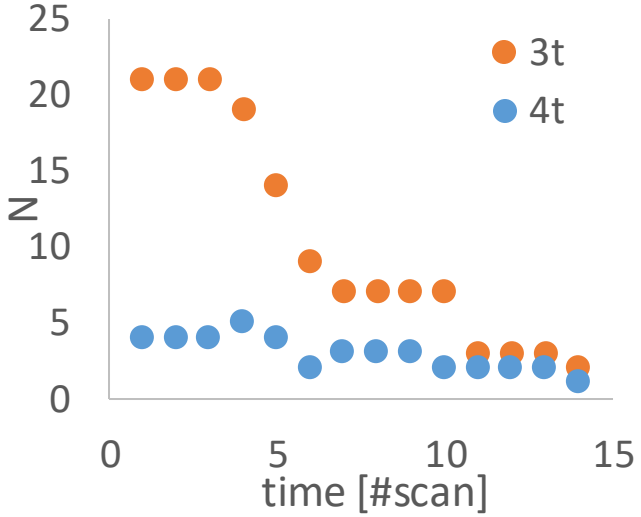


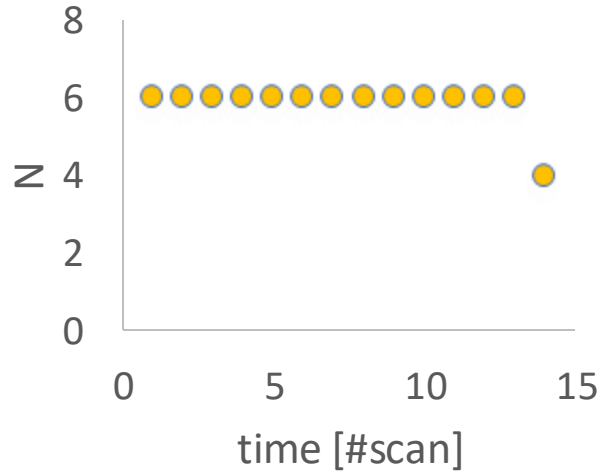


Vaskivskyi, I. *et al.* Controlling the metal-to-insulator relaxation of the metastable hidden quantum state in 1T-TaS2. *Sci Adv* **1**, e1500168 (2015).

Spontaneous relaxation through configurational states





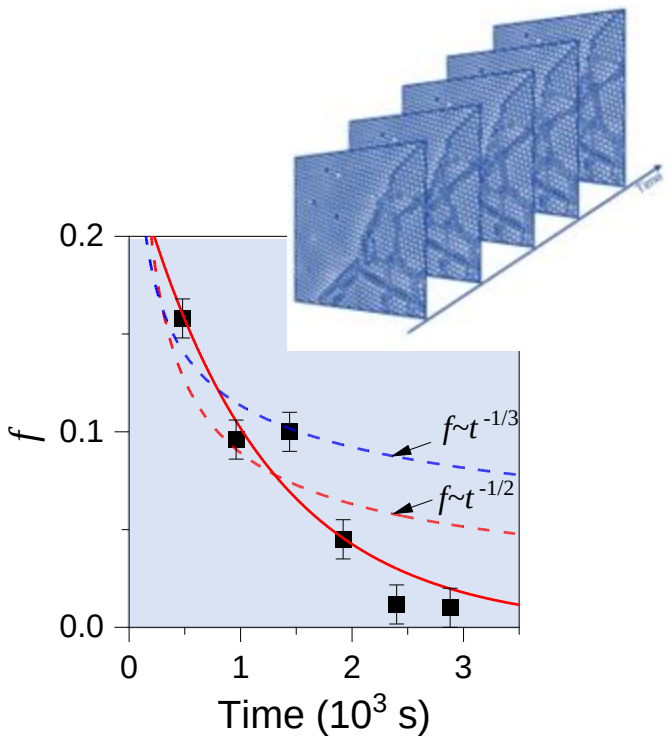


Topologically non-trivial defects stabilize the ‘hidden’ domain state

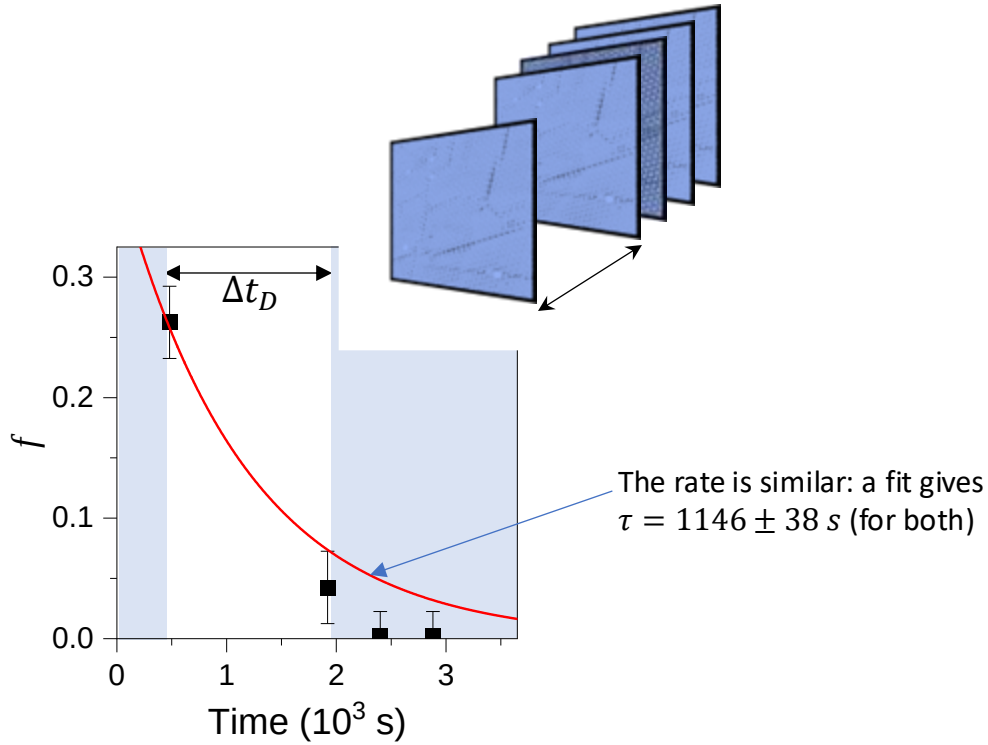
Kranjec et al, *Symmetry* 2022, 14, 926. https:// doi.org/10.3390/sym14050926

Tip-enhanced relaxation?

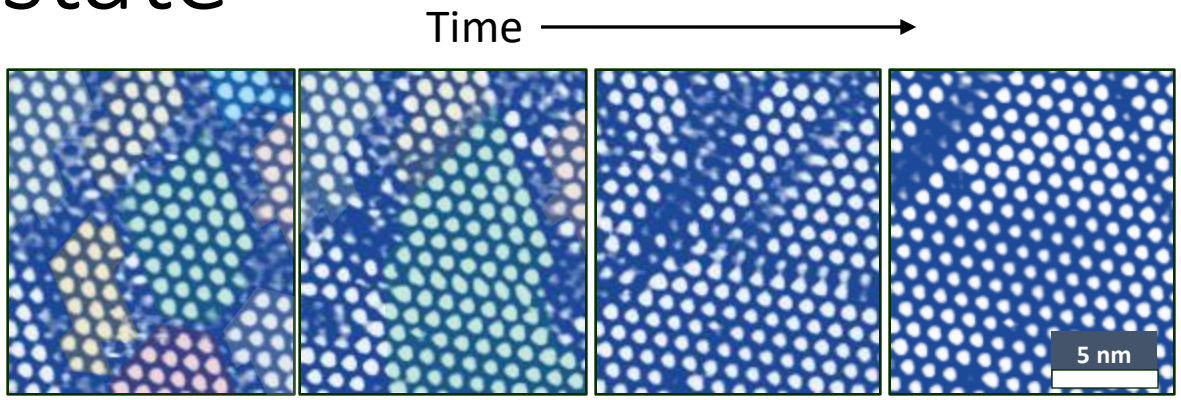
Relaxation with tip scanning

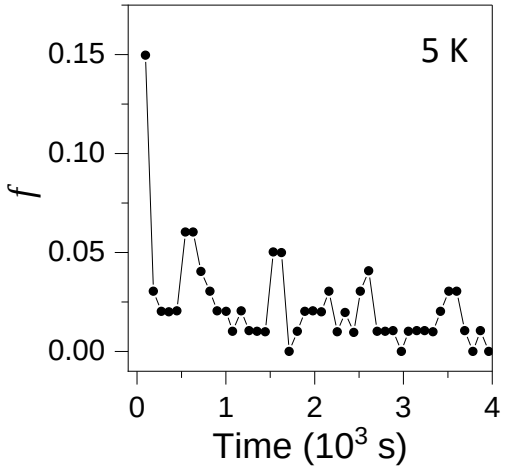


Relaxation with NO tip scanning

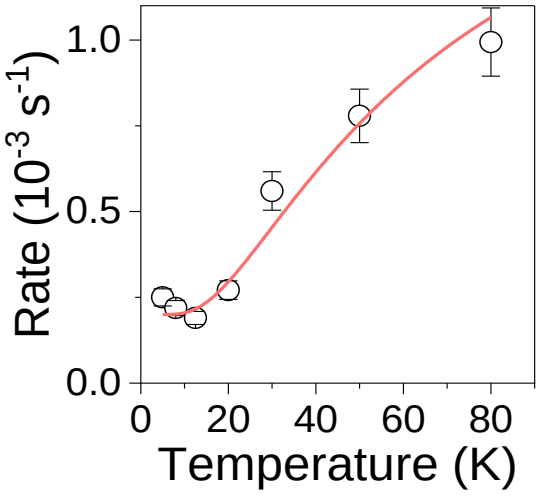


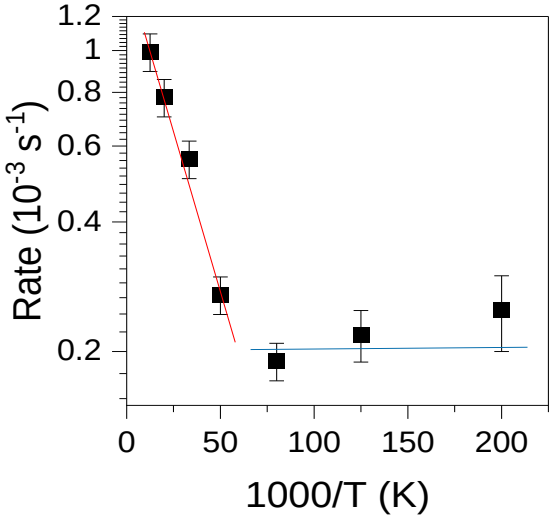
Spontaneous decay dynamics of the domain state





f = 'Hamming distance' (how many polarons have moved from one configuration to another)

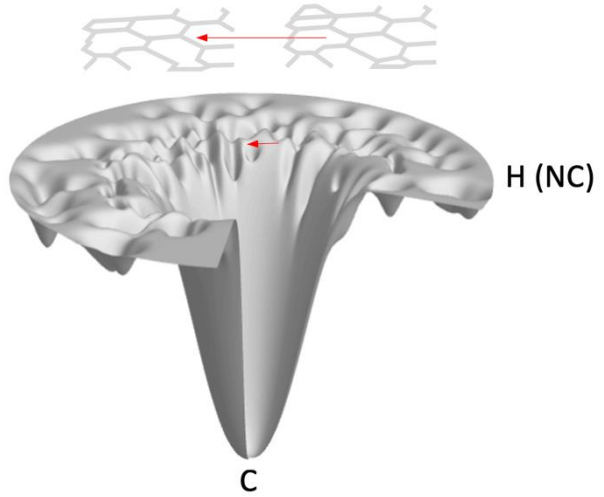




$$R(T) = R_q + R_0 e^{-E_B/k_B T}$$

E_B is determined by the energy difference between configurational states

R_0 is related to the Hamming distance

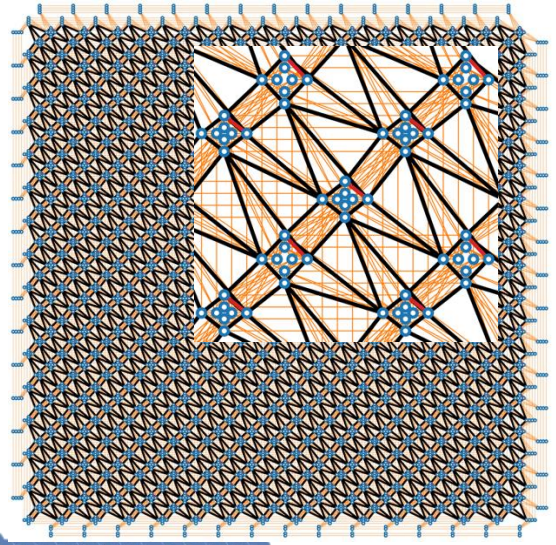


Vodeb et al., Nat. Commun. **15**, 4836 (2024).

