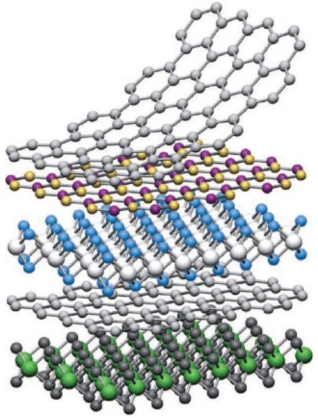
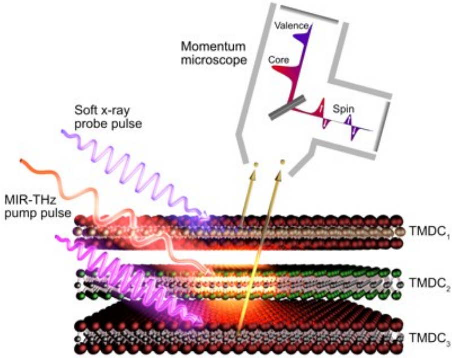
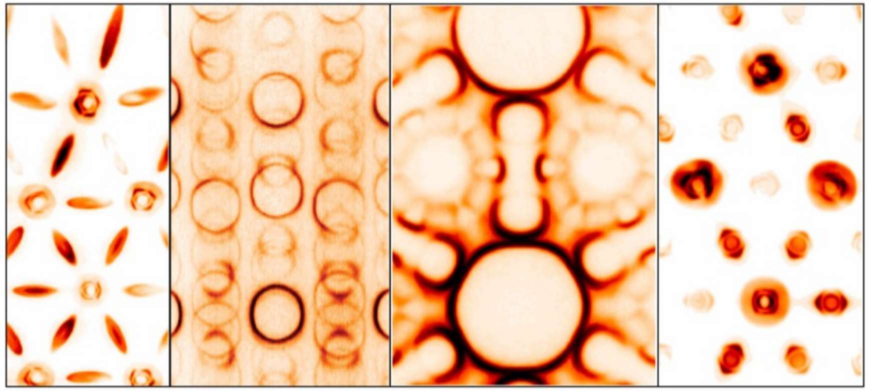
Exploring Quantum Materials with X-ray Spectroscopy







Markus Scholz
Hamburg, 4th August 2025

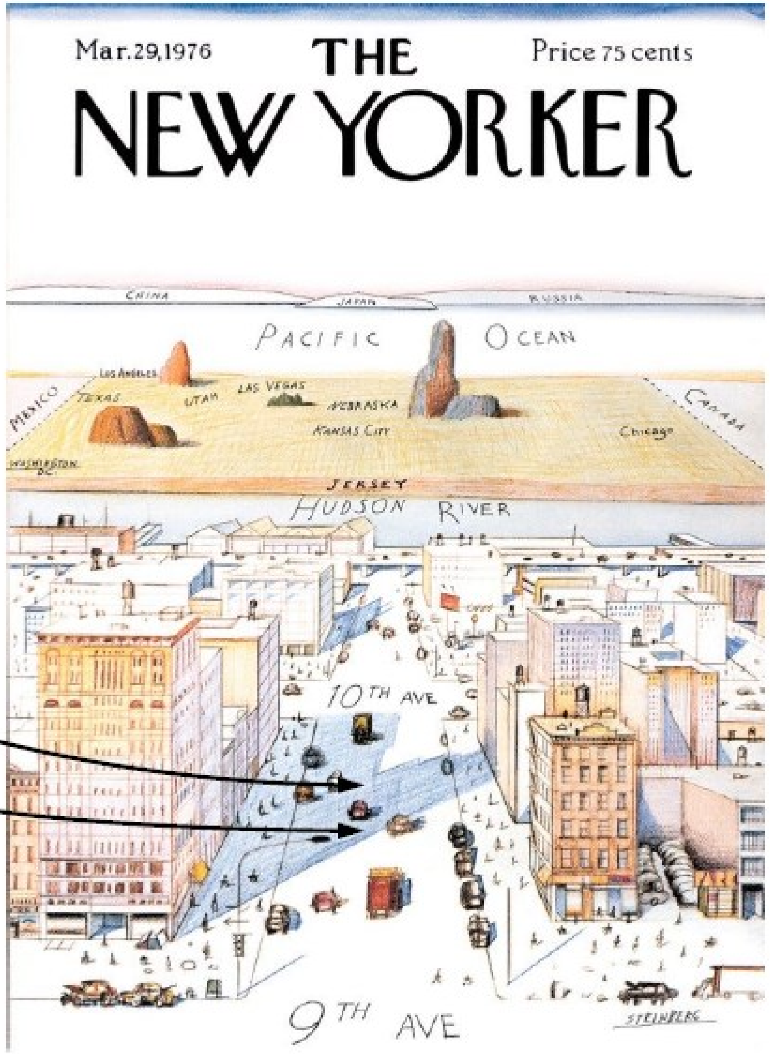
HELMHOLTZ

DESY.

Outline

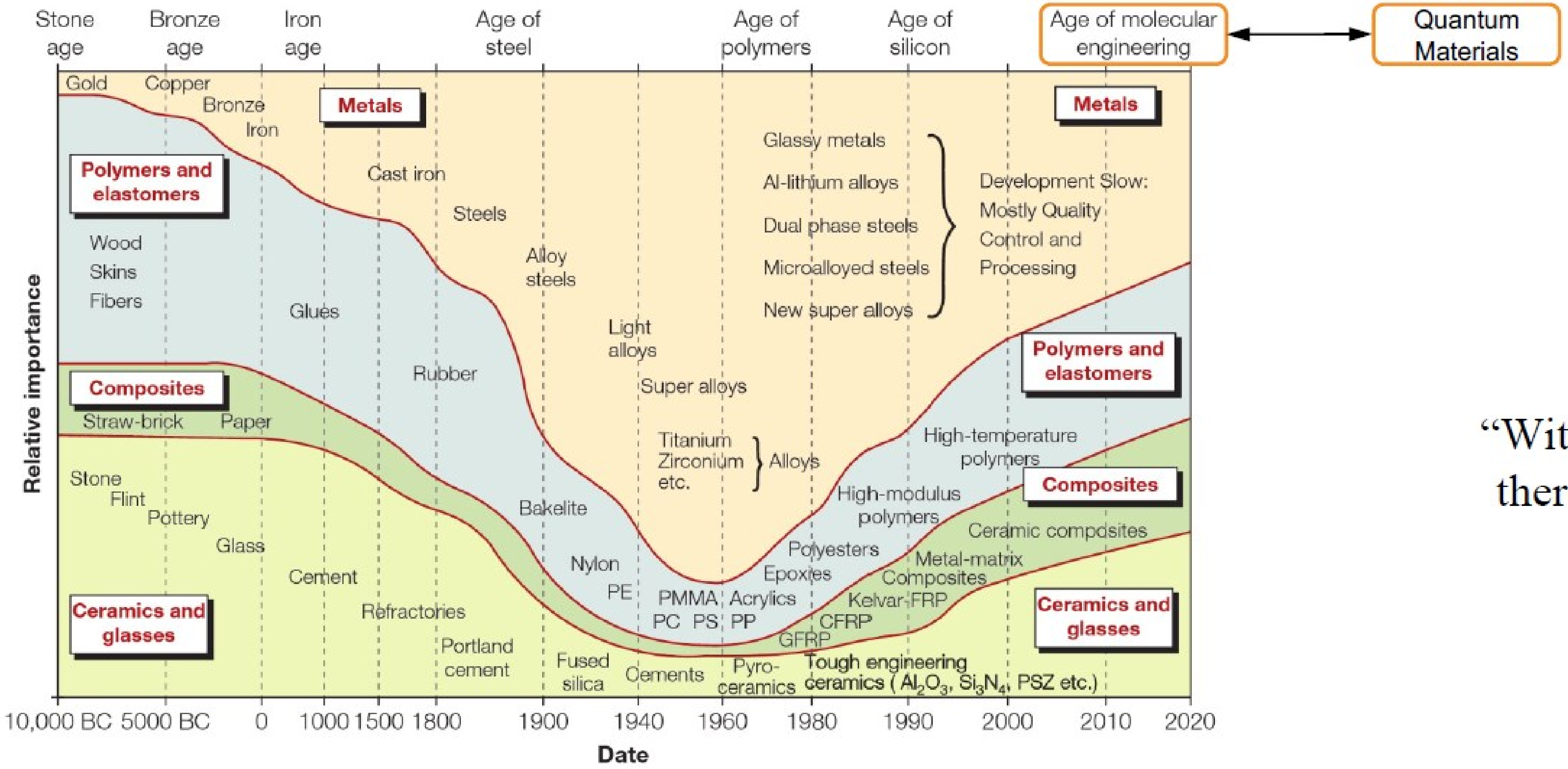
X-ray spectroscopy of Quantum Materials

- **Quantum materials**
  - Electrons in solids
  - Band structure
  - **2D Materials**
- **X-ray spectroscopy**
  - **Photoelectron spectroscopy**
  - Band structure imaging
  - Two advanced examples ("nano & femto")



Engineering materials

History



The evolution of engineering materials with time. "Relative importance" is based on information contained in the books listed under "Further reading"; plus, from 1960 onward, data for the teaching hours allocated to each material family at U.K. and U.S. universities. The projections to 2020 rely on estimates of material usage in automobiles and aircraft by manufacturers. The time scale is nonlinear. The rate of change is far faster today than at any previous time in history.

"Without materials there is nothing."

Michael F. Ashby:
Materials Selection in Mechanical Design

Electrons

… make the world go round (“Si age”)

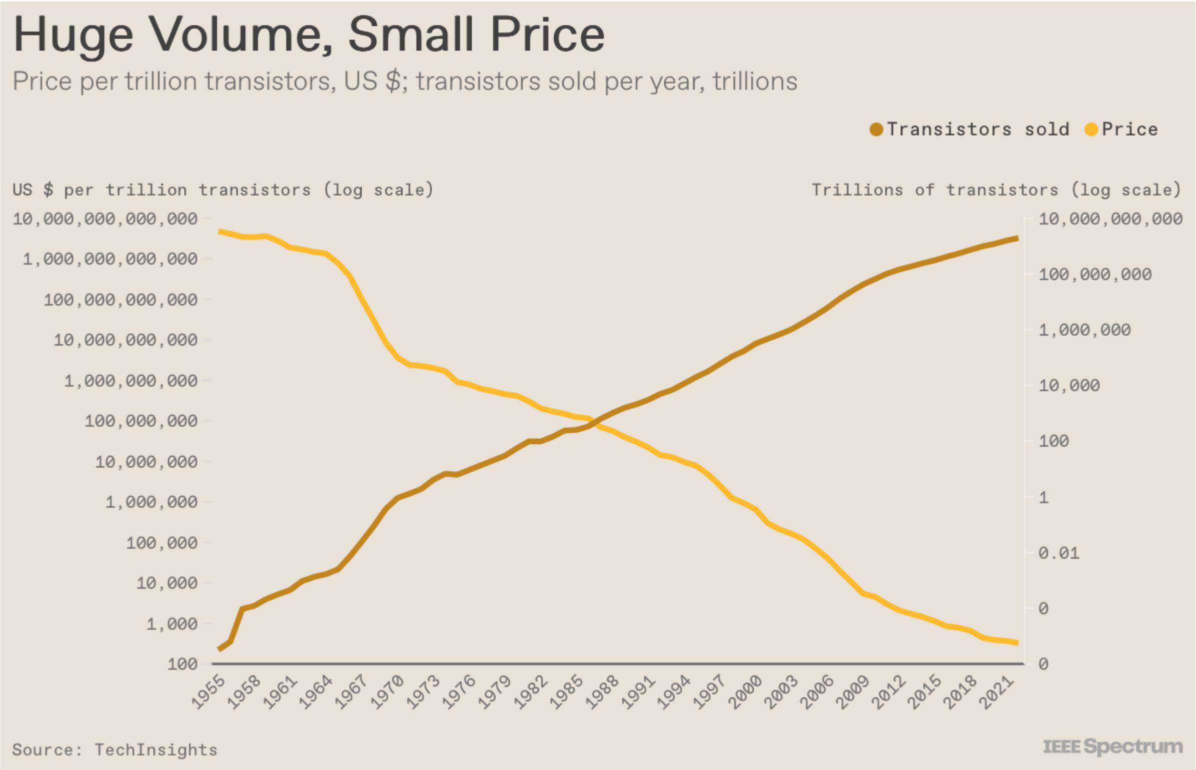



Mass: 9.1×10^{-31} kg (<0.05% m_{Atom})
Charge: $-1\ e = -1.6\times10^{-19}$ C
Size: blurred
Energy: variable

Glue and property giver
Energy & information carrier

Practical appeal of quantum materials

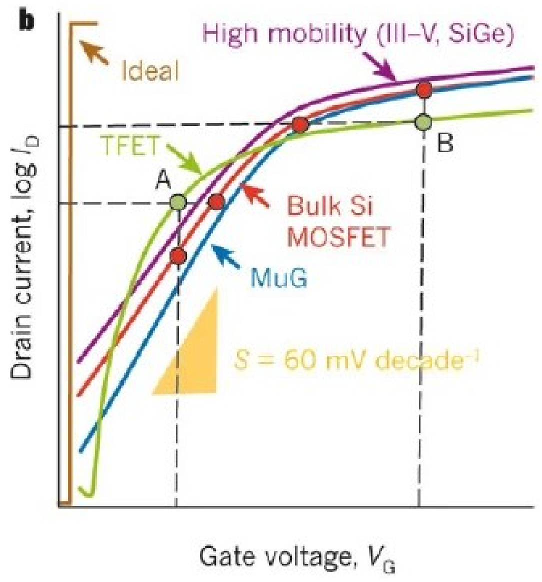
The quest for a better switch



IEEE Spectrum: *The State of the Transistor in 3 Charts* (2022)

$$\underset{\text{transistors}}{10^{22}} \times \underset{\text{bit transitions}}{10^{14}} \times \underset{\text{energy per transition}}{10^{-17}\,\text{J}}$$

≈2% of global primary energy production $= \boxed{10^{19}\,\text{J per year}}$

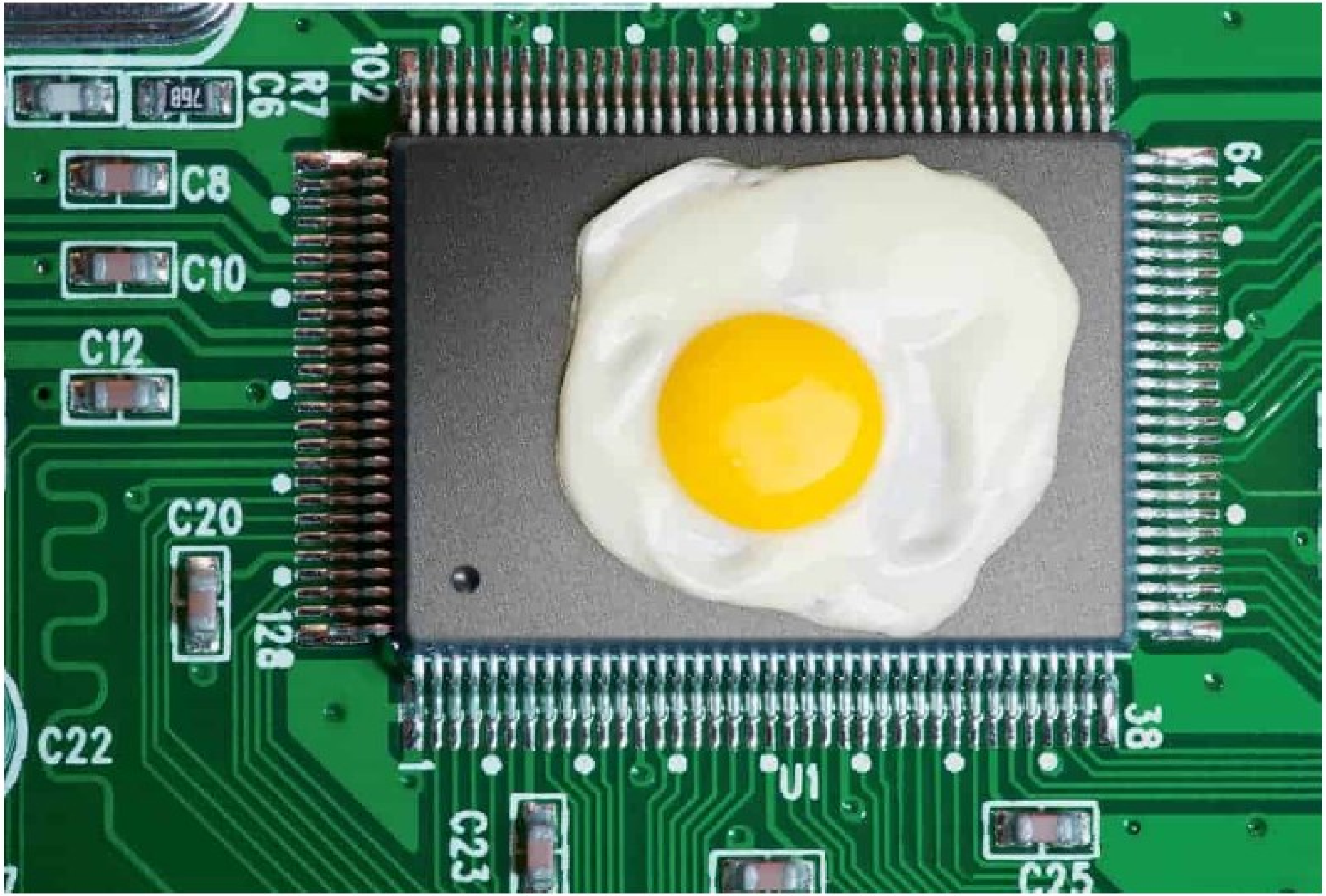


Ionescu & Riel, Nature **479**, 329 (2011)

- **How fast?**
  Sub-vibrational.
- **How efficient?**
  Sub-Boltzmann.
- **How?**
  Electrons or high-energy phonons. Nonthermal. Correlated. Coherent?

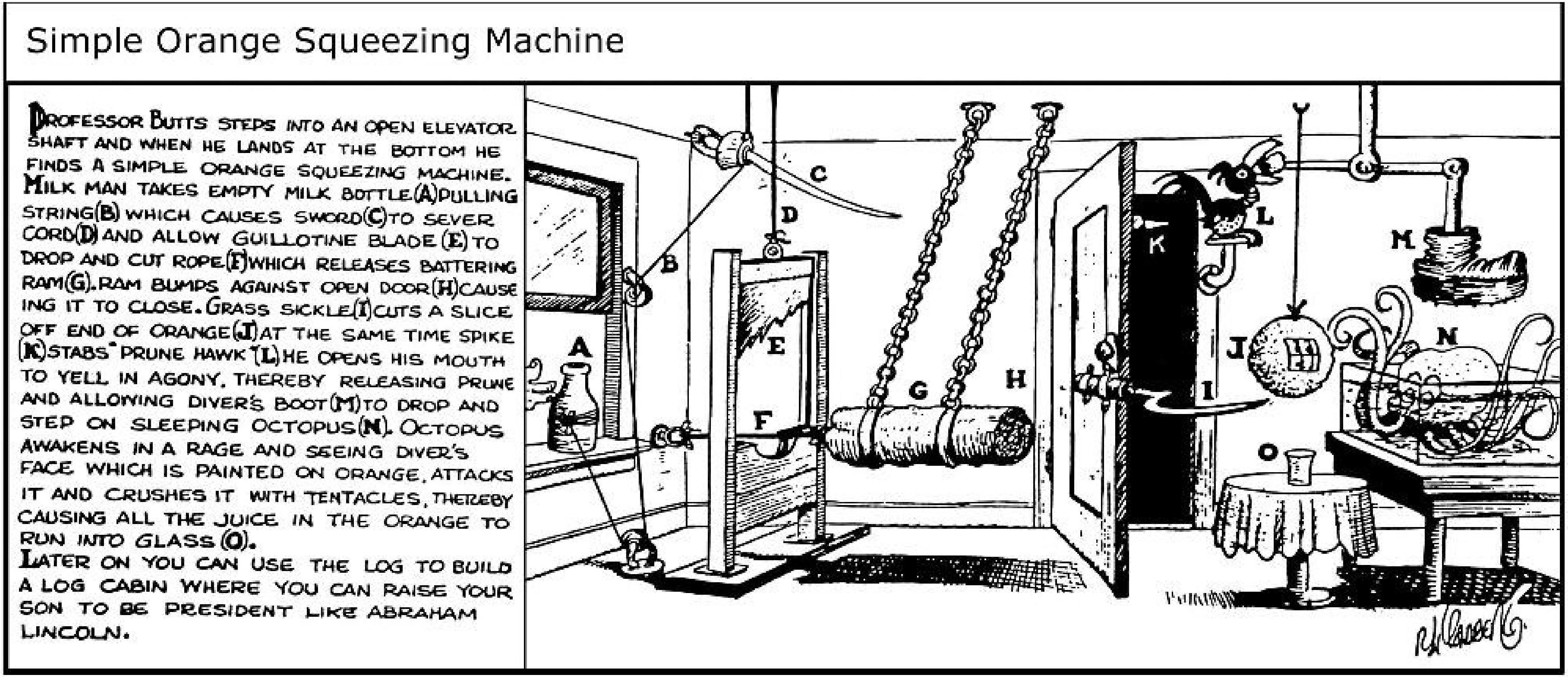
How efficient?

Efficiency means avoiding unwanted excitations.



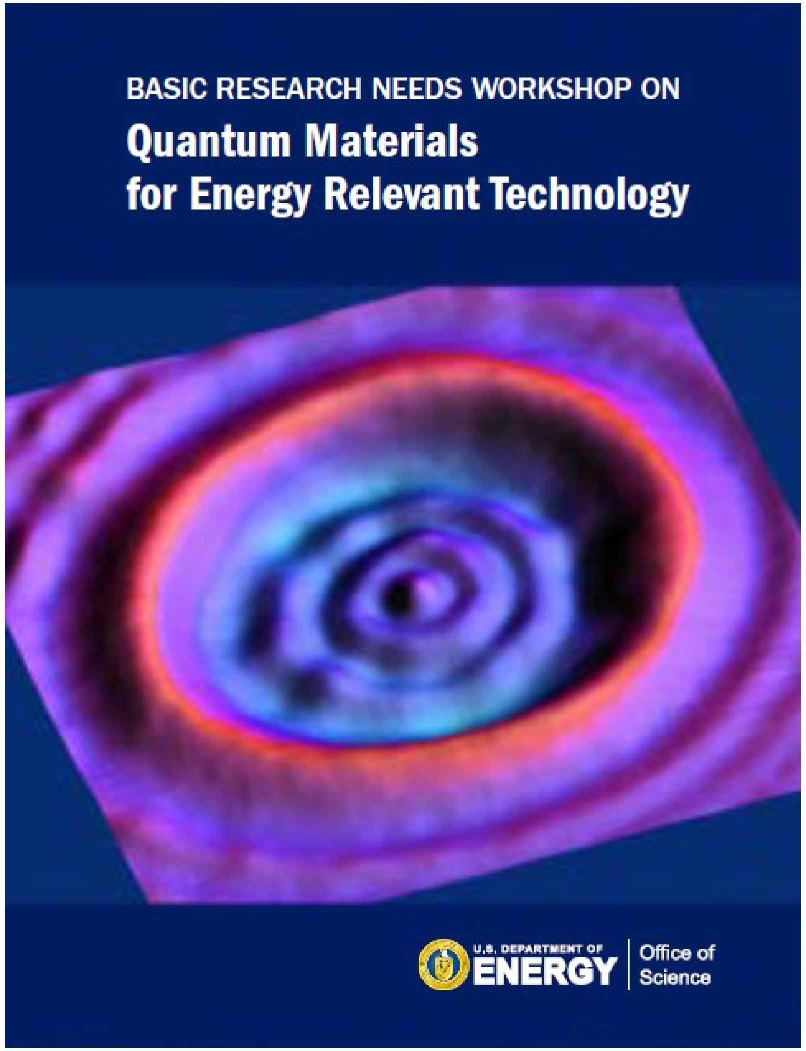
How

Mechanisms can be complicated … and need not be universal



Quantum materials

Definition

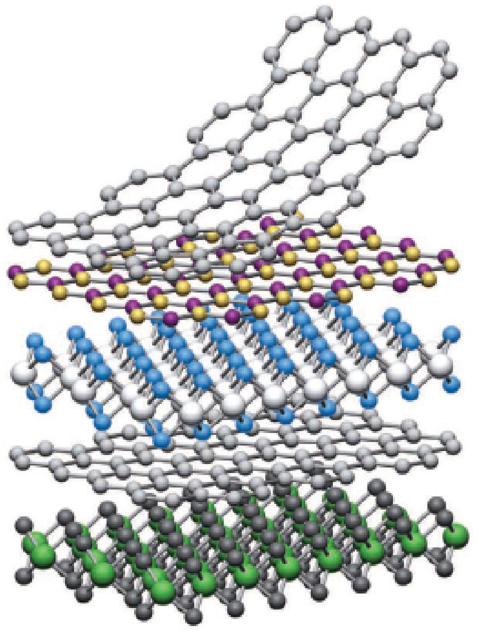


… solids with **exotic physical** properties, arising from the **quantum mechanical** properties of their constituent **electrons**; such materials have great scientific and/or technological potential.