Quantum simulations

From CLG via Jordan-Wigner transformation:

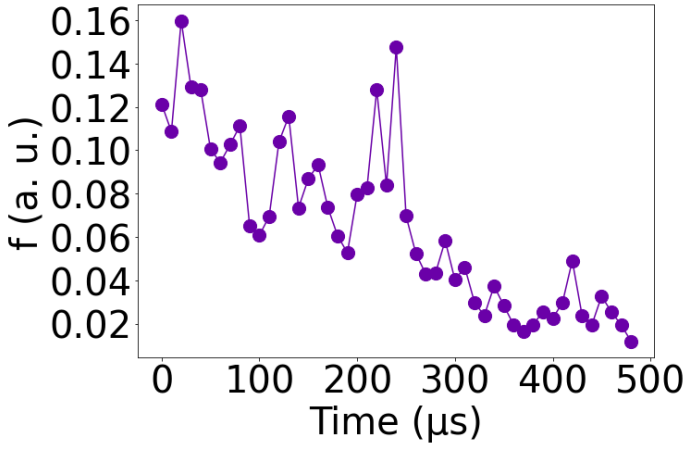
$$H_S = -A(s)\sum_i \sigma_i^x/2 + B(s)\left(\sum_{i<j} J_{i,j}\sigma_i^z\sigma_j^z + \sum_i h_i\sigma_i^z\right)/2$$



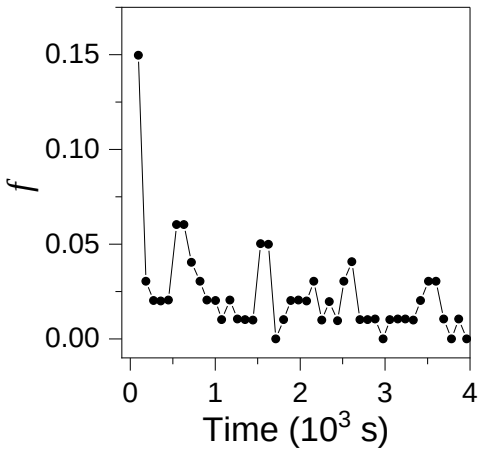
Custom embedding on the D-wave Advantage 6.1 QPU

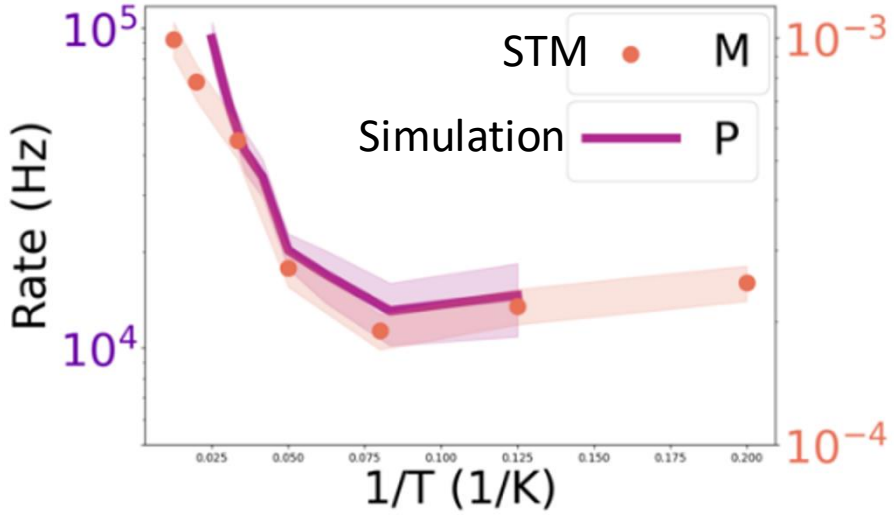
Vodeb et al., Nat. Comm. **15**, 4836 (2024).

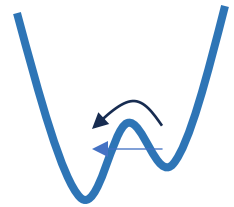
Simulation



Experiment (STM)

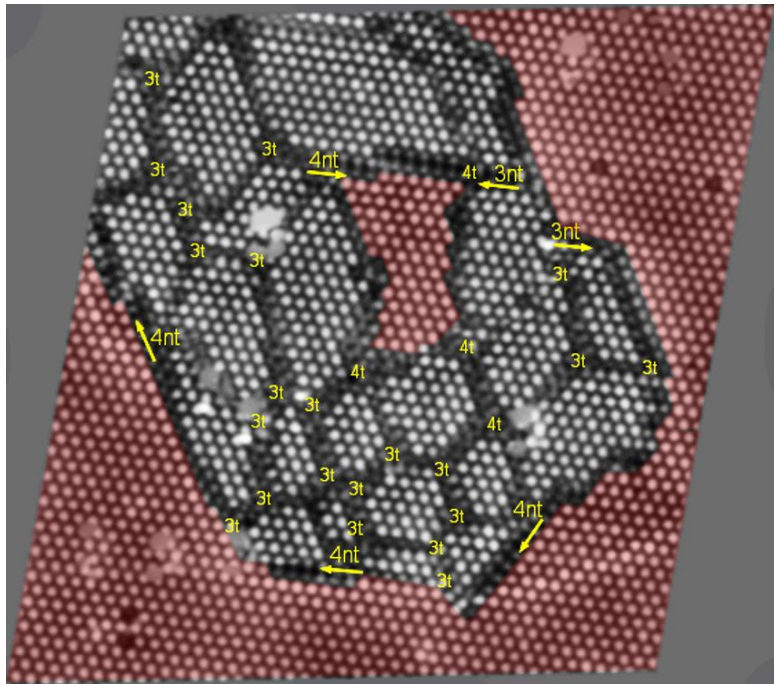




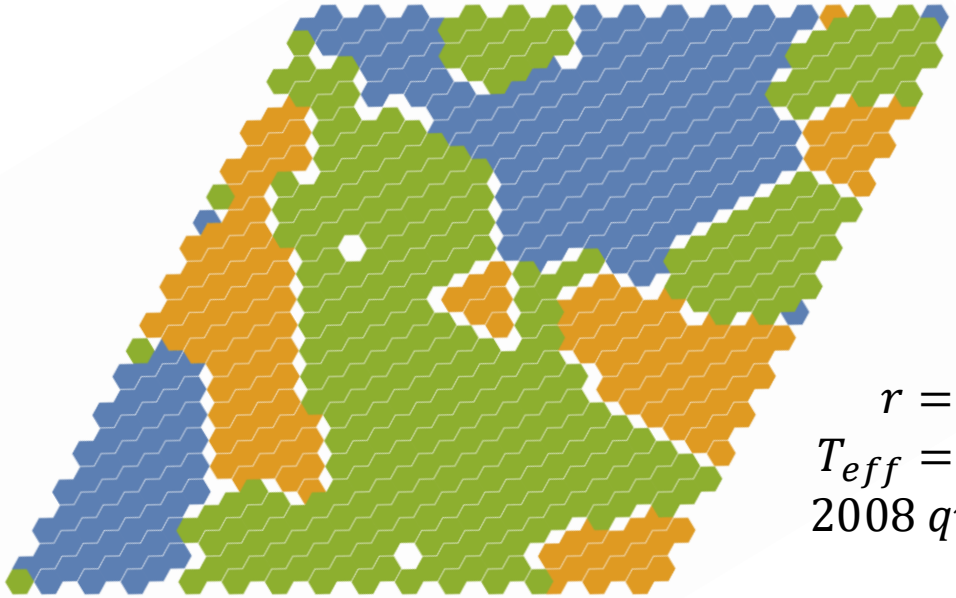


Experiment and simulation of quantum decay

Sequence of STM images
~30 minutes per image



STM topography:
Domain state decay at 4 K in 1T-TaS_2



$r = 9$
$T_{eff} = 1.33$
$2008\ qubits$

Simulation on D-Wave quantum annealer

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

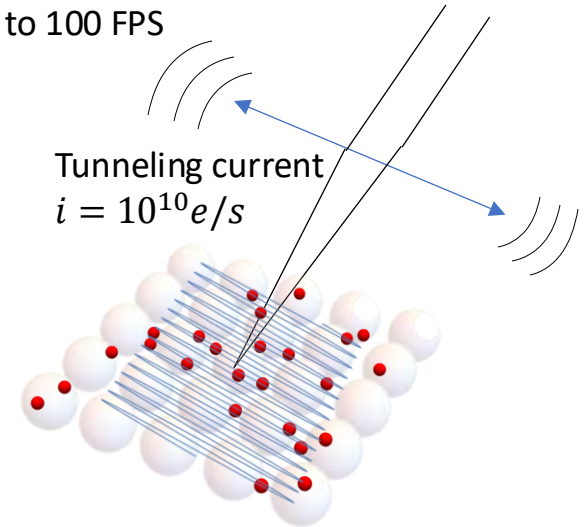
Vodeb et al., Nat. Comm. **15**, 4836 (2024).