Grand challenges

Quantum materials research

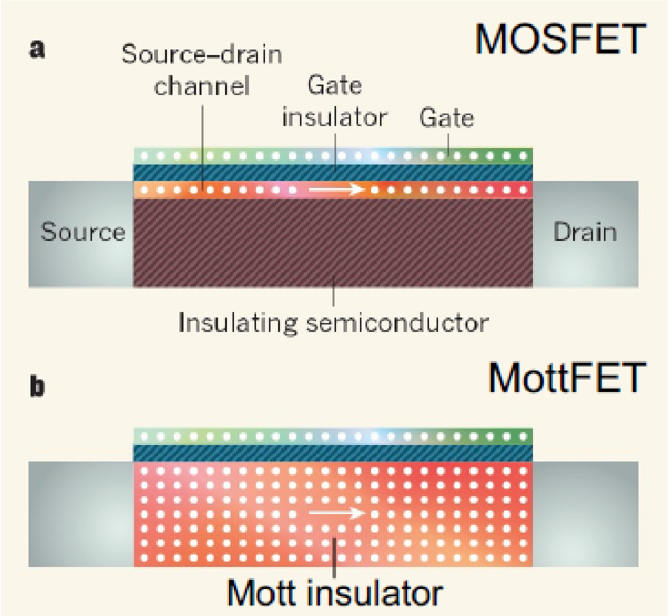
Room-temperature superconductor



"Mimic layered superconductors by using atomic-scale Lego"

Geim & Grigorieva, Nature **499**, 419 (2013)

Ultrafast "sub-Boltzmann" switch



"Exploit strong correlation: toggle one, switch all"

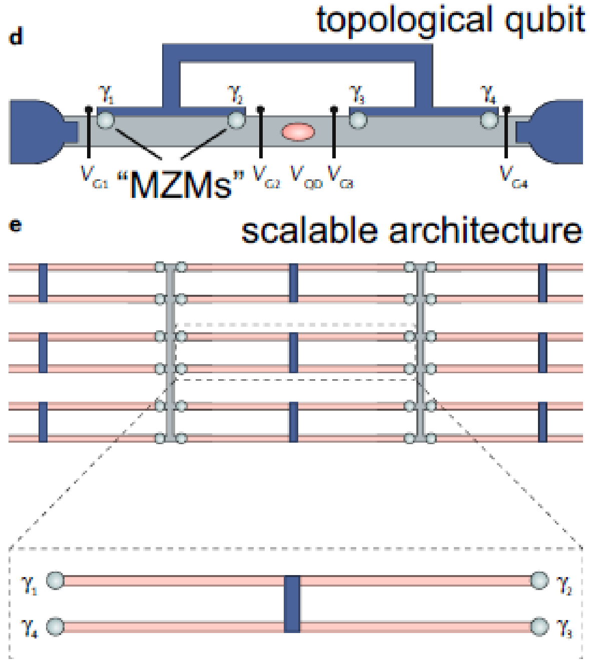
Mannhart & Haensch, Nature **487**, 436 (2012)

SOPHIA CHEN SCIENCE 03.09.2020 08:00 AM WIRED

Two Physicists Bet Over a Quantum Computing Moon Shot

Topological quantum computing has long been a beautiful dream. Two top scientists are now facing off over whether it will exist by 2030.

Topological quantum computer



"Store and manipulate quantum information in a nonlocal manner"

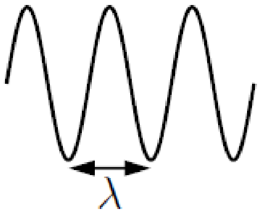
Lutchyn *et al.*, Nat. Rev. Mat. **3**, 52 (2018)

Electrons

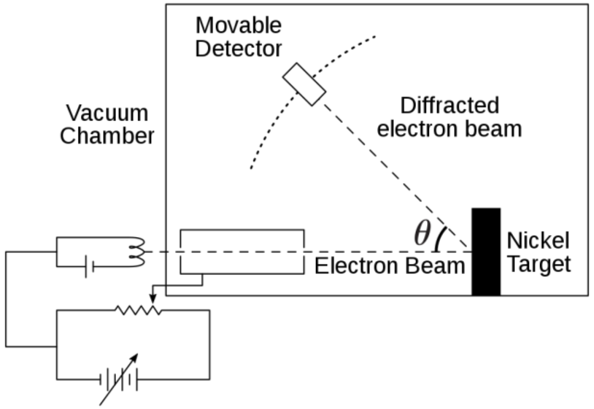
..are wave-like

de Broglie

$$\lambda = \frac{h}{p}$$



Davisson & Germer



$$\lambda(\text{nm}) = \sqrt{\frac{1.5}{E(\text{eV})}}$$

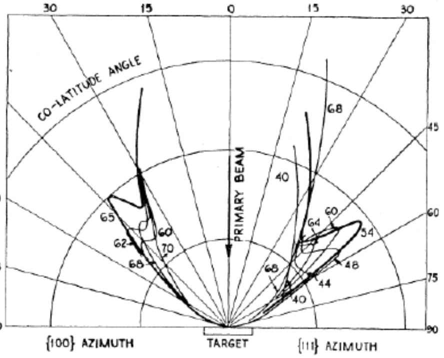
Second Series *December, 1927* *Vol. 30, No. 6*

THE

PHYSICAL REVIEW

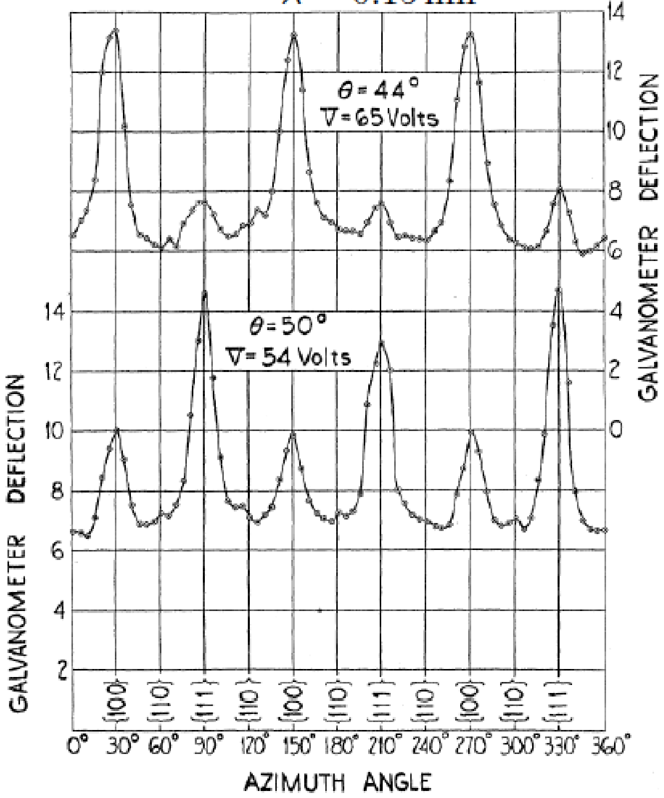
DIFFRACTION OF ELECTRONS BY A CRYSTAL OF NICKEL

By C. Davisson and L. H. Germer



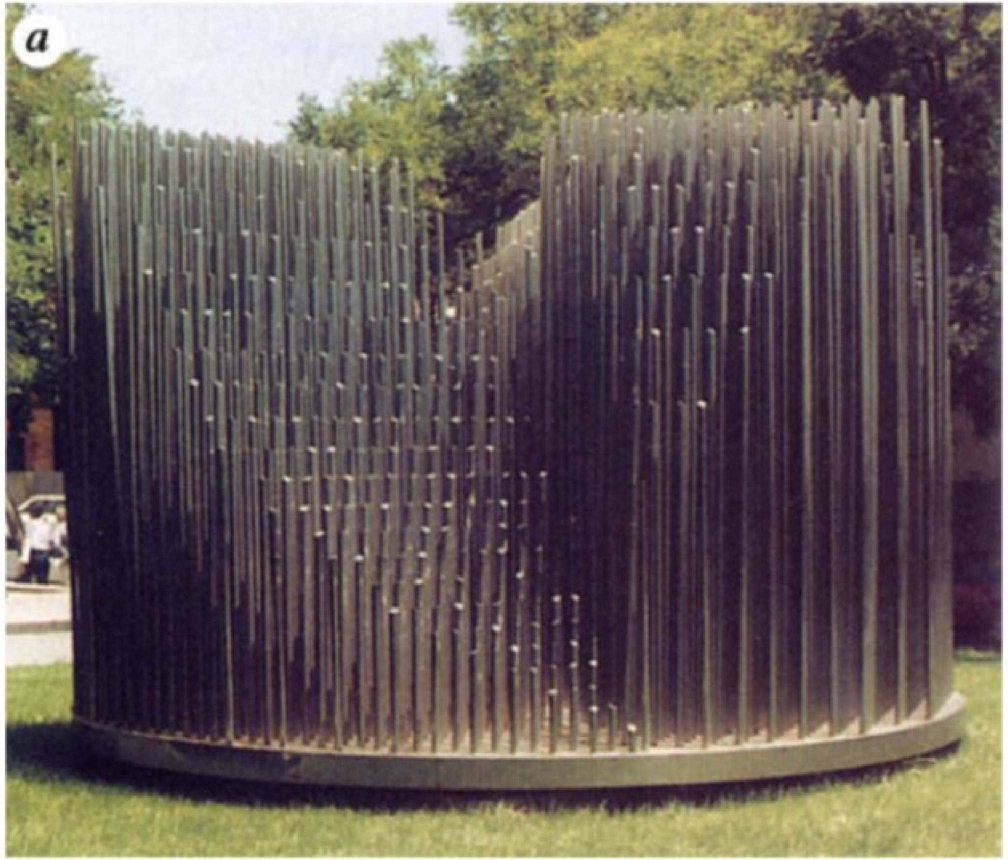
$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{h^2}{2m}\frac{1}{\lambda^2}$$

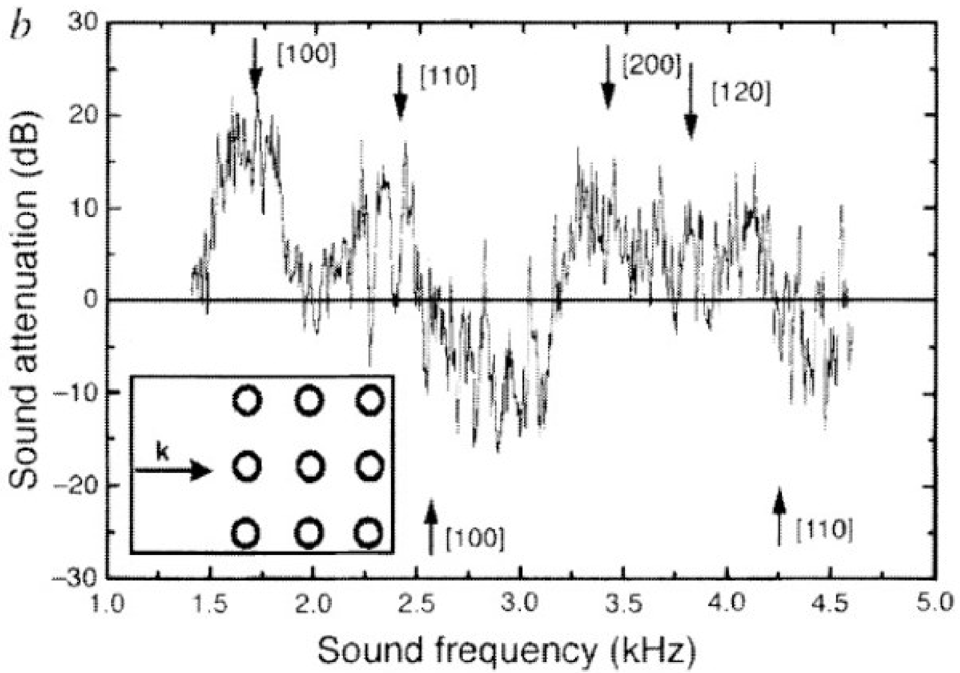
$\lambda = 0.15\,\text{nm}$



Waves + lattice = band structure

Wavelength-dependent transmission



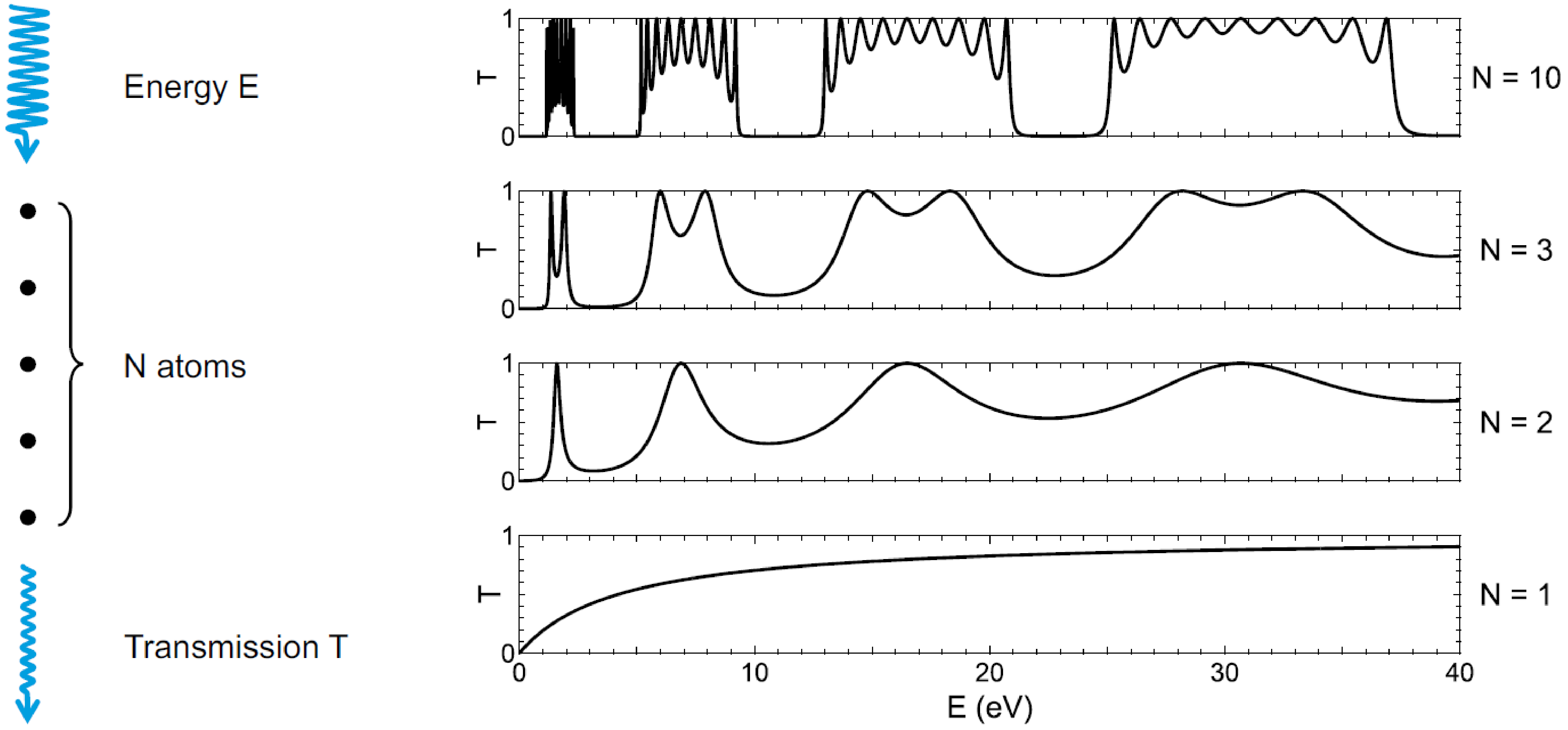


a, Kinematic sculpture by Eusebio Sempere. *b*, Sound attenuation results as a function of the sound frequency. The wave vector is along the (100) direction as shown in the inset. Arrows indicate the calculated maxima and minima due to interference from the different crystal planes of the sculpture.