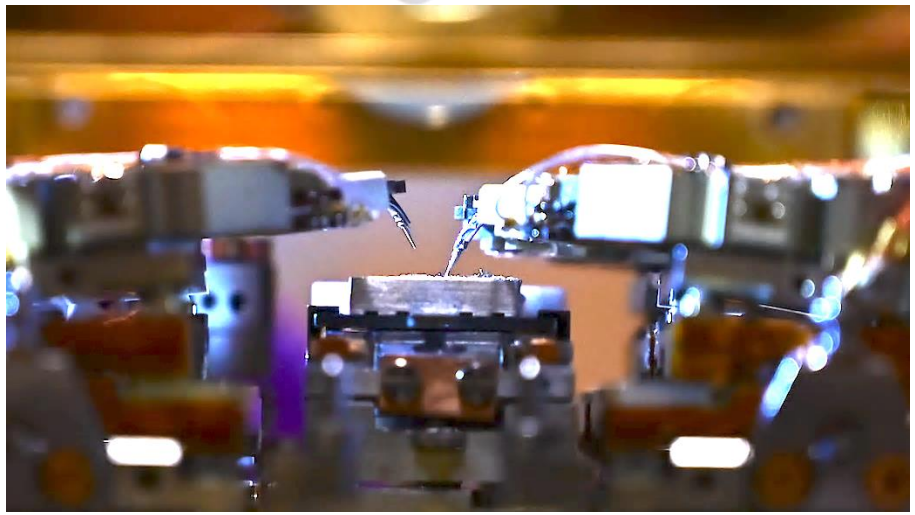
Fast-STM imaging of domain fluctuations in the H state of 1T-TaS_2

FAST scanning STM

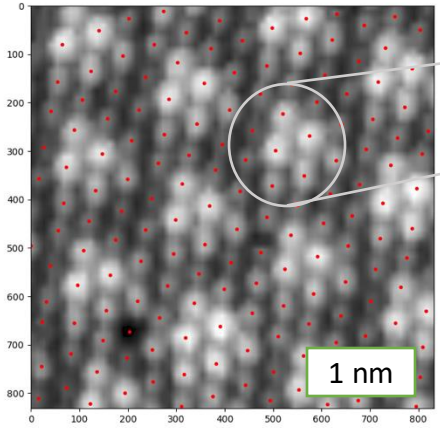
Up to 100 MHz sampling per pixel

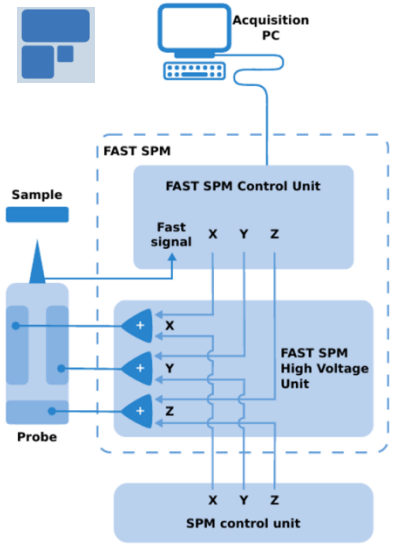
up to 100 FPS



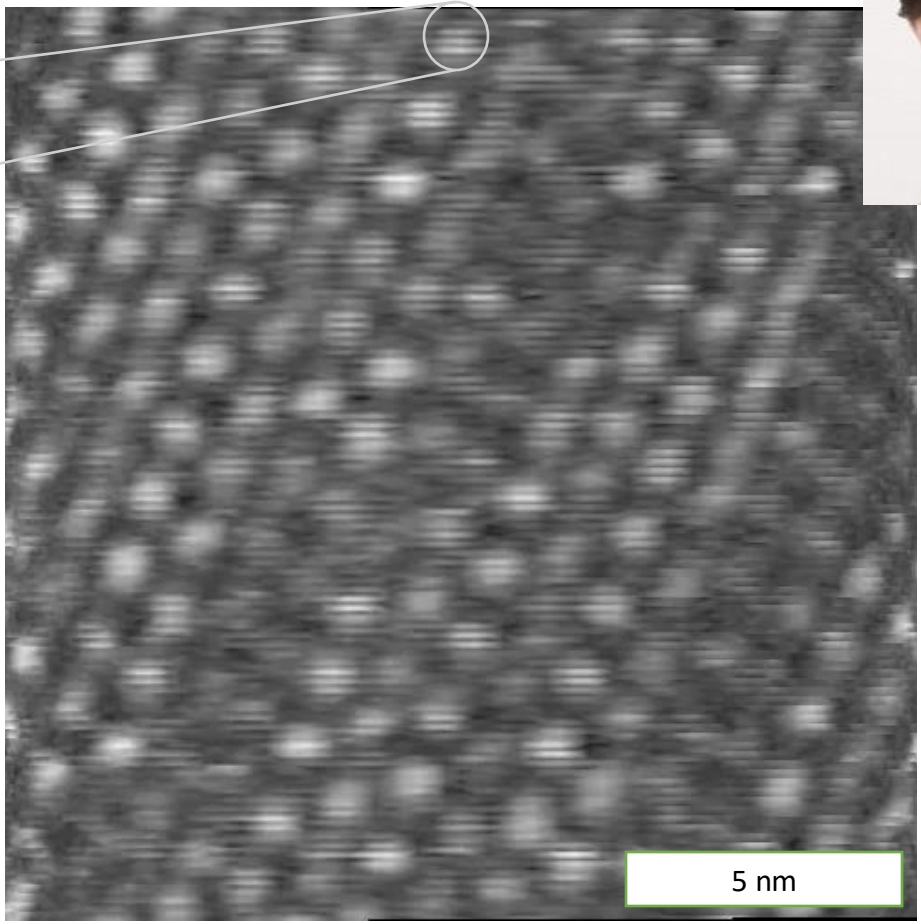


Atomic resolution





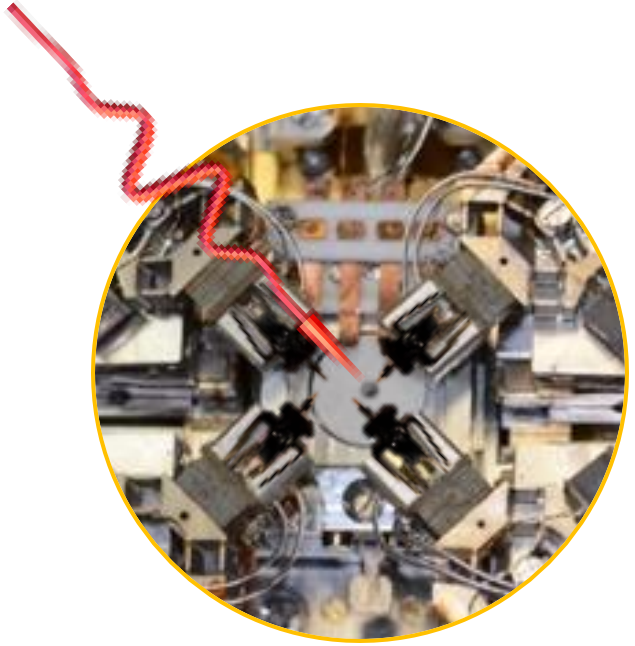
Raw real-time movie at 6 Hz framerate



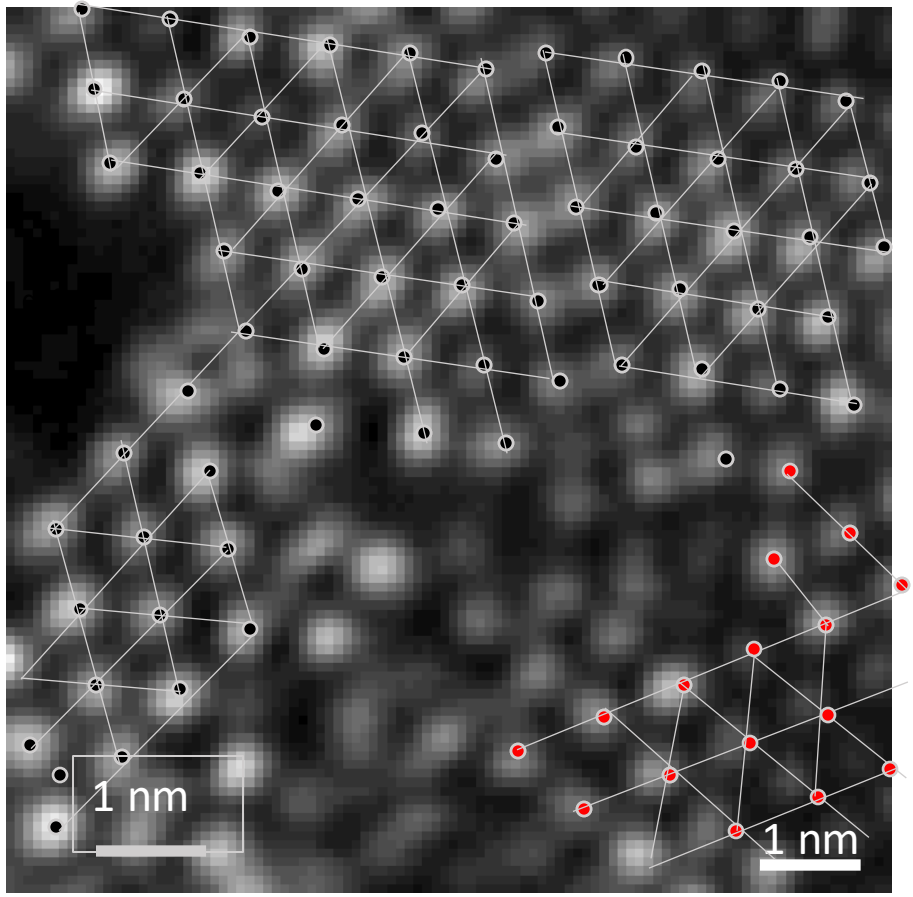
$i = 1\,nA, V = 0.8\,V$

Yevhenii Vaskivskyi

A L-R domain vertex

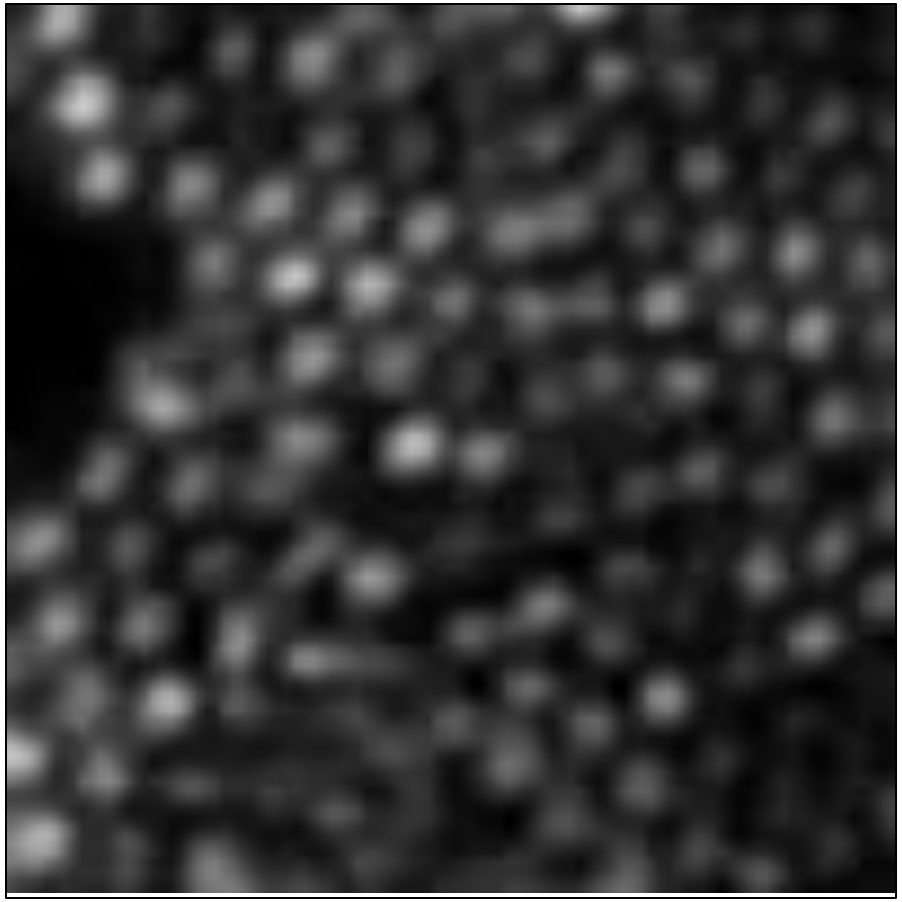


Quench



$i = 1\,nA, V = 0.8\,V$

Fast STM polaron dynamics in real time

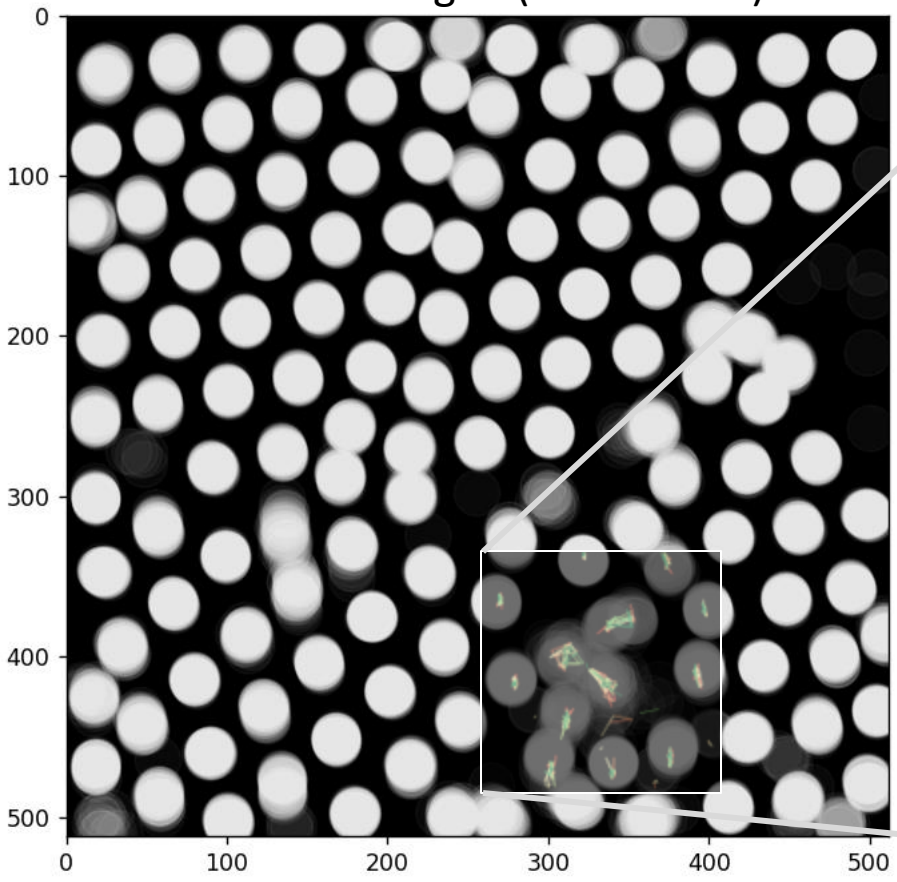


1T-TaS_2 6 Hz STM real time video

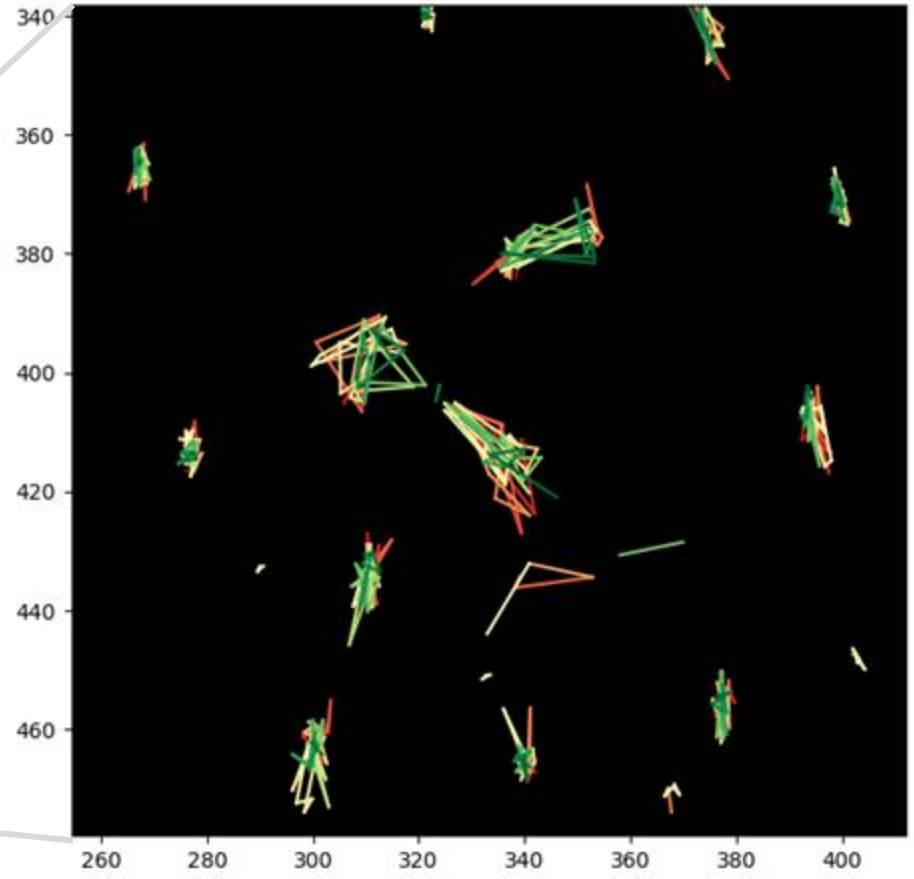
$i = 1\ nA, V = 0.8\ V$
T=77K

Electron ‘trajectories’

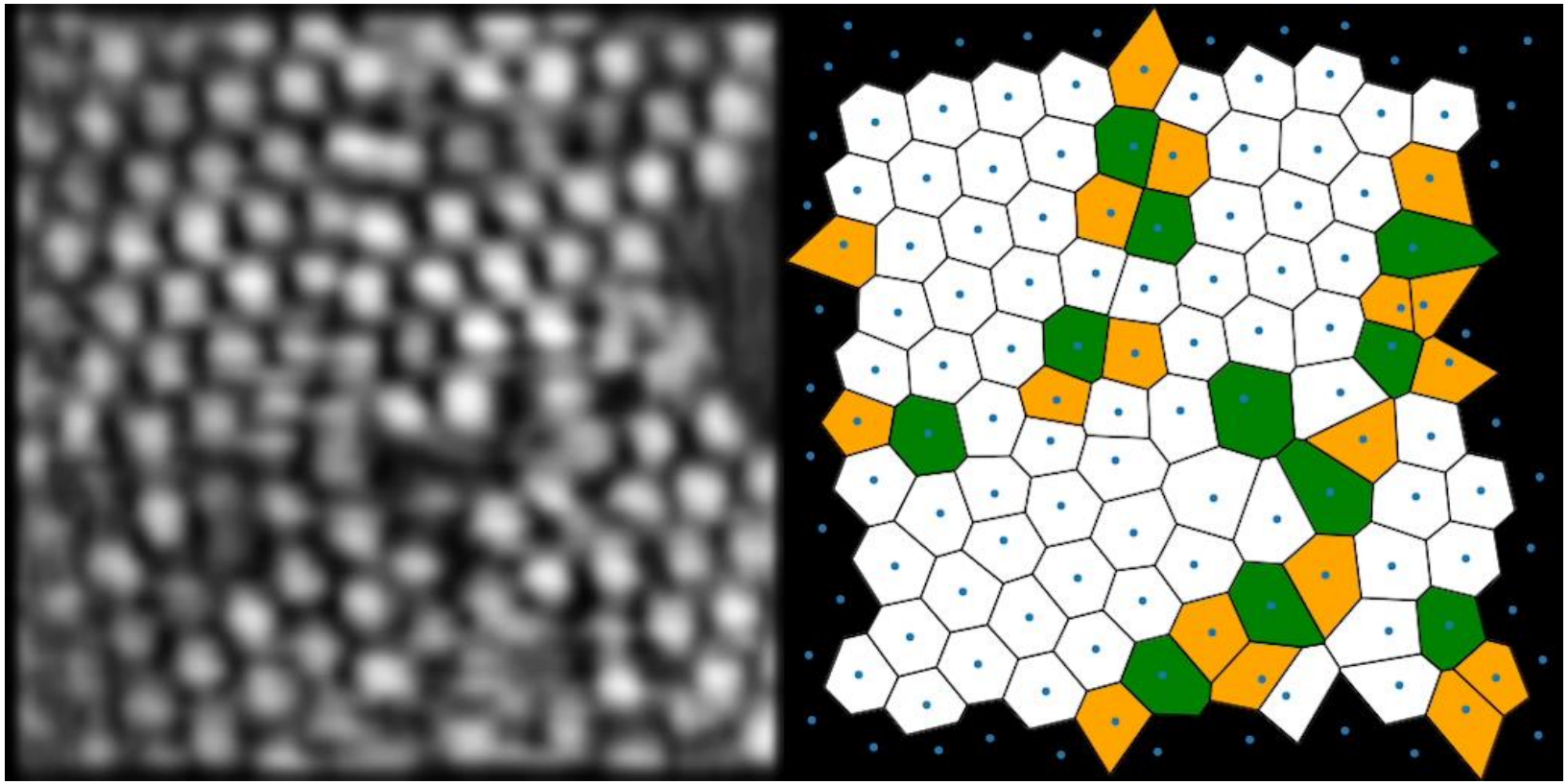
Time-averaged (= slow STM)



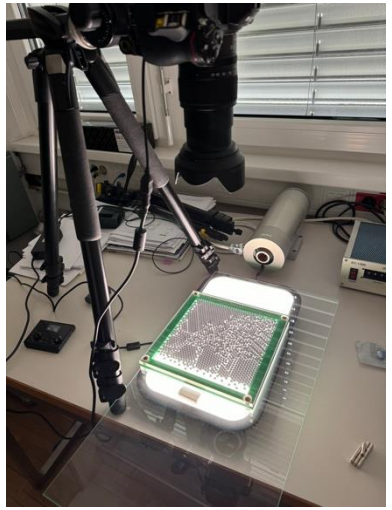
Frame sequence



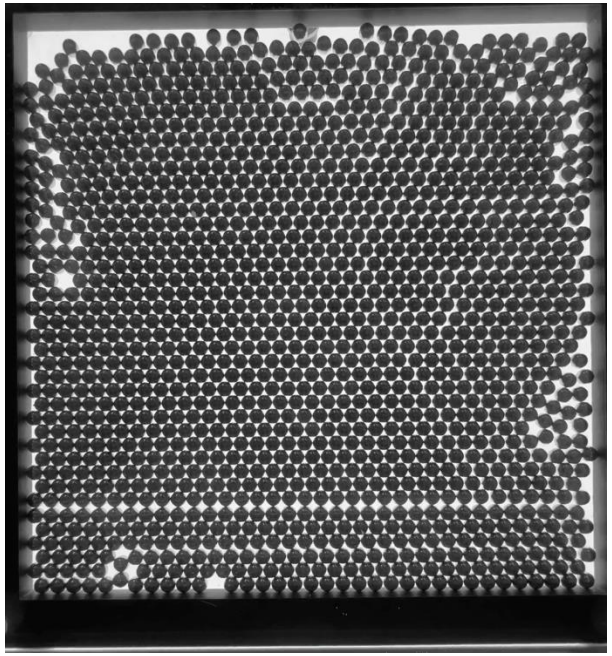
Tesselated Wigner-Seitz structure reveals motion of dislocations and disclinations



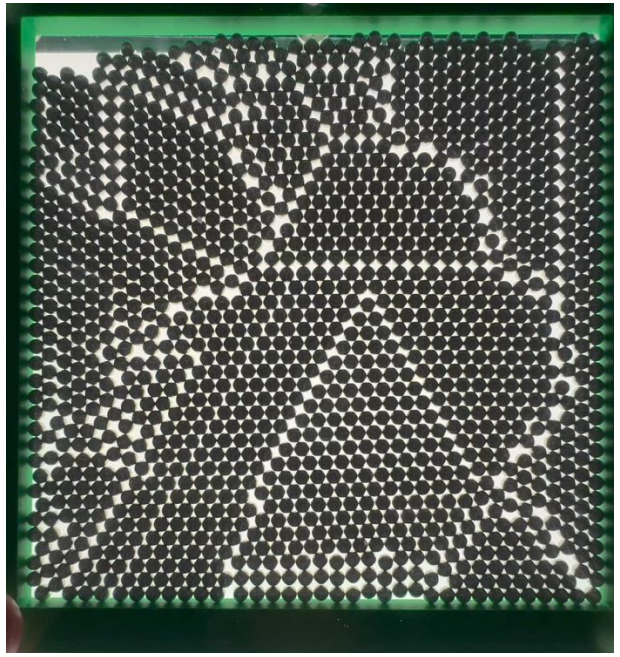
Classical packing in 2D – the effect of temperature and strain