NATURE · VOL 378 · 16 NOVEMBER 1995

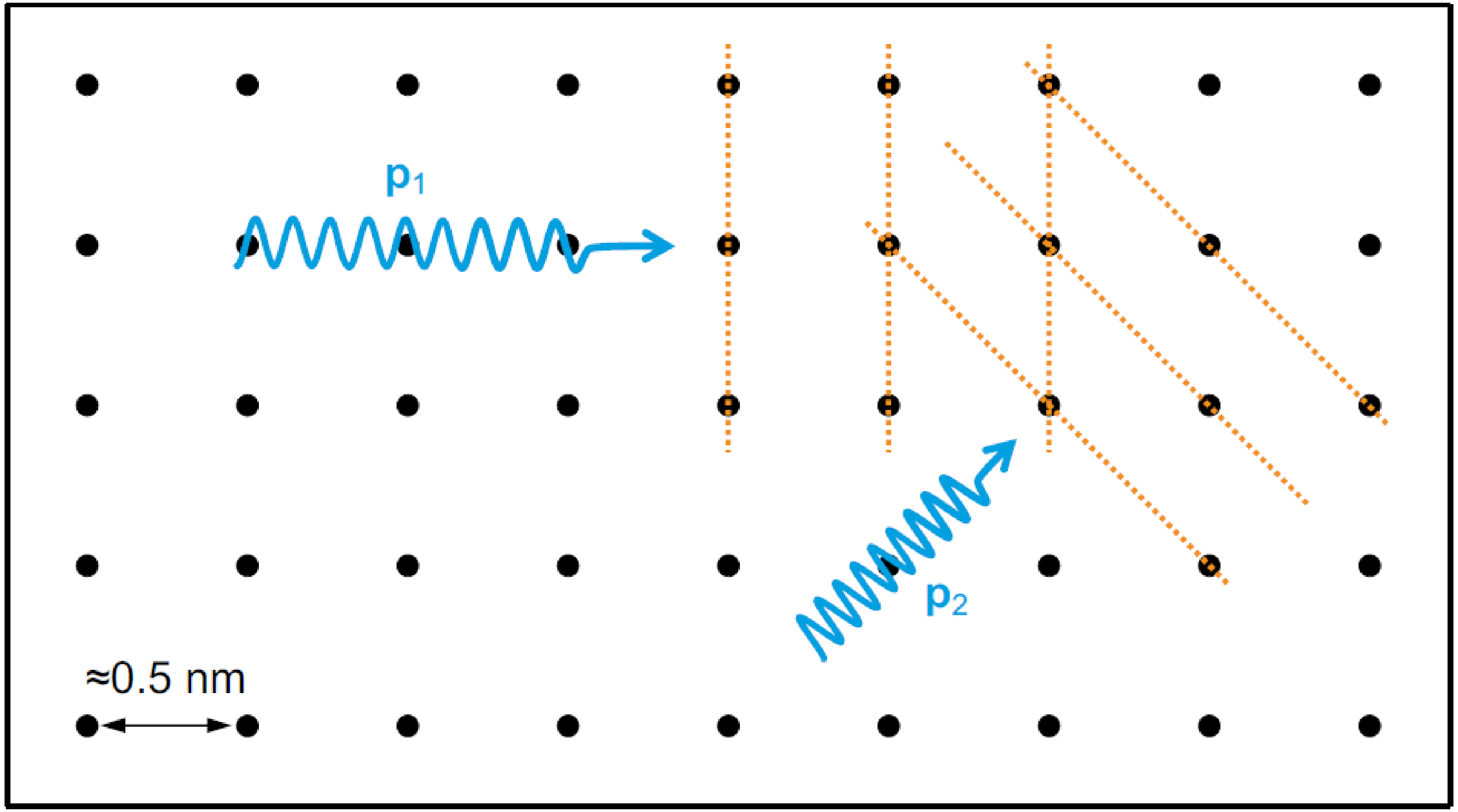
Electrons through a 1D lattice

Energy-dependent transmission



Electrons on a 2D lattice

Wavelength- & direction-dependent propagation (energy)



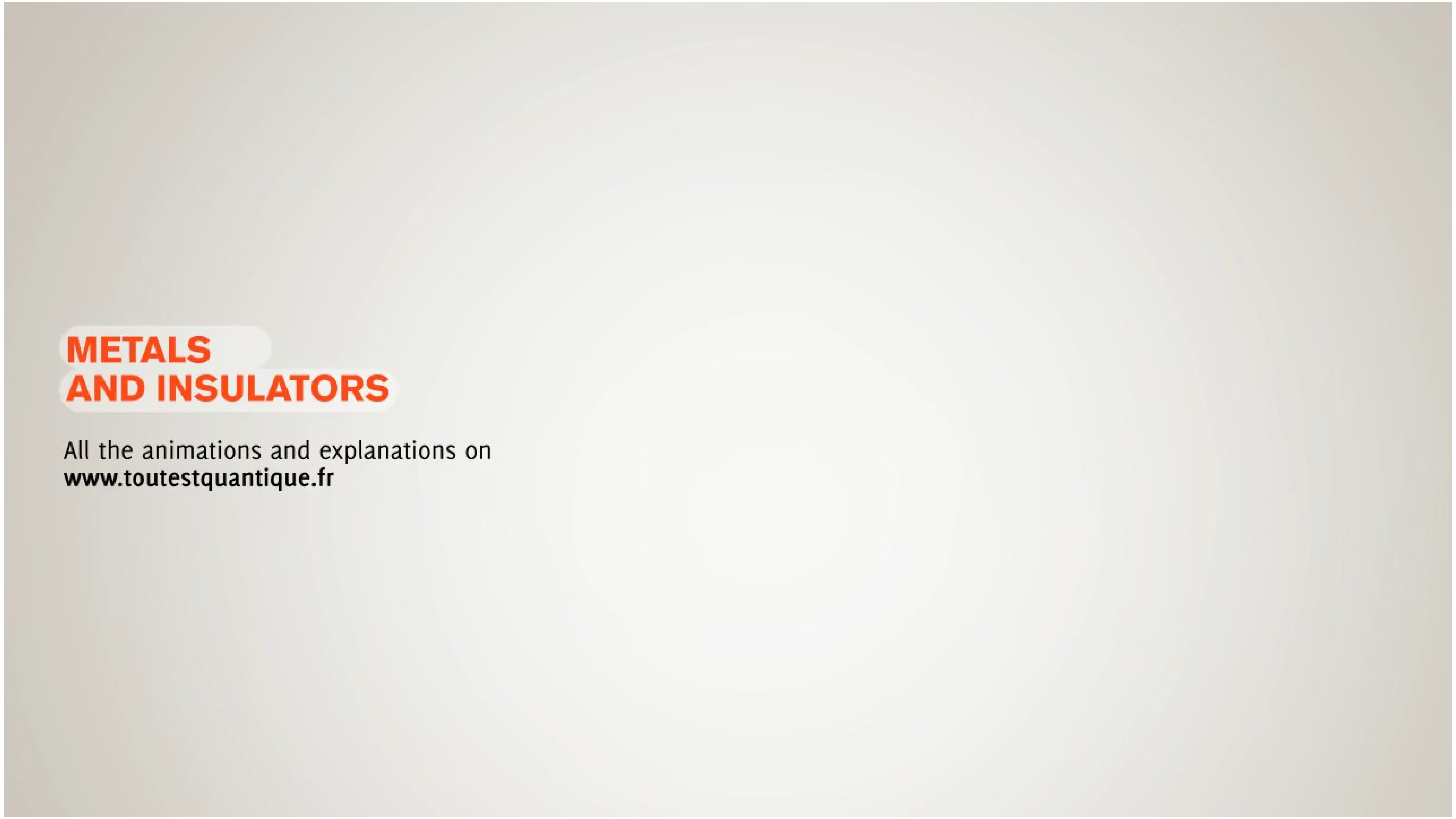
$$E(\mathbf{p})$$

$$\mathbf{p} = \hbar \mathbf{k}$$

$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{h^2}{2m}\frac{1}{\lambda^2}$$

Metals and insulators

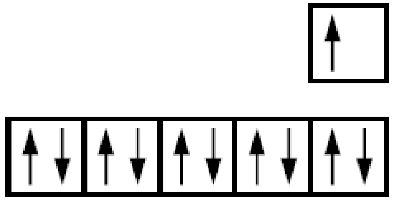
toutestquantique.fr

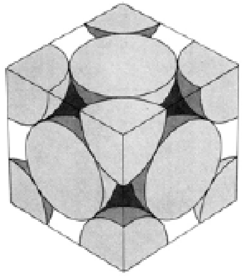


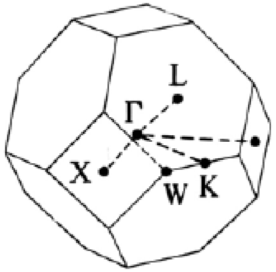
Band structure of copper

Why is copper conductive & reddish?

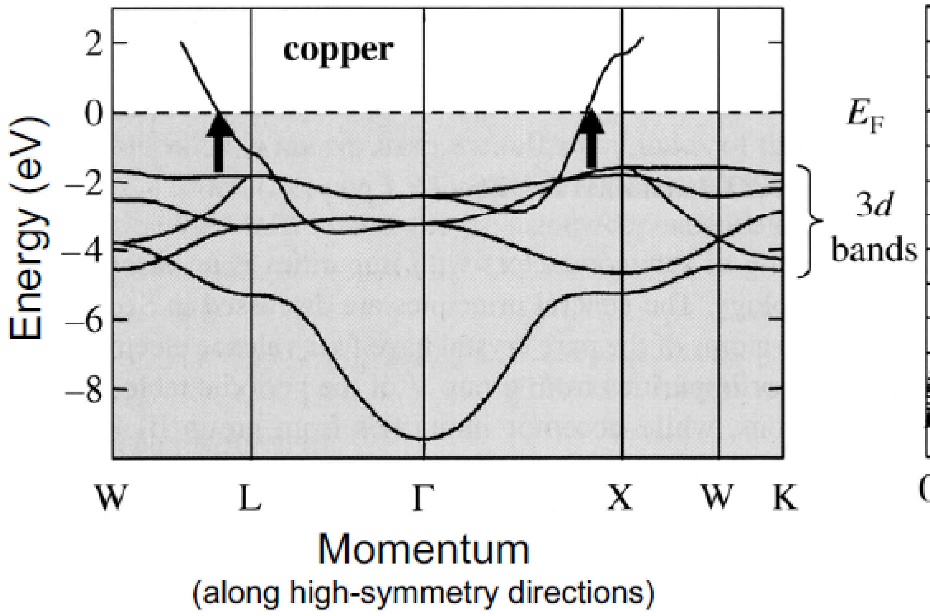
Cu: [Ar] $3d^{10}\ 4s^{1}$

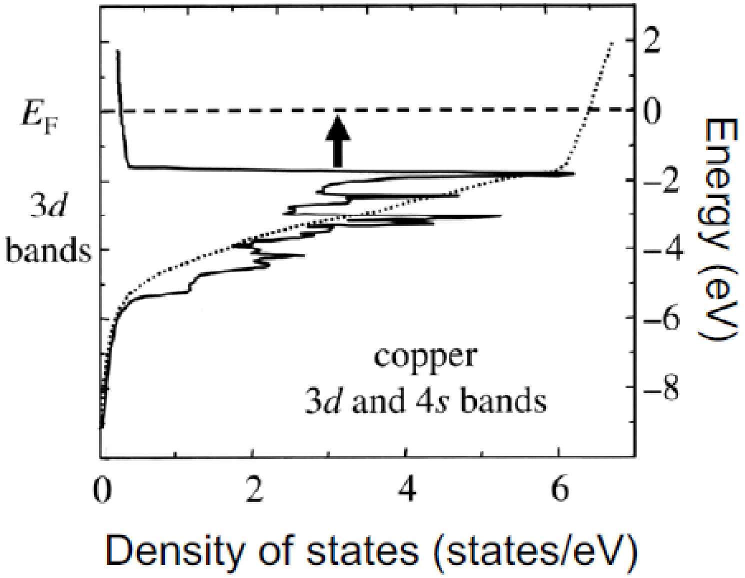






$$E = \frac{p^2}{2m} = \frac{h^2}{2m}\frac{1}{\lambda^2}$$





conductive

$$v = \frac{p}{m^*} = \frac{dE}{dp} \approx 1.6 \times 10^6\ \mathrm{m/s}$$

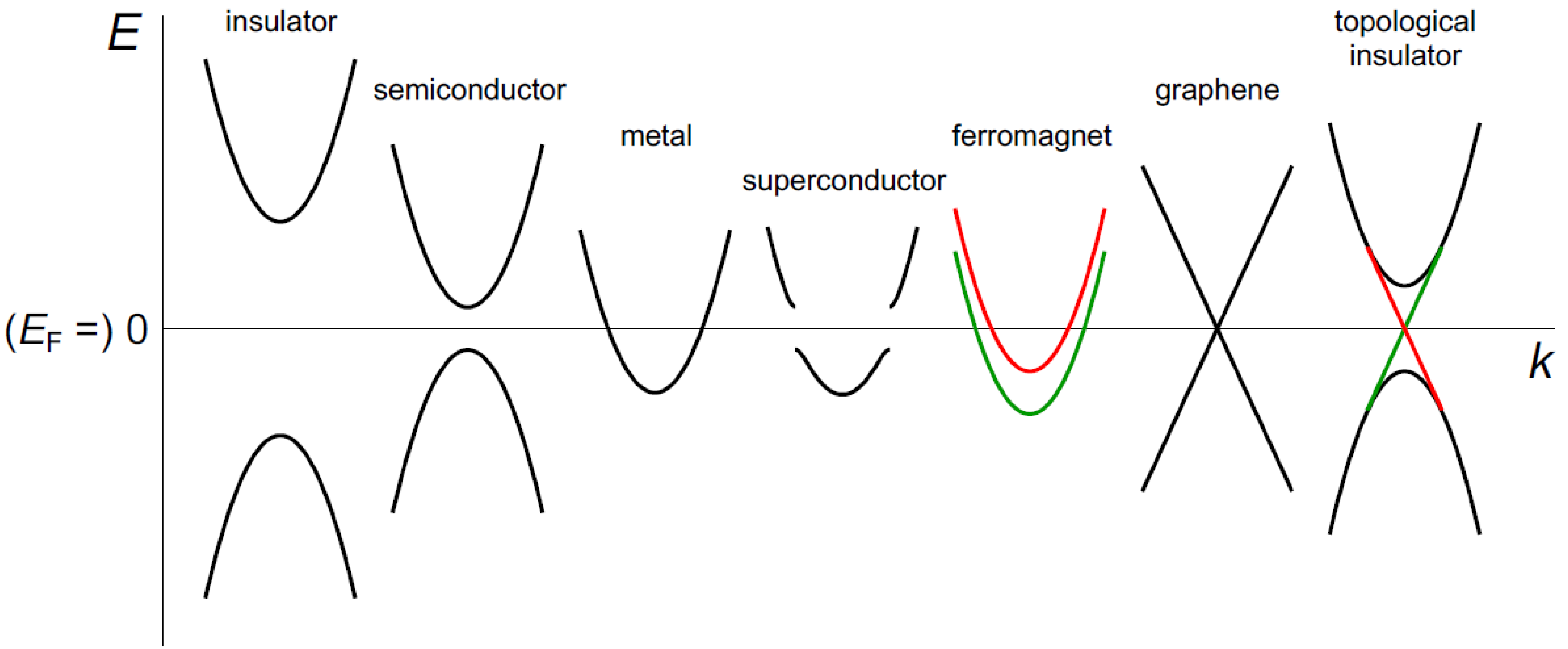
reddish

$$2\,\mathrm{eV} \approx 620\,\mathrm{nm}$$

Quantum materials

“Exotic” band structures

… solids with **exotic** physical properties, arising from the **quantum mechanical** properties of their constituent **electrons**; such materials have great scientific and/or technological potential.



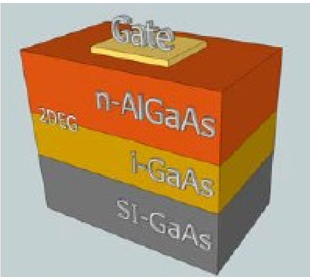
Brief history of quantum materials

Spanning ≳4500 years

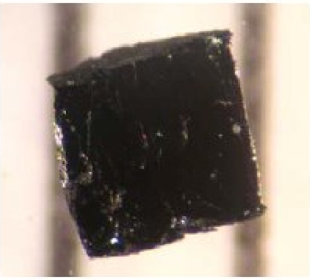
≲ −2500 years
Magnetite (Fe_3O_4)
Ferromagnetism

Symmetry

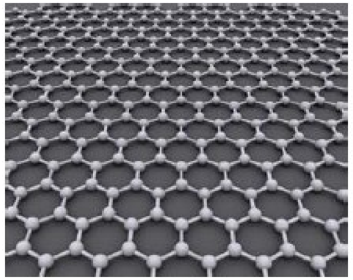
1911
Mercury (Hg)
Superconductivity



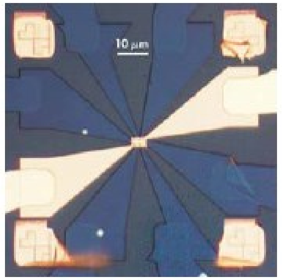
1980
2D electron gas
Quantum Hall effect
Topology & Dimensionality



1986
$La_{1.85}Ba_{0.15}CuO_4$
High-temperature SC
Interaction



2004
Graphene (C)
2D materials
Dimensionality



2007
(Hg,Cd)Te quantum well
Topological insulator (2D)

Topology

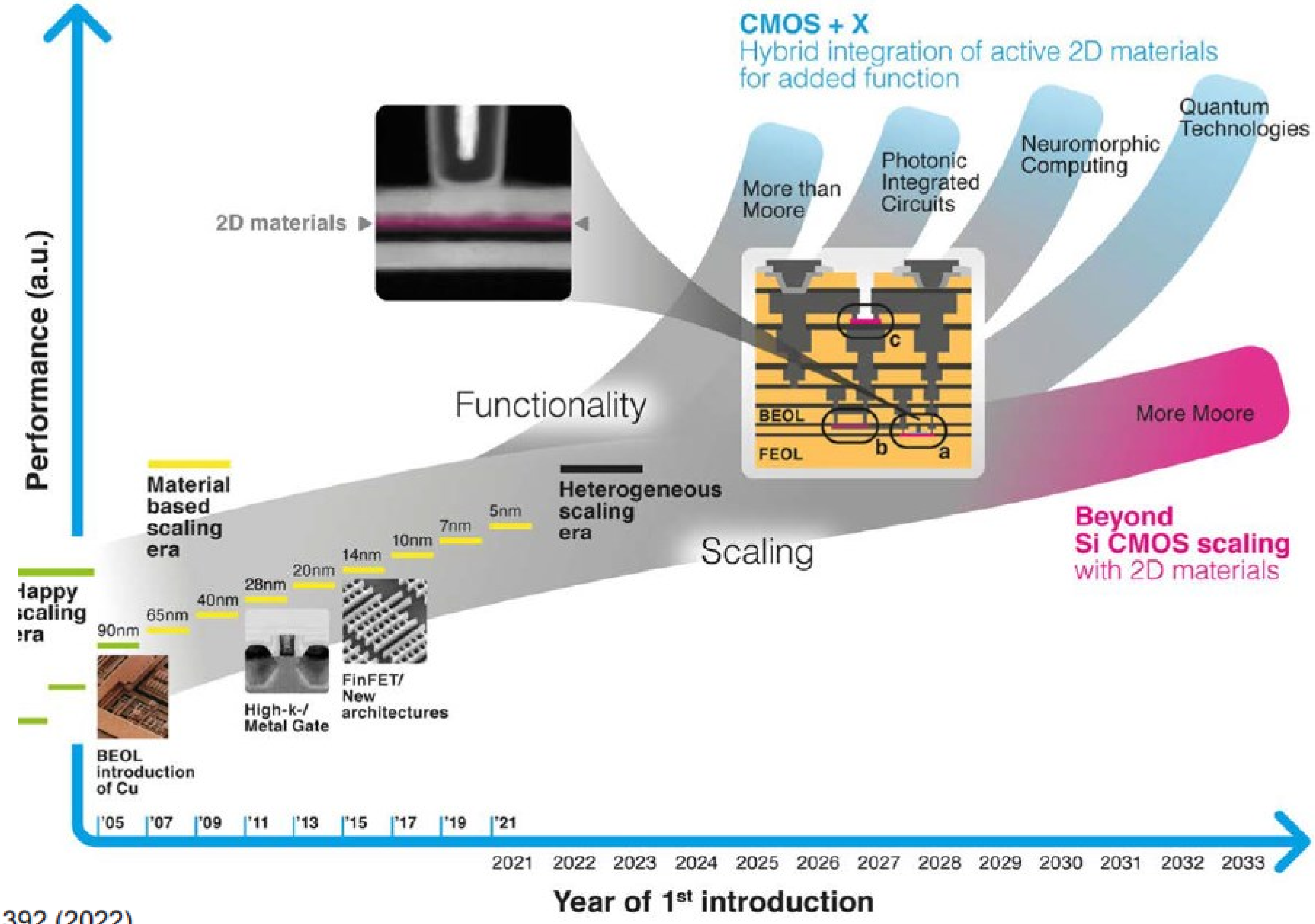
2008
$Bi_{1-x}Sb_x$
Topological insulator (3D)

Graphene

toutestquantique.fr

Towards 2D material electronics

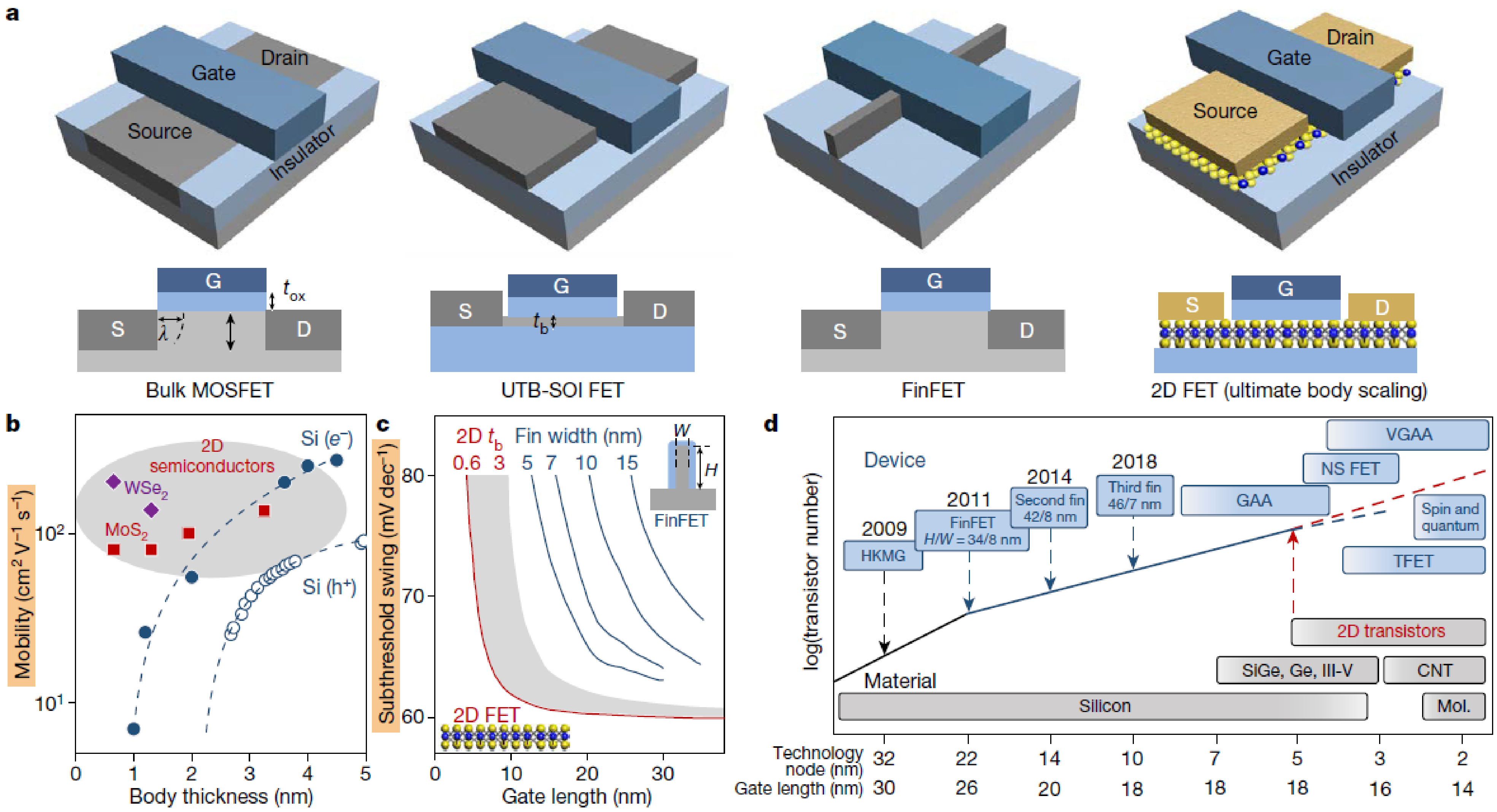
"CMOS + X"



Lemme *et al.*, Nat. Commun. **13**, 1392 (2022)