Temperature (pseudorandom shaking)

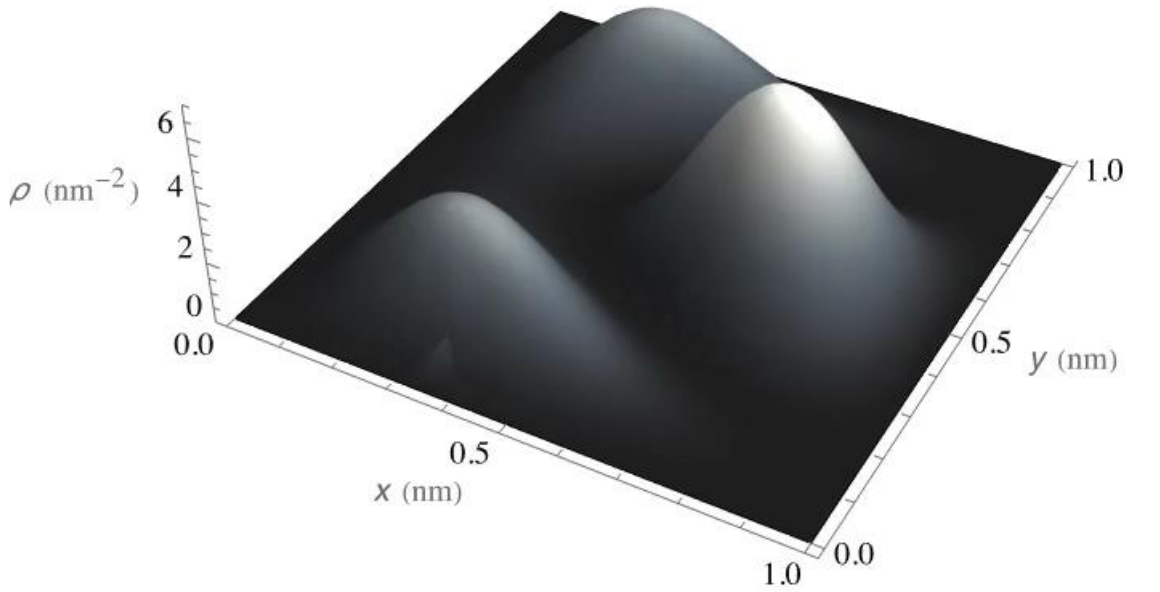


Jamming of steel balls under uniaxial pressure (gravity)



Non-interactiong particle in a box

(time-dependent Schrödinger equation solution)



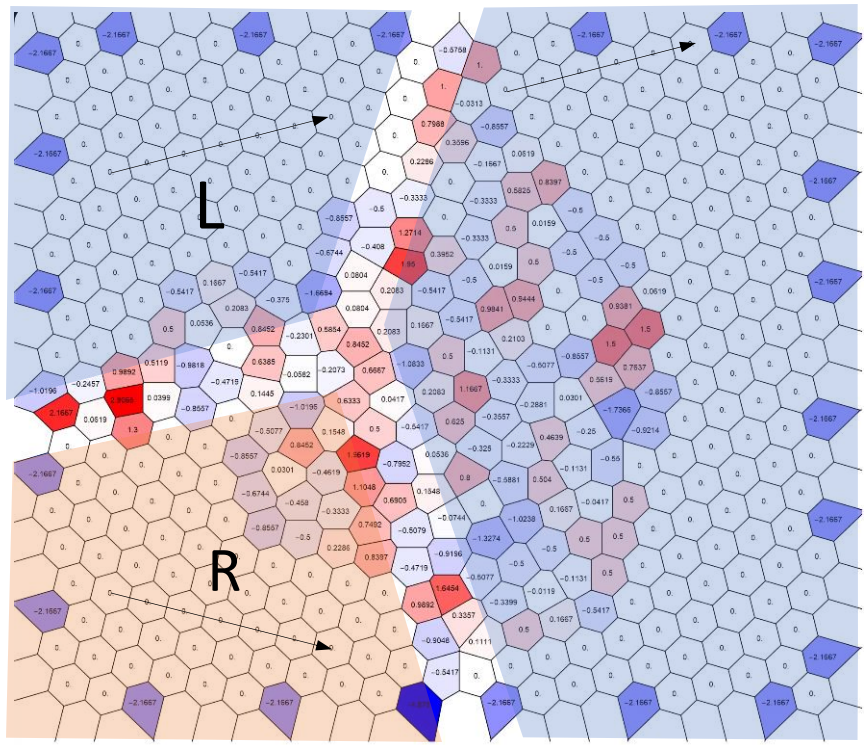
Timescale = 20 fs

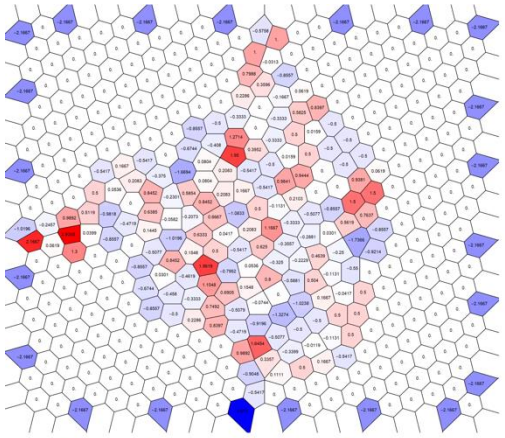
E_F = 1 eV

Model dynamics

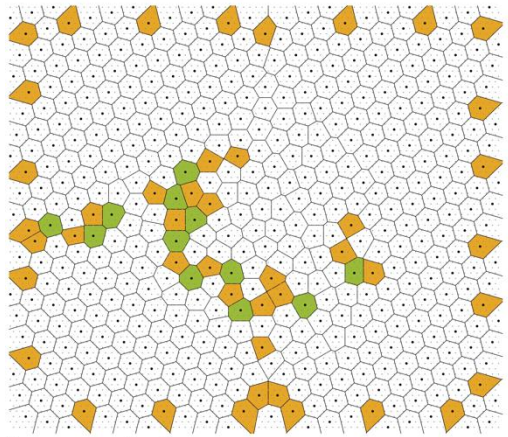
$$\mathcal{H} = \sum_{i<j} V(i,j) n_i n_j,$$

Boundary conditions mimic the Fast STM experiment (L and R domains)

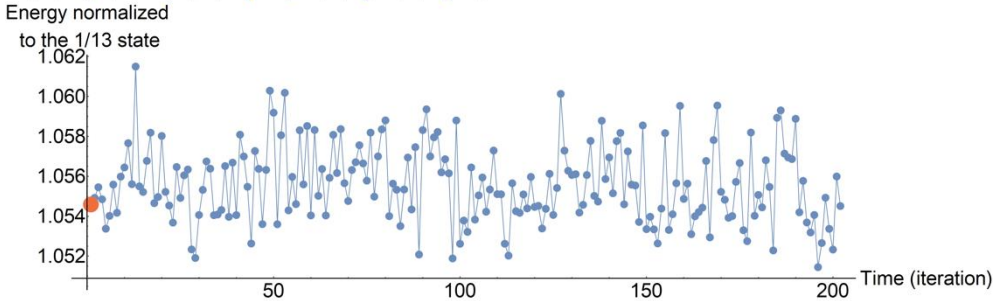




Charge density
(white is neutral f=1/13)

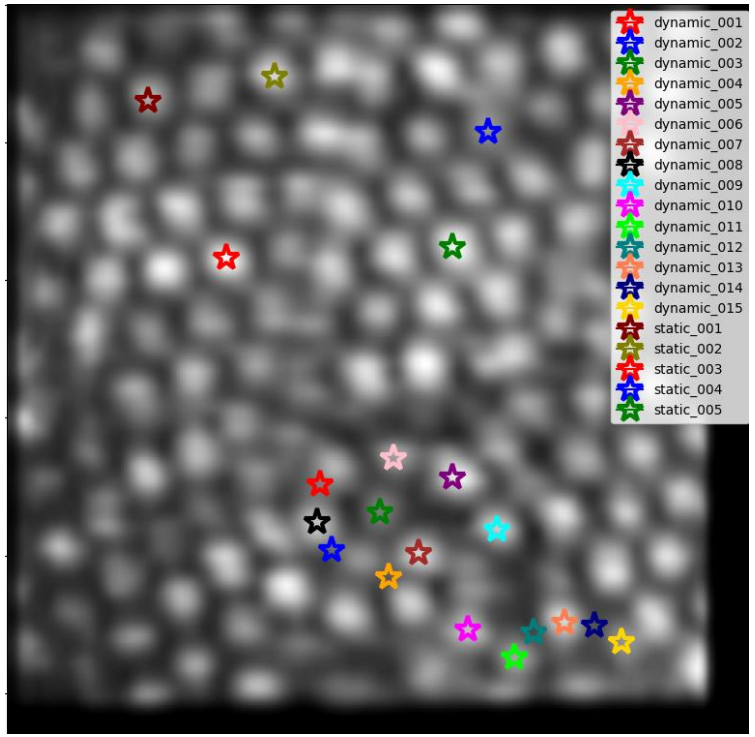


Defect density

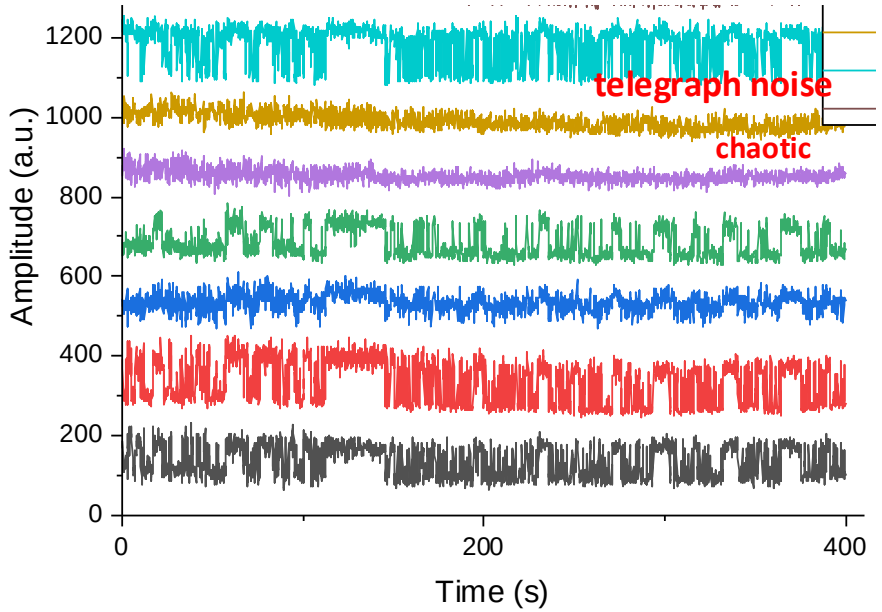


J.Vodeb (unpub)

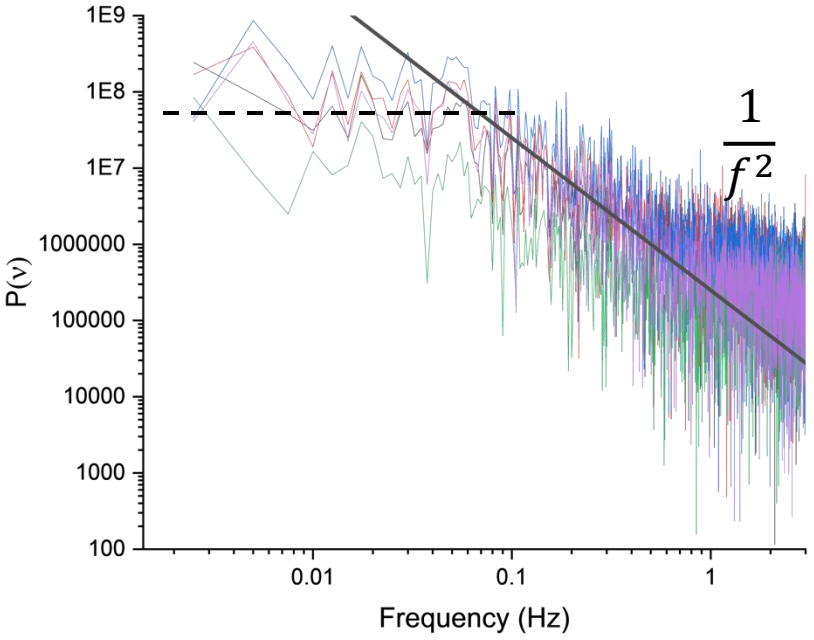
Noise analysis: ‘telegraph noise’ and chaotic dynamics observed at different points



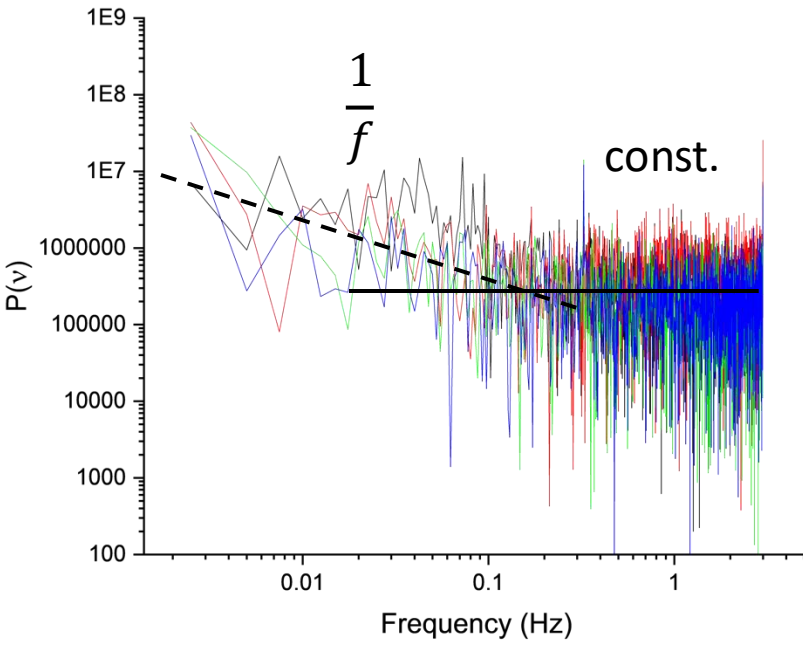
Noise at different points



Dynamical point noise shows **telegraph noise**



Static point noise **is ‘chaotic’**



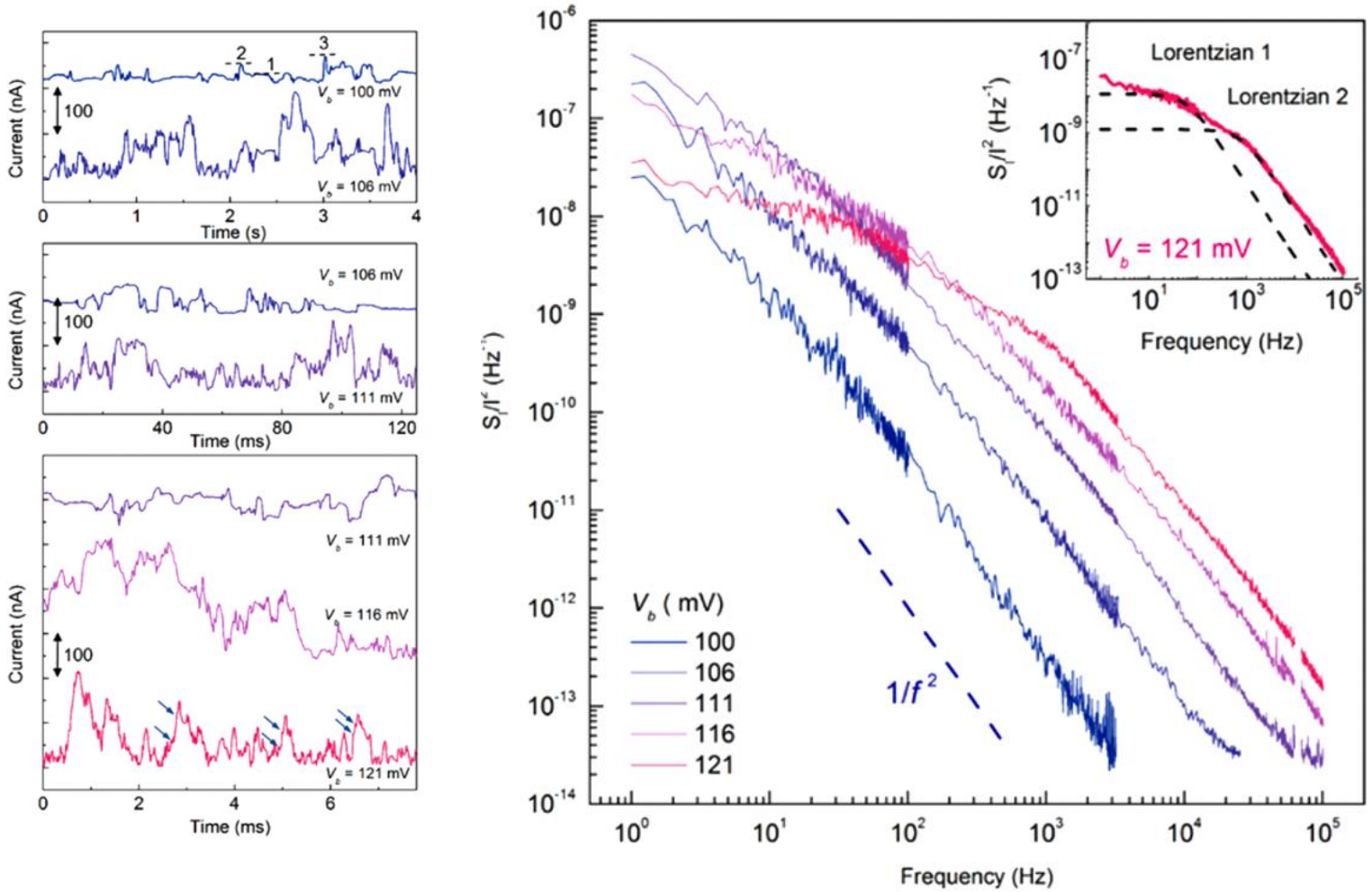
NANO LETTERS Cite This: *Nano Lett.* 2018, 18, 3630–3636

Chaos test: Toker, et al (2020).

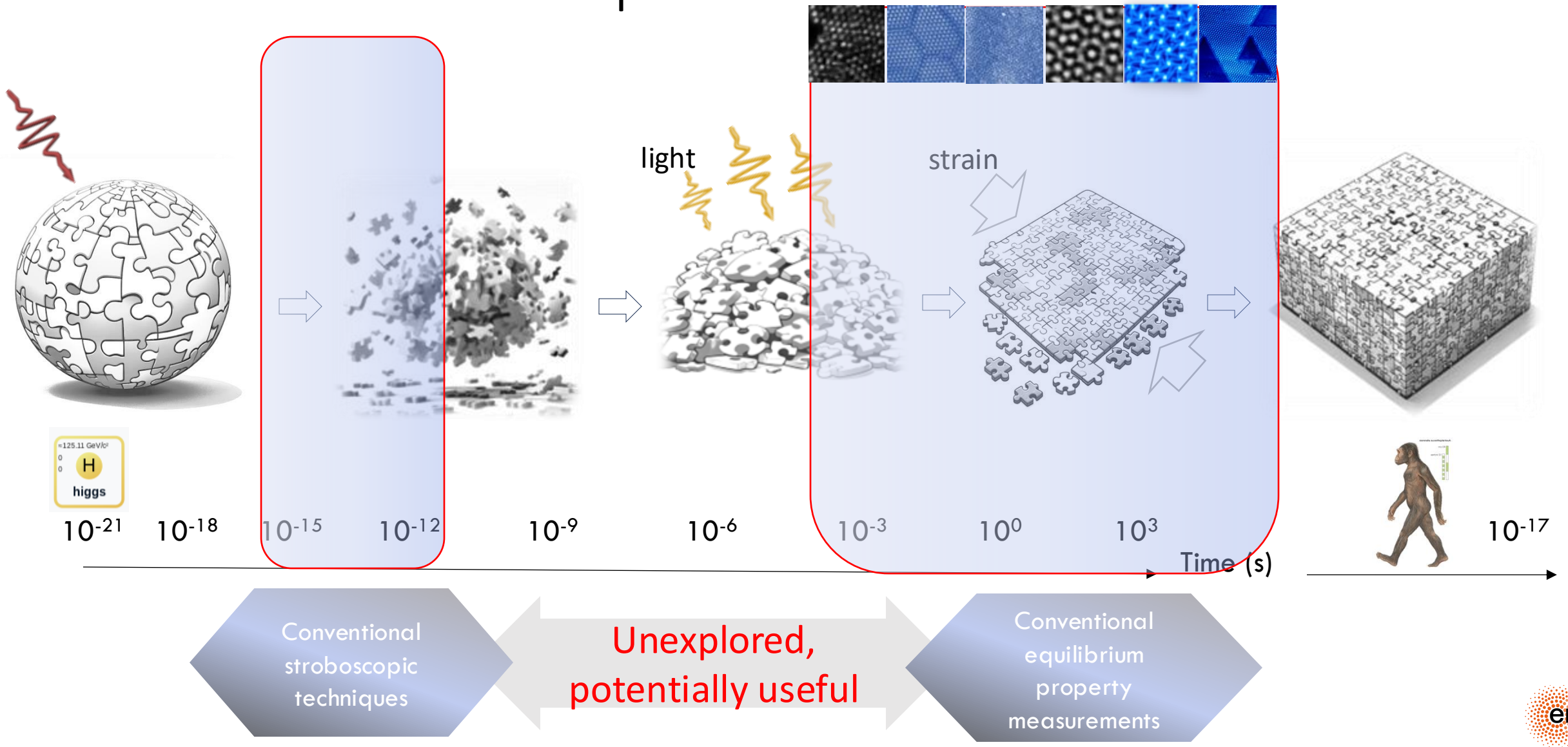
Low-Frequency Current Fluctuations and Sliding of the Charge Density Waves in Two-Dimensional Materials

Guanxiong Liu,[†] Sergey Rumyantsev,[†,‡] Matthew A. Bloodgood,[§] Tina T. Salguero,[§] and Alexander A. Balandin*[,†]