2D transistors

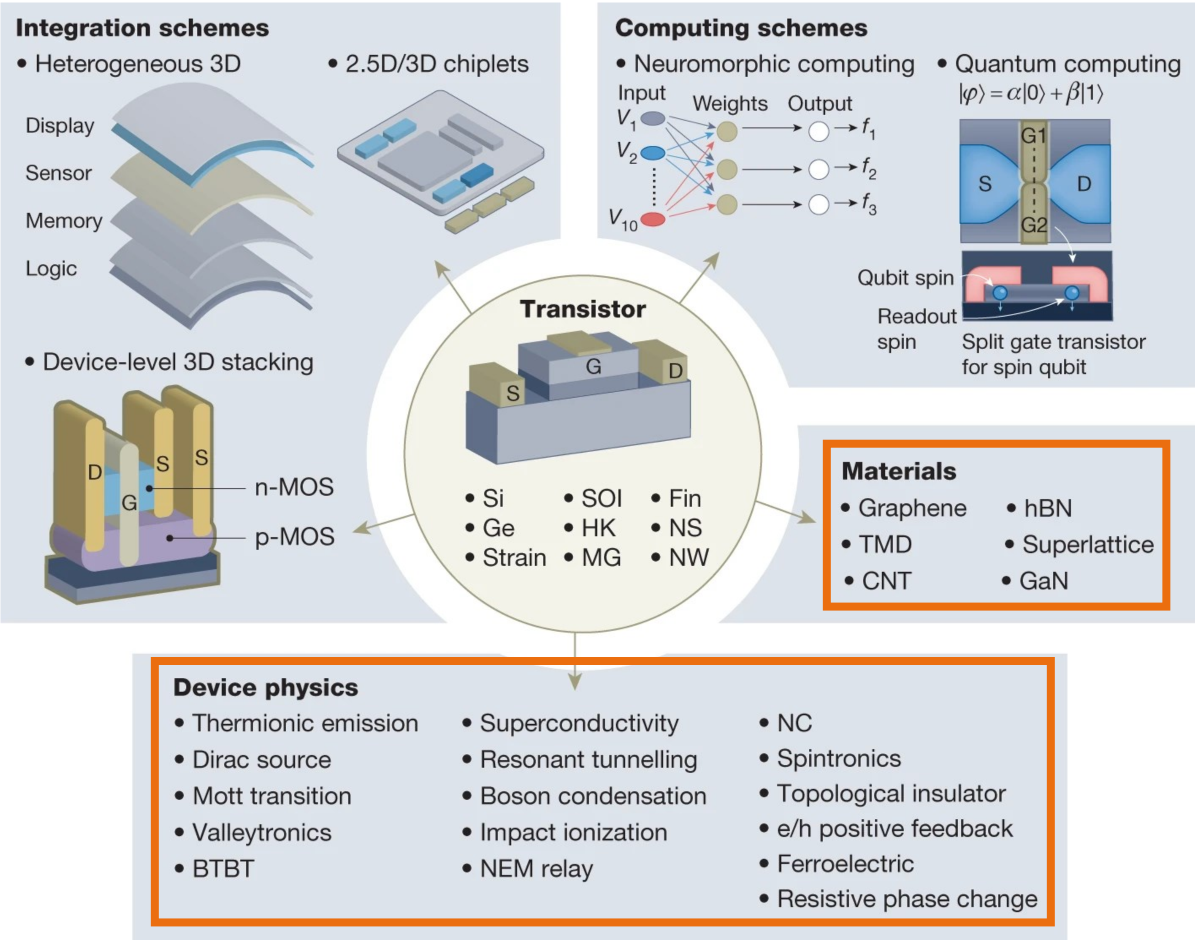
Beyond Si CMOS scaling



Liu *et al.*, Nature **591**, 43 (2021)

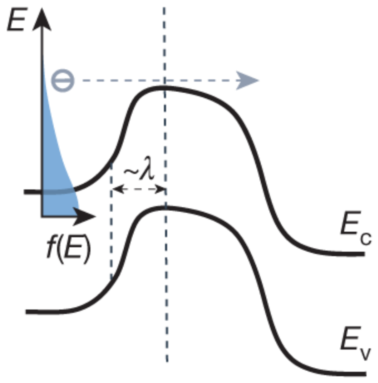
Future transistors

The need for new (quantum) materials & mechanisms

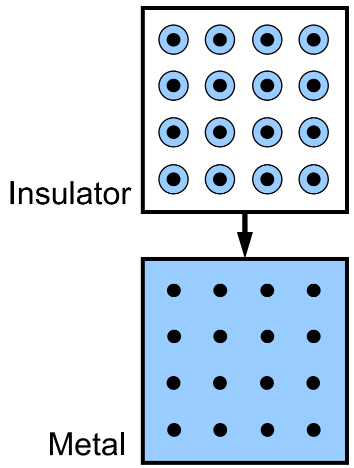


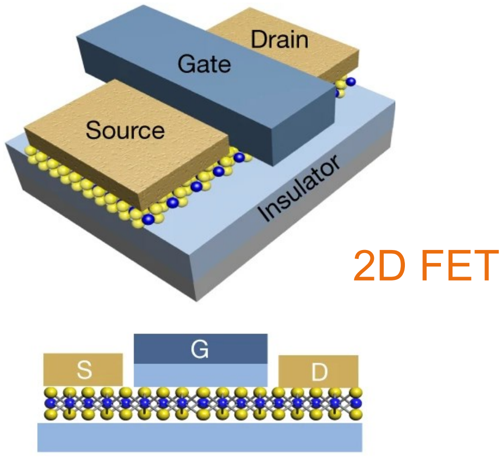
Cao *et al.*, Nature **620**, 501 (2023)

Thermionic emission

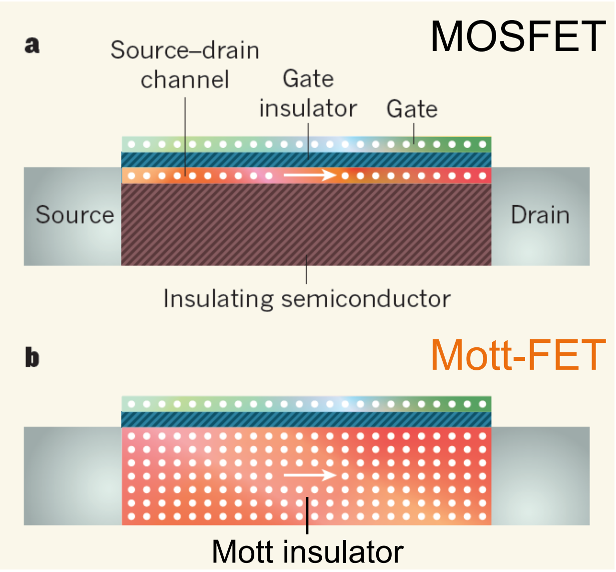


Mott transition





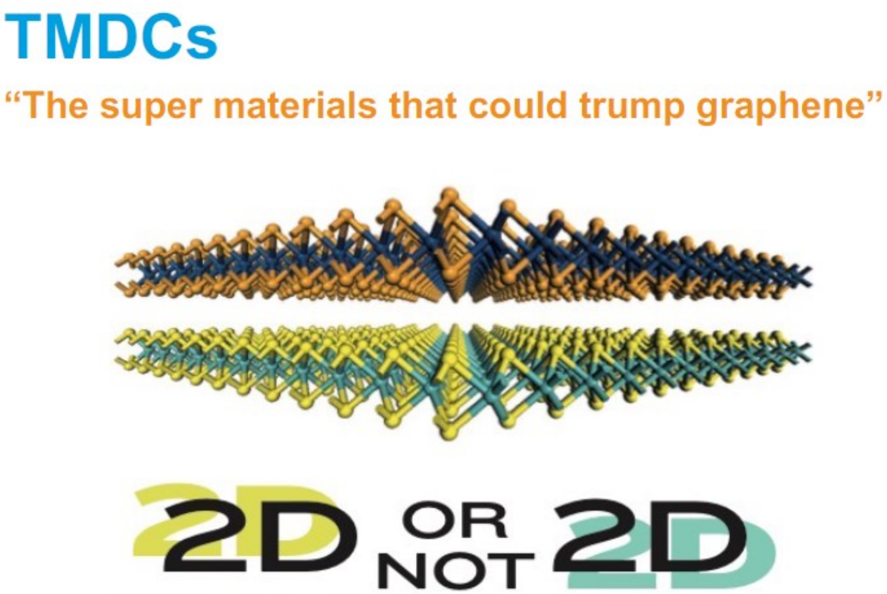
Liu *et al.*, Nature **591**, 43 (2021)



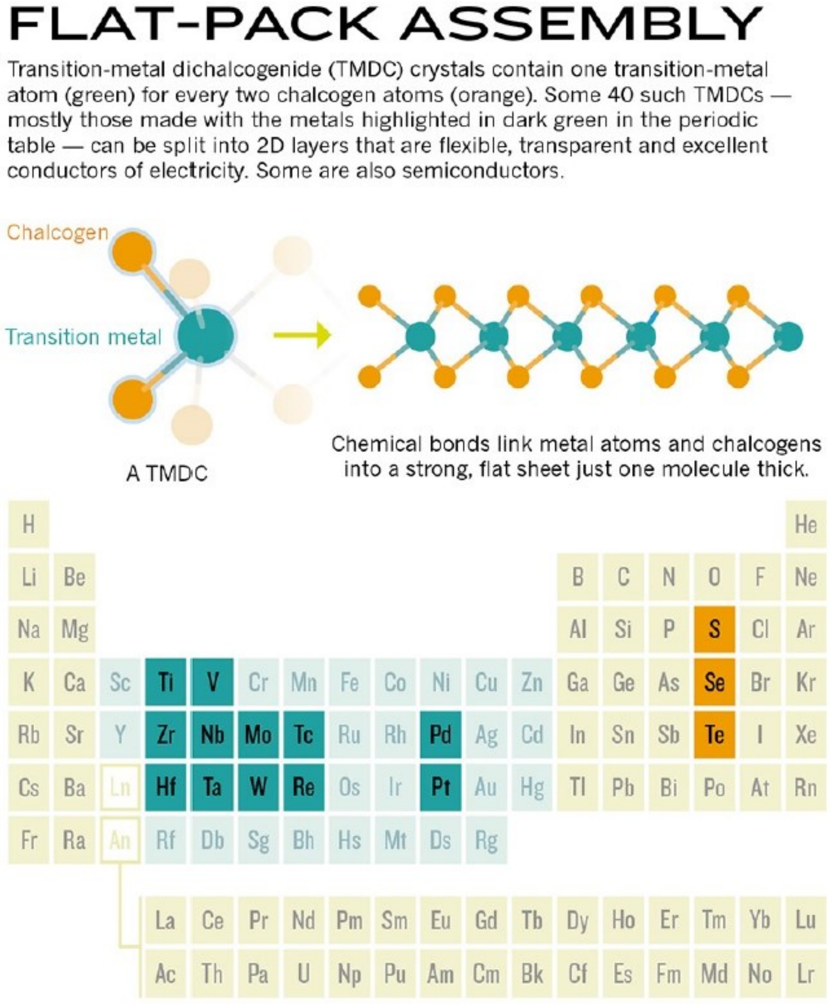
Mannhart & Haensch, Nature **487**, 436 (2012)

Beyond Graphene

“The super materials that could trump graphene”



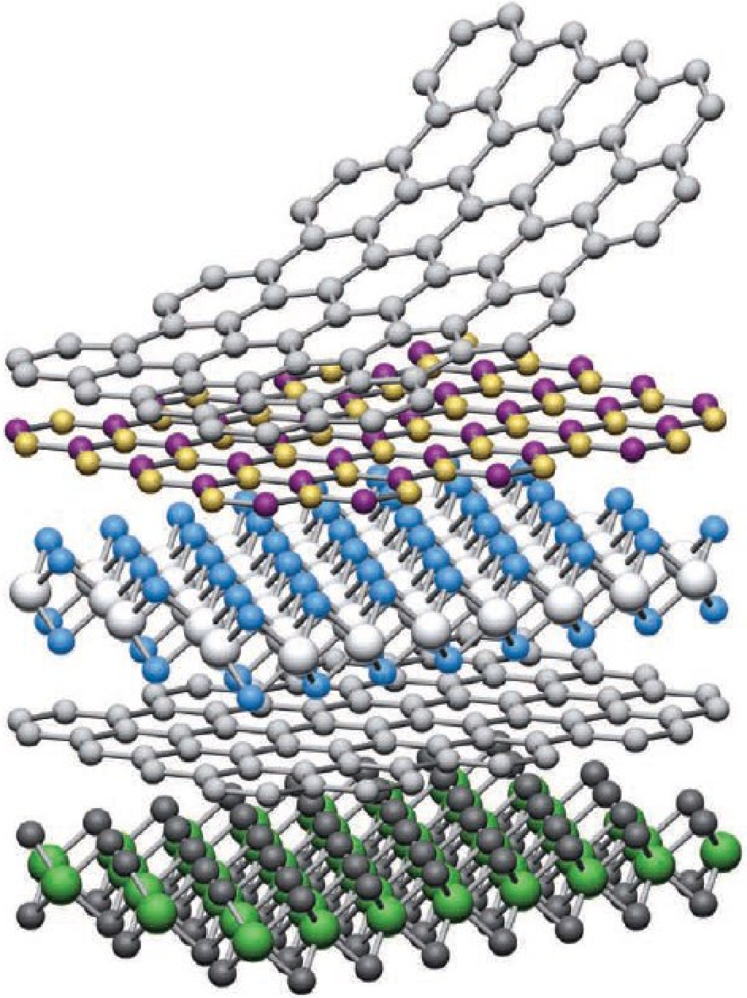
E. Gibney, Nature **522**, 274 (2015)

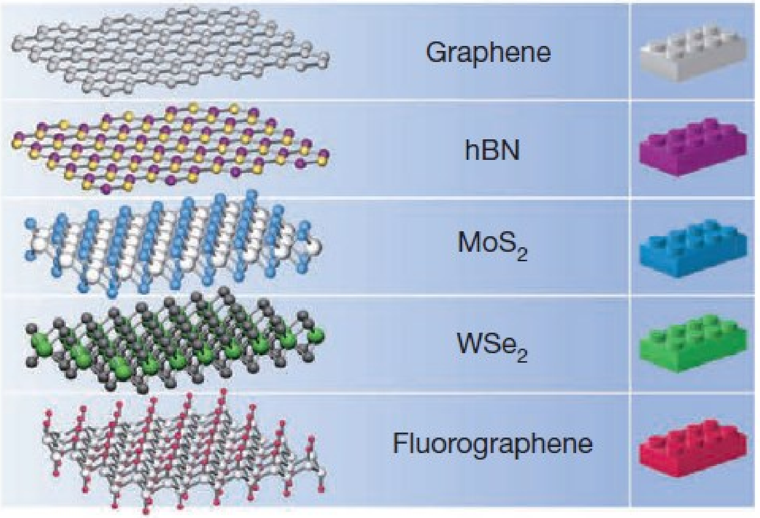


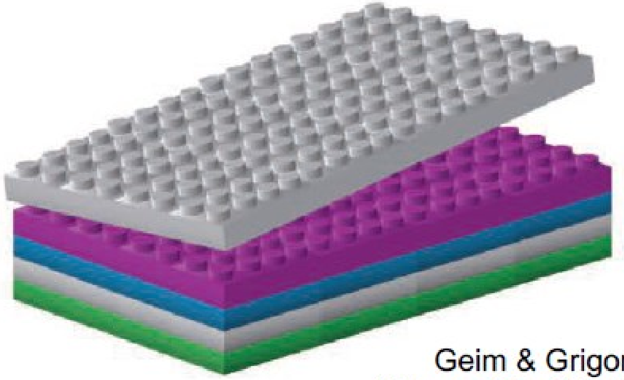
Van der Waals heterostructures

“What if we mimic layered superconductors by atomic-scale LEGO?”