NANO LETTERS
Cite This: *Nano Lett.* 2018, 18, 3630−3636



The aftermath of a phase transition



Conventional stroboscopic techniques

Unexplored, potentially useful

Conventional equilibrium property measurements

Article

Cavity-mediated thermal control of metal-to-insulator transition in 1T-TaS_2

https://doi.org/10.1038/s41586-023-06596-2

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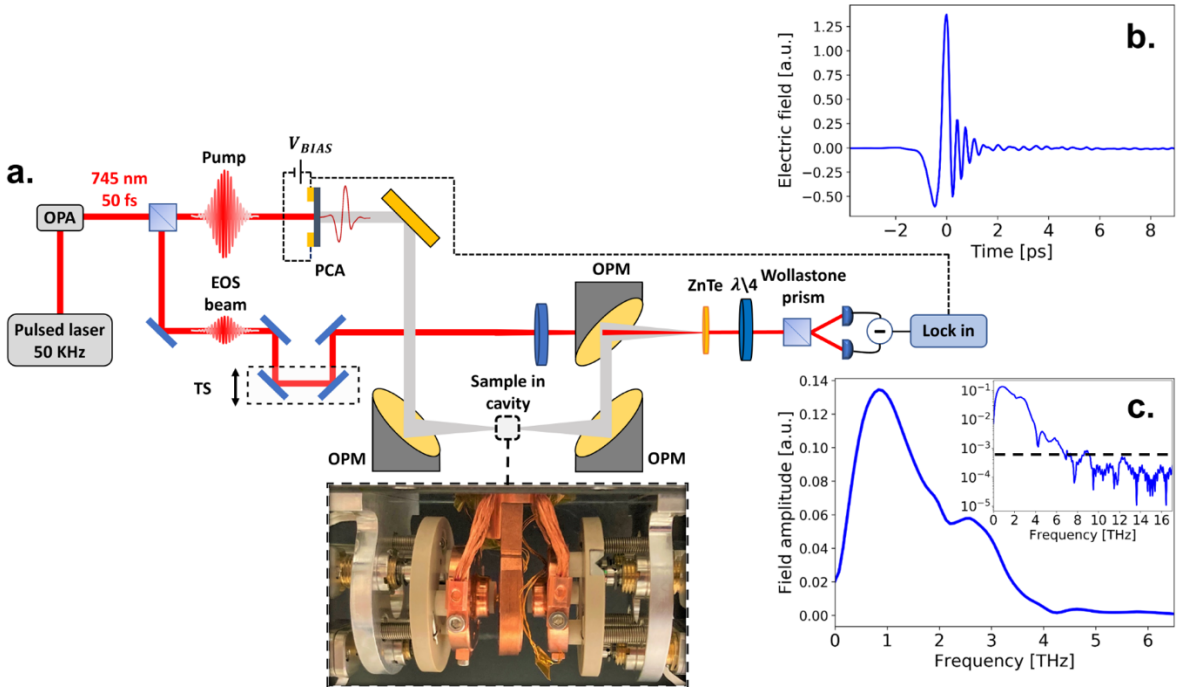
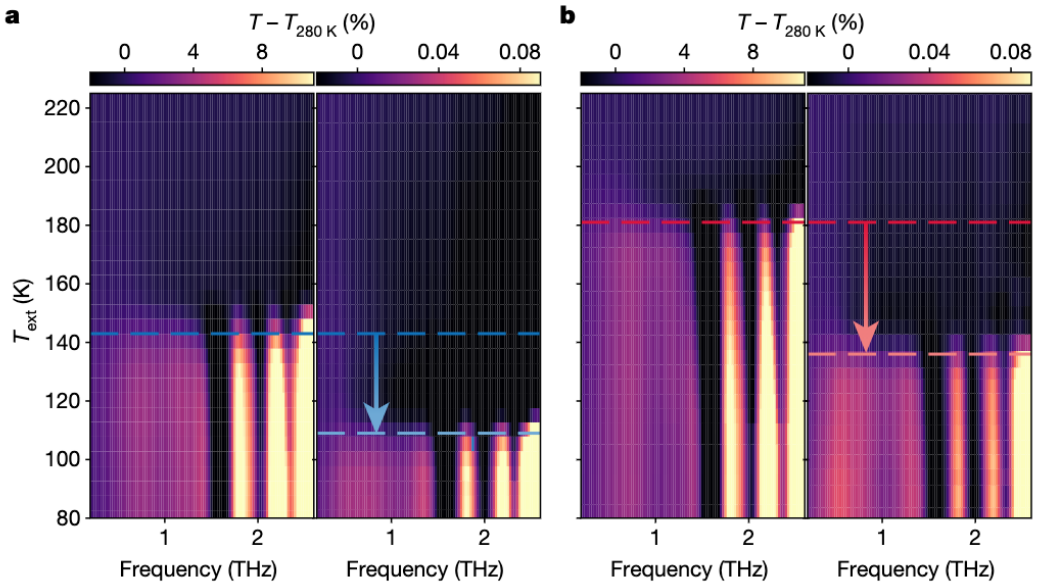
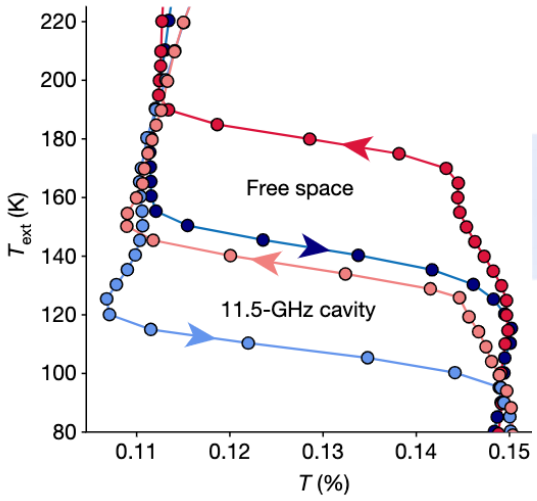
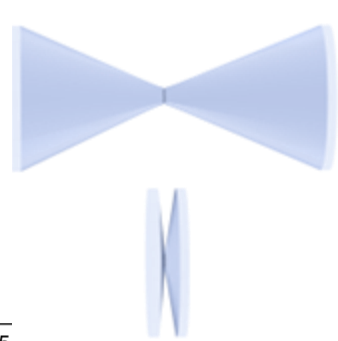
Accepted: 31 August 2023

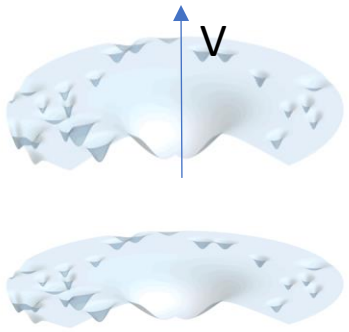
Giacomo Jarc[1,2], Shahla Yasmin Mathengattil[1,2], Angela Montanaro[1,2,3], Francesca Giusti[1,2], Enrico Maria Rigoni[1,2], Rudi Sergo[2], Francesca Fassioli[3,4], Stephan Winnerl[5], Simone Dal Zilio[6], Dragan Mihailovic[7], Peter Prelovšek[7], Martin Eckstein[8] & Daniele Fausti[1,2,3]✉





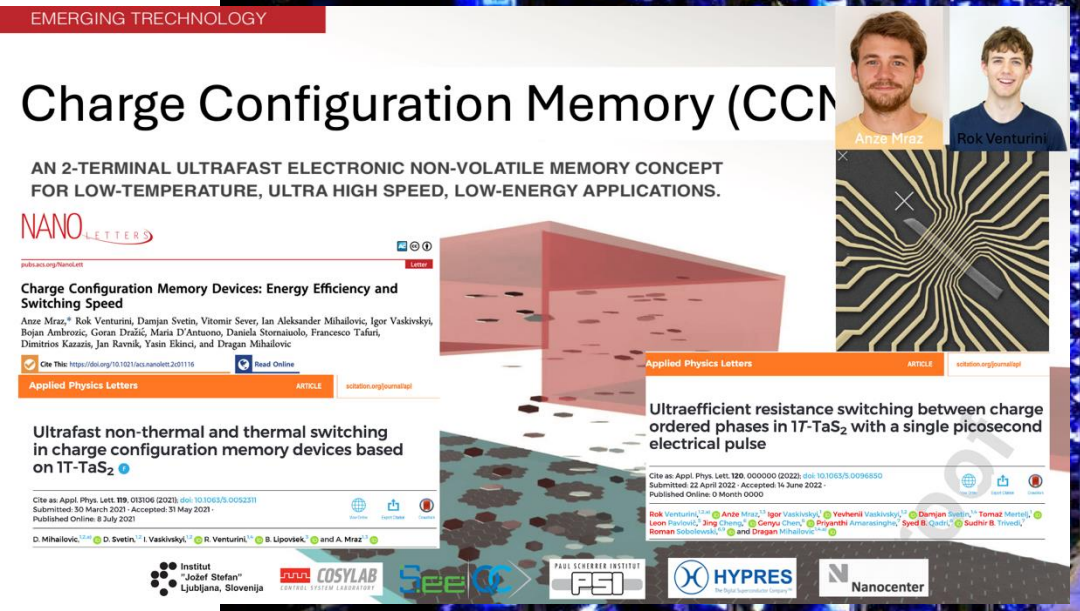


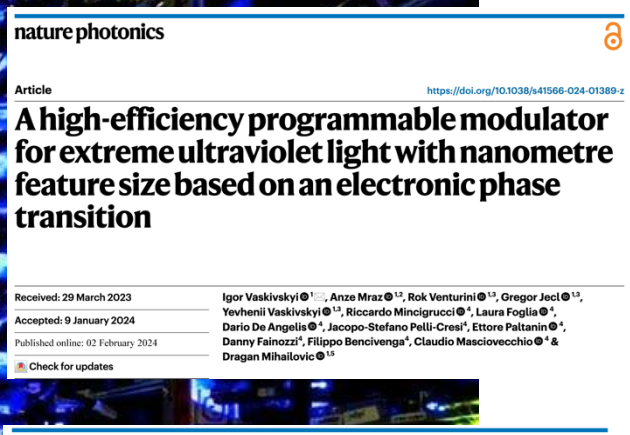


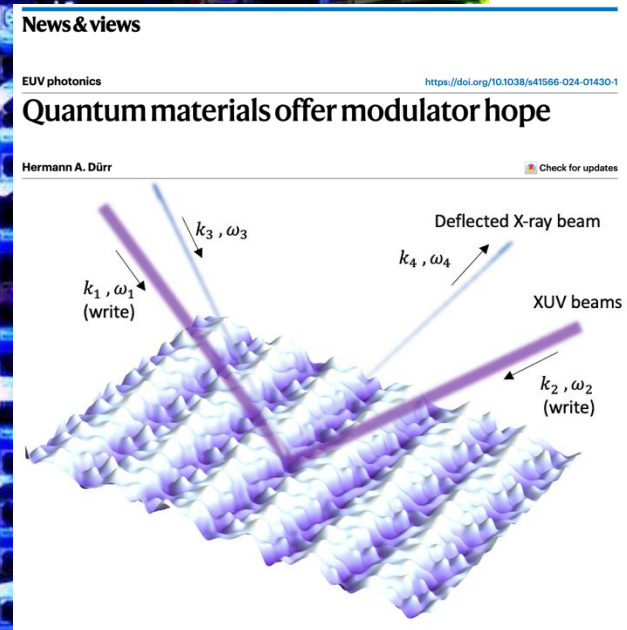


Metastable state devices

-
-





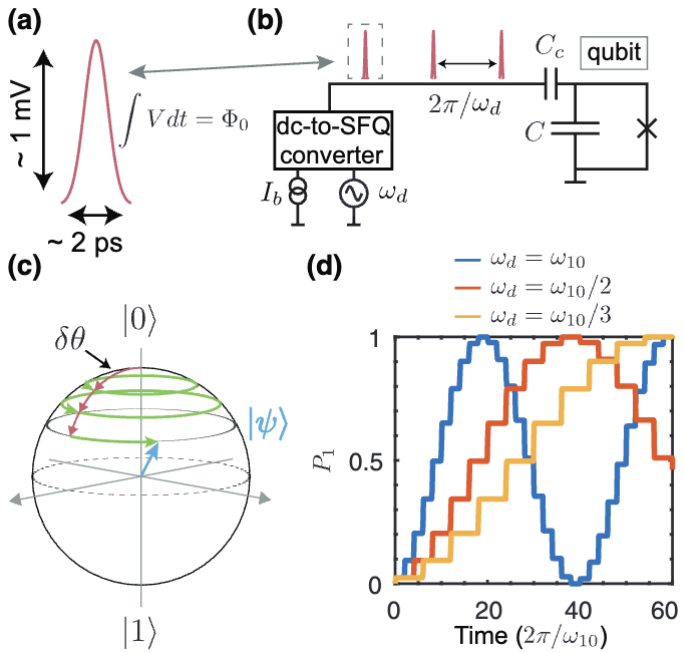


Digital Coherent Control of a Superconducting Qubit

E. Leonard Jr.,[1,†,‡] M. A. Beck,[1,†,§] J. Nelson,[2,¶] B.G. Christensen,[1] T. Thorbeck,[1,§] C. Howington,[2] A. Opremcak,[1] I.V. Pechenezhskiy,[1,‖] K. Dodge,[2] N.P. Dupuis,[1,**] M.D. Hutchings,[2,††] J. Ku,[2] F. Schlenker,[1] J. Suttle,[1,§] C. Wilen,[1] S. Zhu,[1] M.G. Vavilov,[1] B.L.T. Plourde,[2] and R. McDermott[1,*]