- clean, strain-free **atomically sharp interfaces**
- (gate) tunable, emergent **electronic properties**
- new kinds of **devices** & **electronics**







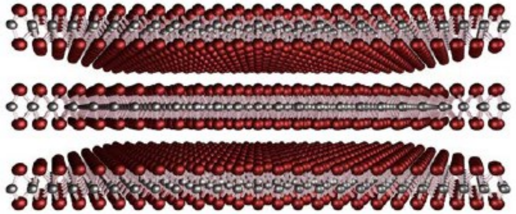
Geim & Grigorieva, Nature **499**, 419 (2013)

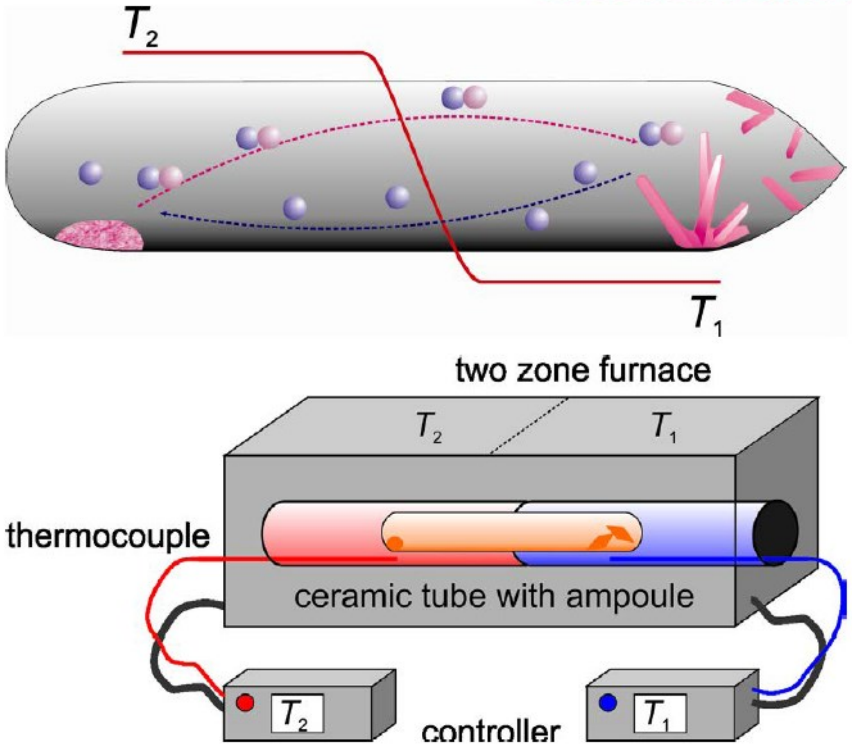
TMDC crystal growth

Chemical vapor transport

Group of Kai Rossnagel

Christian-Albrechts-Universität zu Kiel





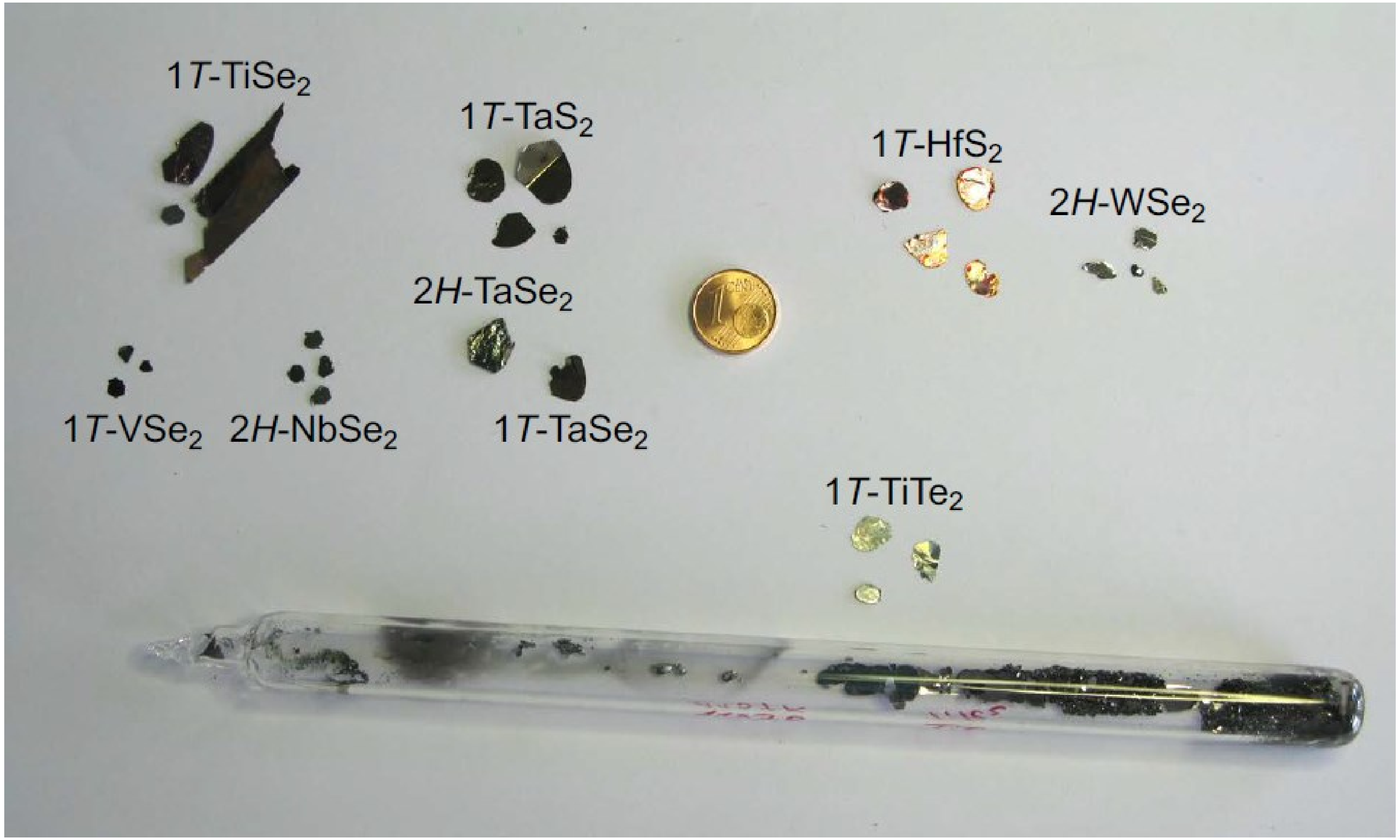
Schmidt *et al.*, *Chemical Vapor Transport Reactions—Methods, Materials, Modeling*