[1] *Department of Physics, University of Wisconsin-Madison, Madison, Wisconsin 53706, USA*

[2] *Department of Physics, Syracuse University, Syracuse, New York 13244, USA*



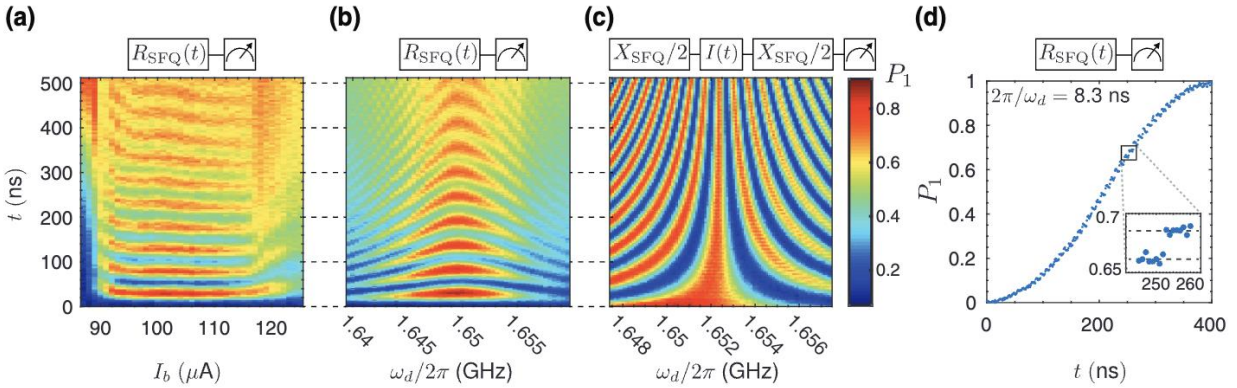
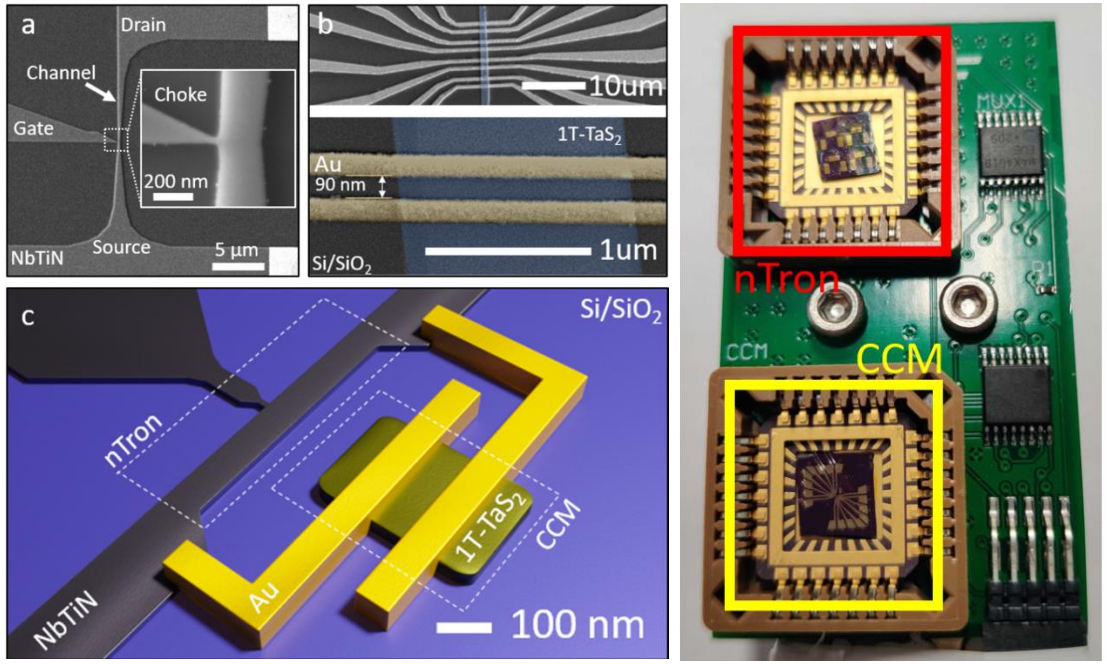


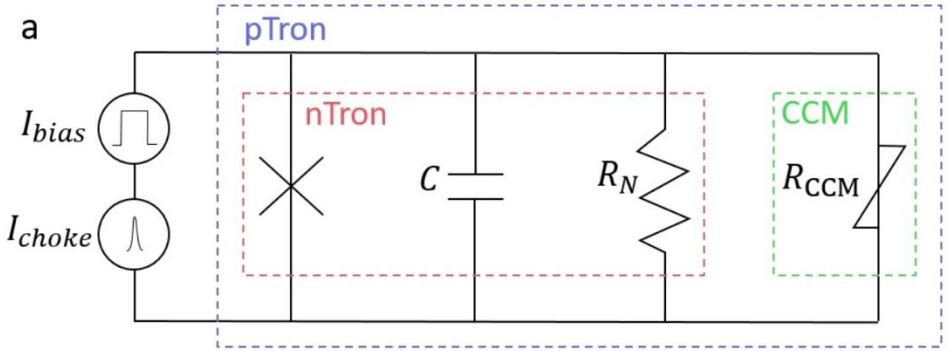
FIG. 3. Basic qubit operations driven by SFQ pulses. (a) SFQ-based Rabi oscillations as a function of bias current I_b to the SFQ driver circuit. Here, $\omega_d = \omega_{10}/3 \approx 1.65$ GHz. (b) Rabi chevron experiment and (c) Ramsey fringe experiment where the SFQ pulse frequency ω_d is varied slightly in the vicinity of $\omega_{10}/3$. (d) Time trace of a SFQ-based Rabi flop obtained with a pulse rate $\omega_{10}/41 = 120.90$ MHz. Inset: An enlargement of the discrete steps in $P_1(t)$ occurring every 8.3 ns, the SFQ pulse-to-pulse timing interval.

A CCM/superconductor hybrid memory device: The pTron (nTron amplifier and 1T-TaS_2 CCM)



Discrete implementation of nTron and CCM

NB. NbTiN films were kindly provided by Wallraff's group (ETHZ)



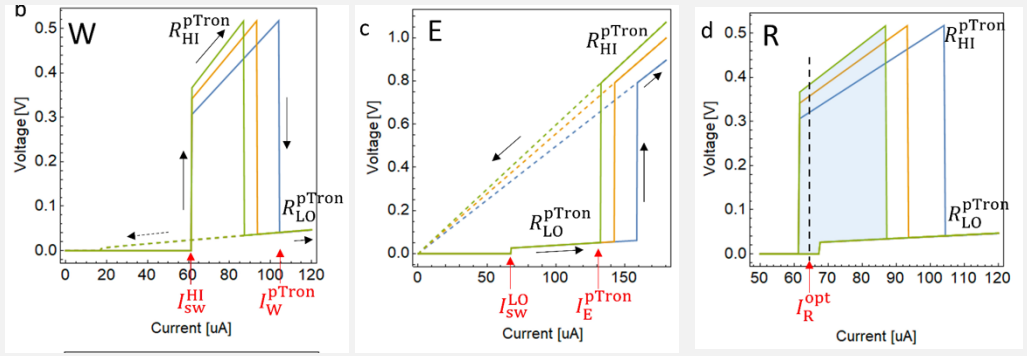
pTron equivalent circuit

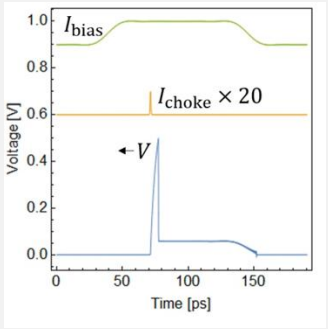
pTron switching

V-I curves

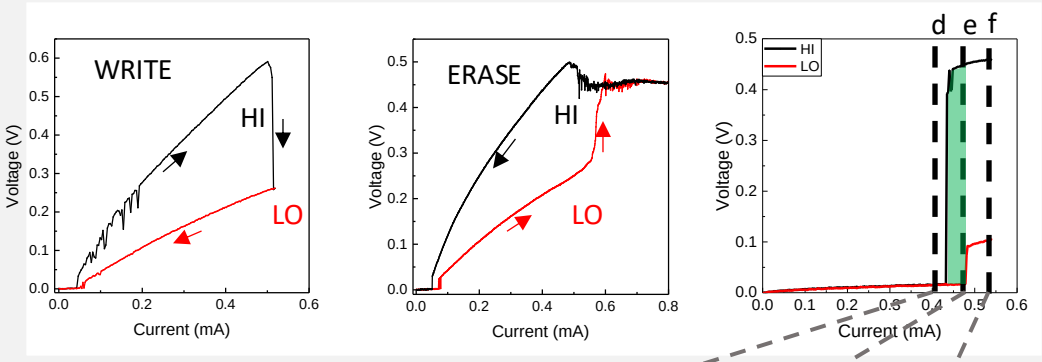
Time dynamics

Model predictions

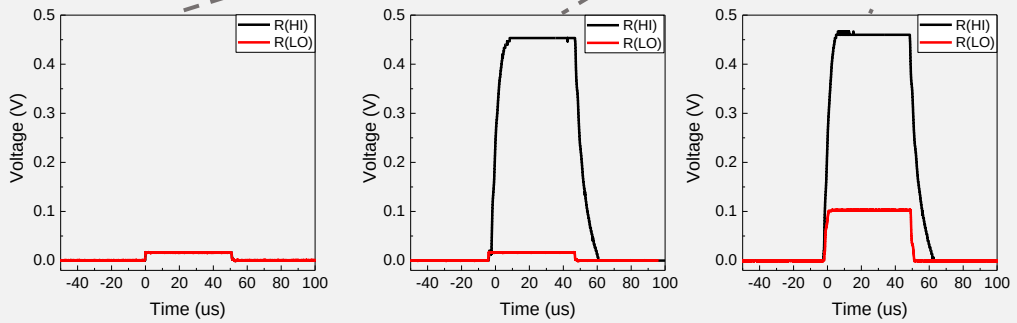




Measured behaviour with NbTiN NW - CCMs



Readout



https://arxiv.org/pdf/2203.14586.pdf

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PSI	Corinna Burri, Yasin Ekcinci, Dimitrios Kazazis, Simon Gerber, Jan Ravnik, Gabriel Aeppli
Elettra collaboration	Riccardo Mincigrucci, Filippo Bencivenga, Laura Foglia, Dario De Angelis, Jacopo-Stefano Pelli-Cresi, Ettore Paltanin, Danny Fainozzi, Claudio Masciovecchio
Cavity experiments	Giacomo Jarc, Shahla Yasmin Mathengattil, Angela Montanaro, Francesca Giusti, Enrico Maria Rigoni, Rudi Sergo, Francesca Fassioli, Stephan Winnerl, Simone Dal Zilio, Peter Prelovšek7, Martin Eckstein, and Daniele Fausti
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