Commercial break

TMDC crystal growth

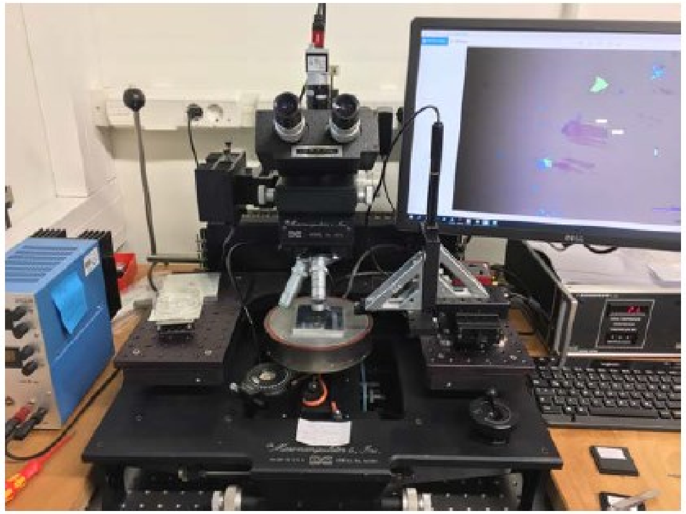
Group Rossnagel

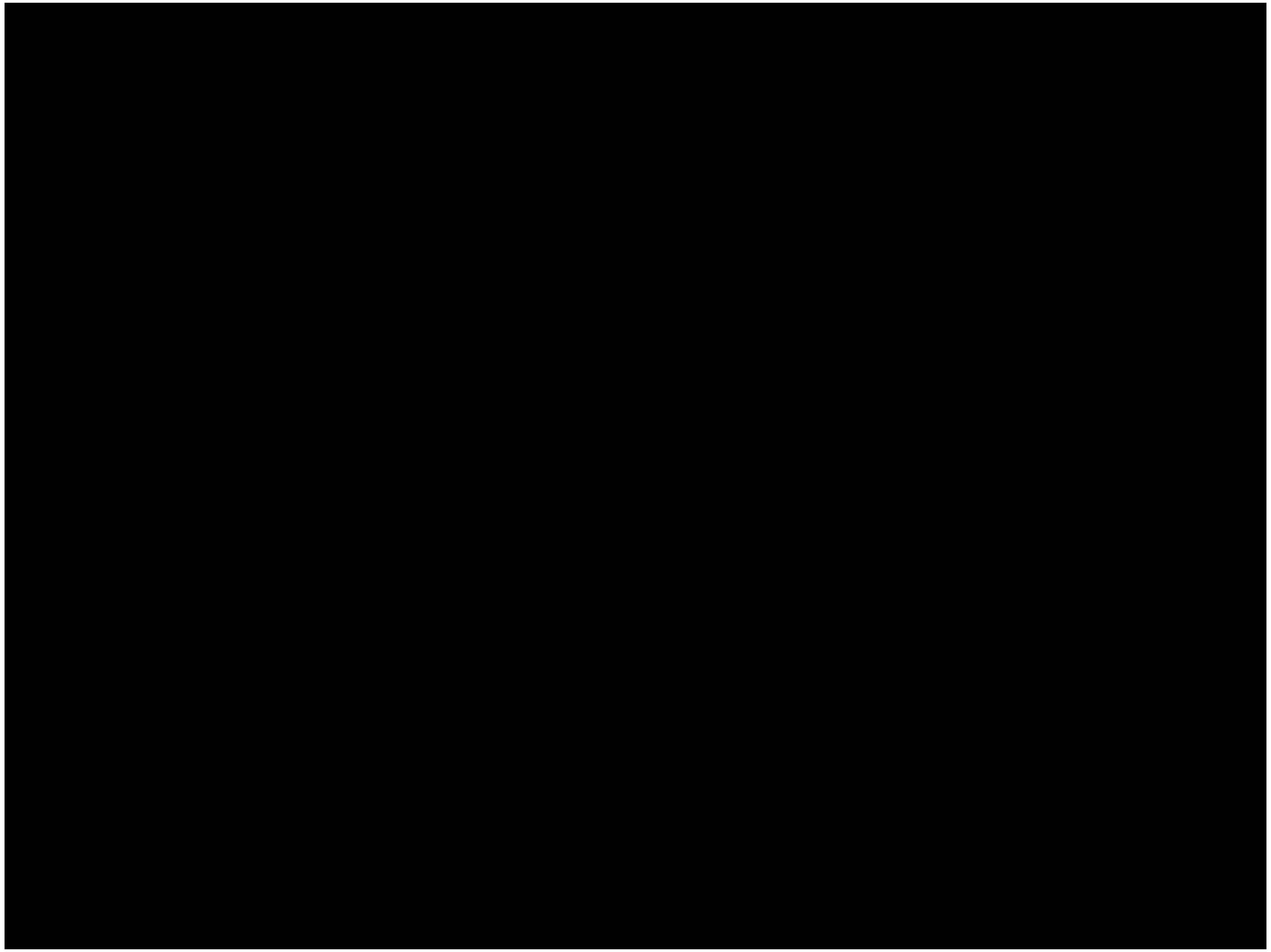
Christian-Albrechts-Universität zu Kiel



Scotch tape method

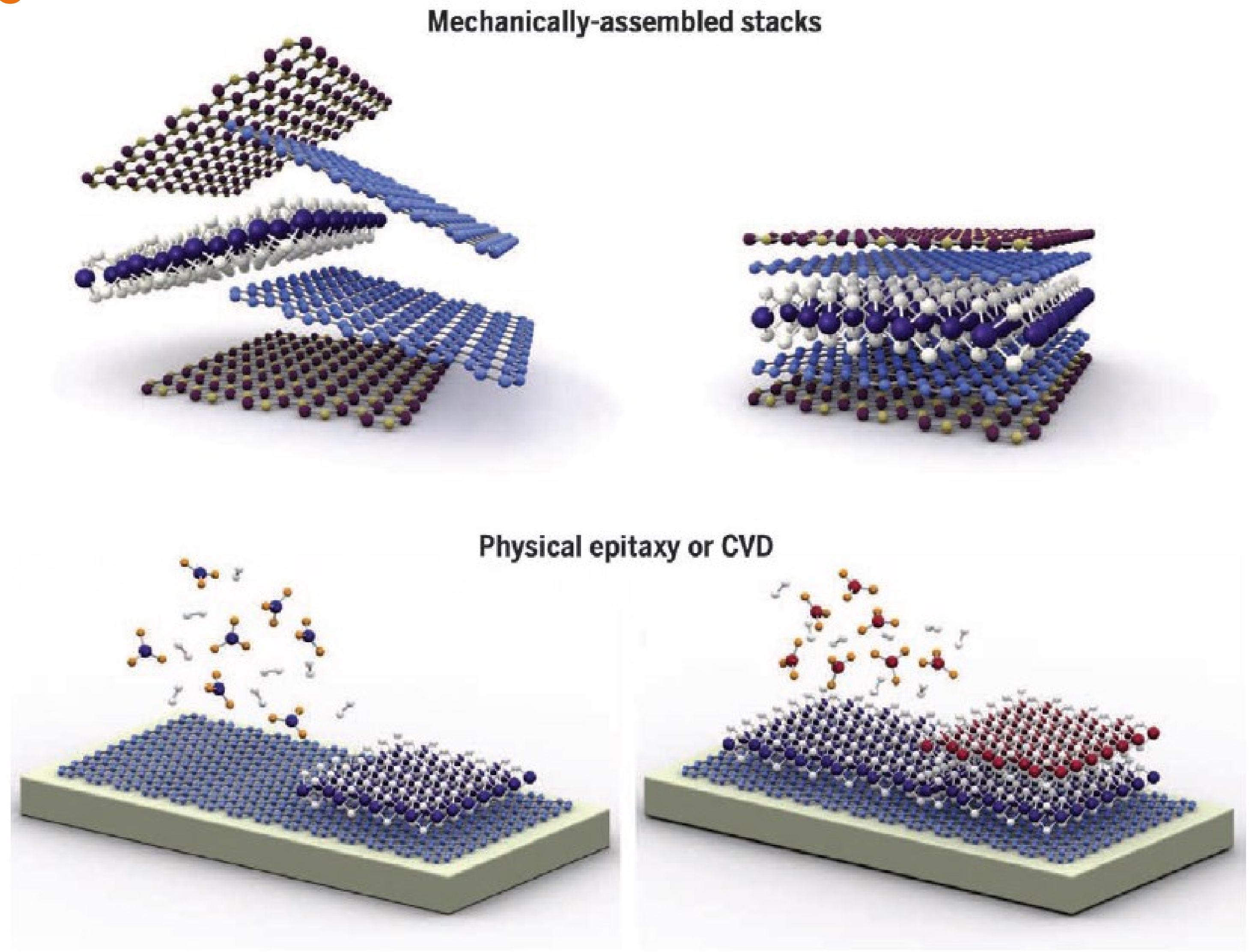
Mechanical exfoliation





Van der Waals heterostructures

Quantum LEGO

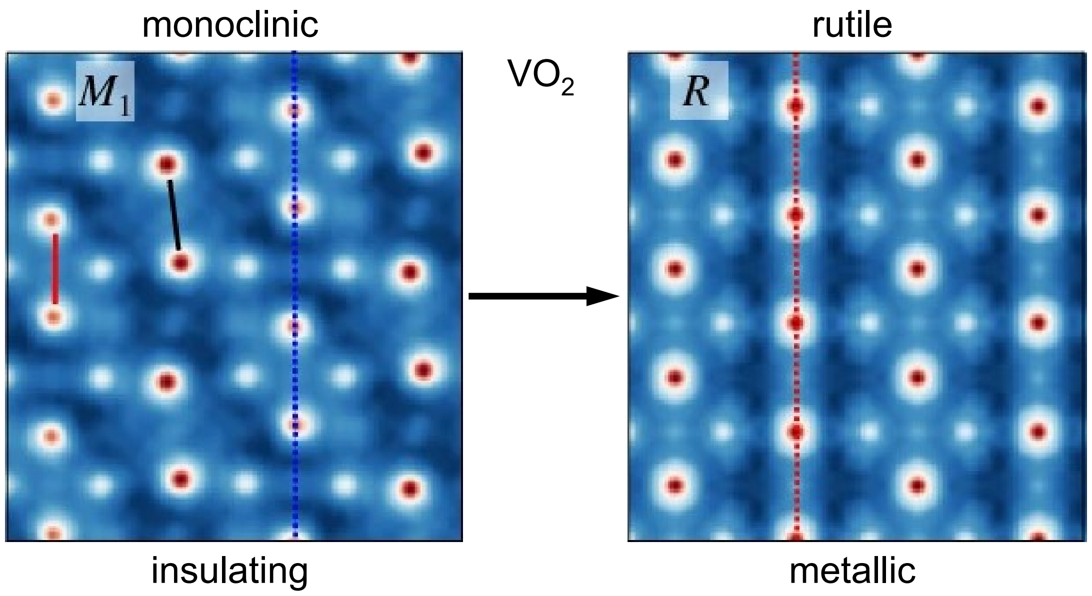


Novoselov *et al.*,
Science **353**, 461 (2016)

Intellectual appeal of quantum materials

The physics of ultrafast switching: complex coupled lattice & electron dynamics

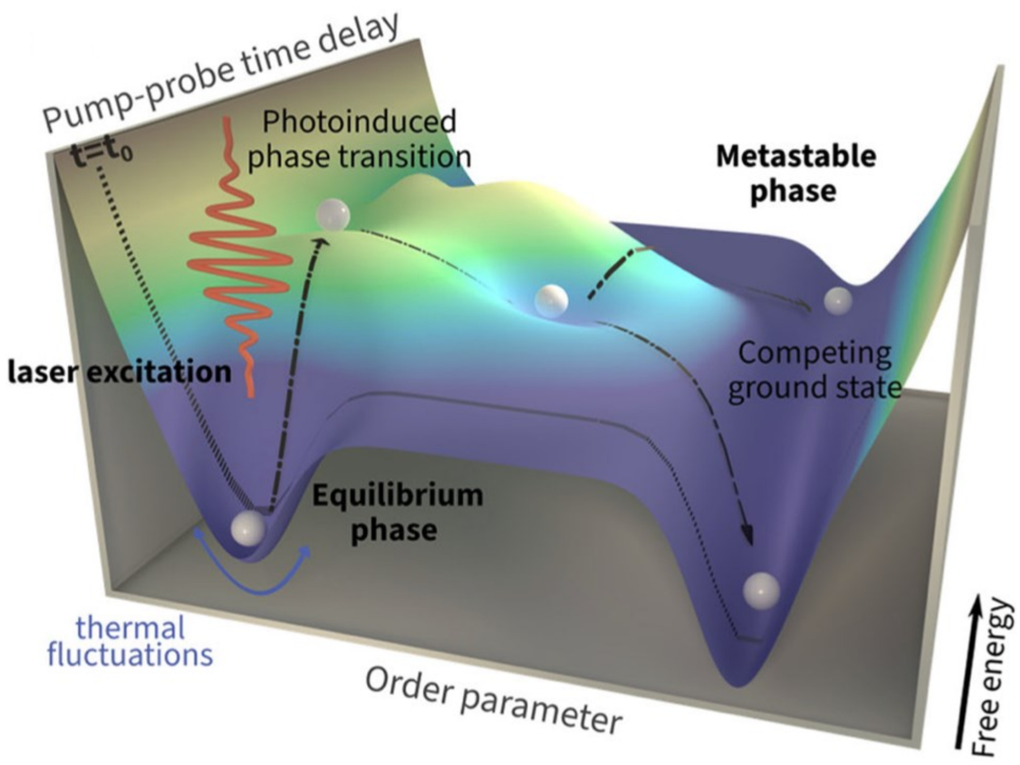
Electrostatic potential



- Speed?
- Efficiency?
- Mechanism?

Otto *et al.*, PNAS **116**, 450 (2019)

Free energy

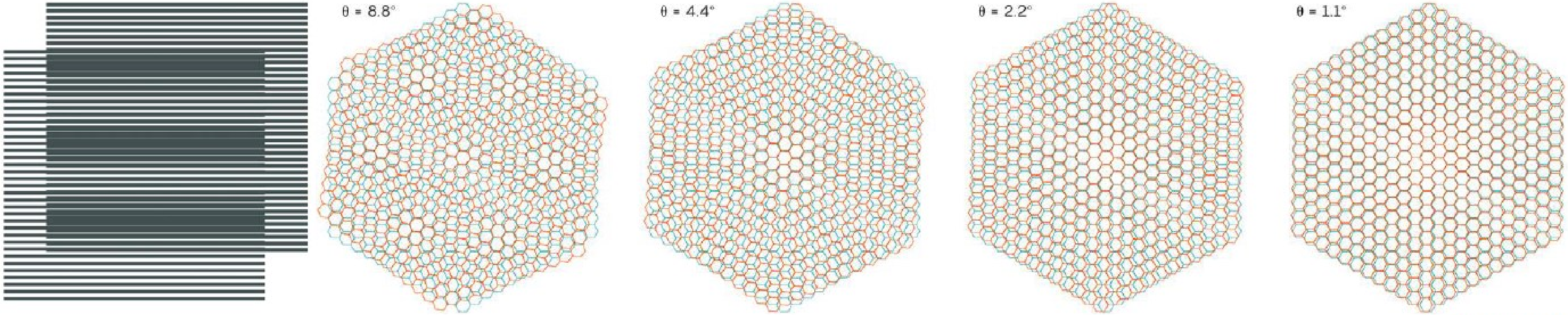


$$F = F_{\text{electr.}} + F_{\text{latt.}}$$

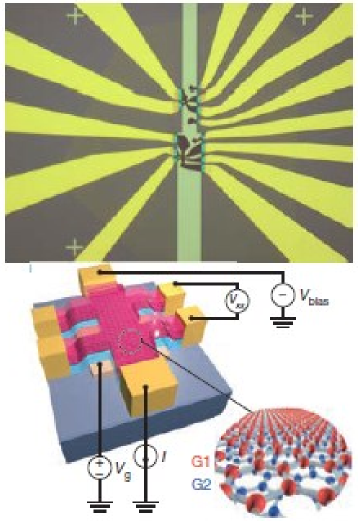
Filippetto *et al.*, Rev. Mod. Phys. **94**, 045004 (2022)

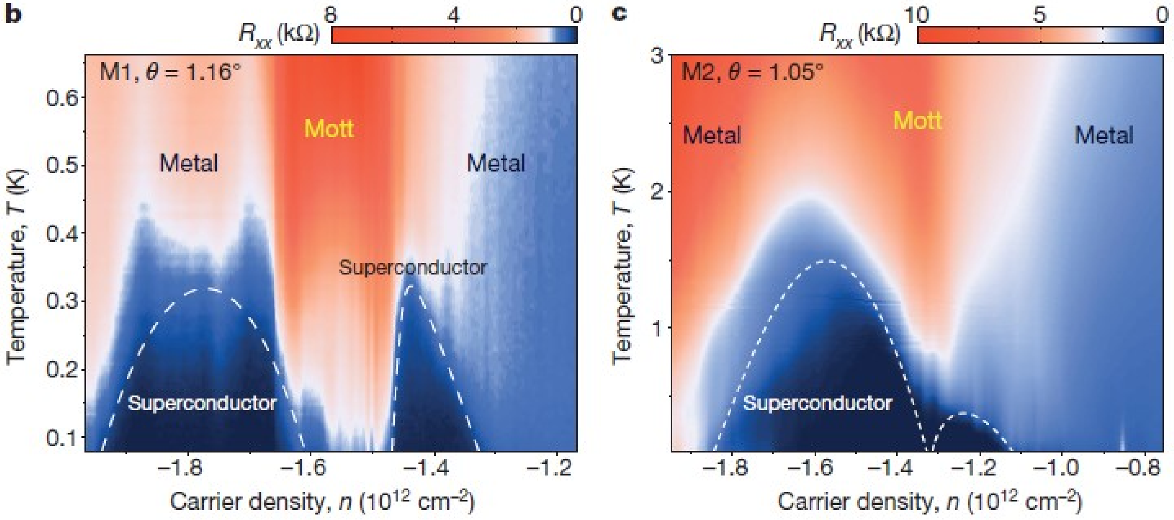
Twistronics

“With a simple twist, a ‘magic’ material is now the big thing in physics.”



quantamagazine.org





Y. Cao *et al.*,
Nature **556**, 43 (2018)

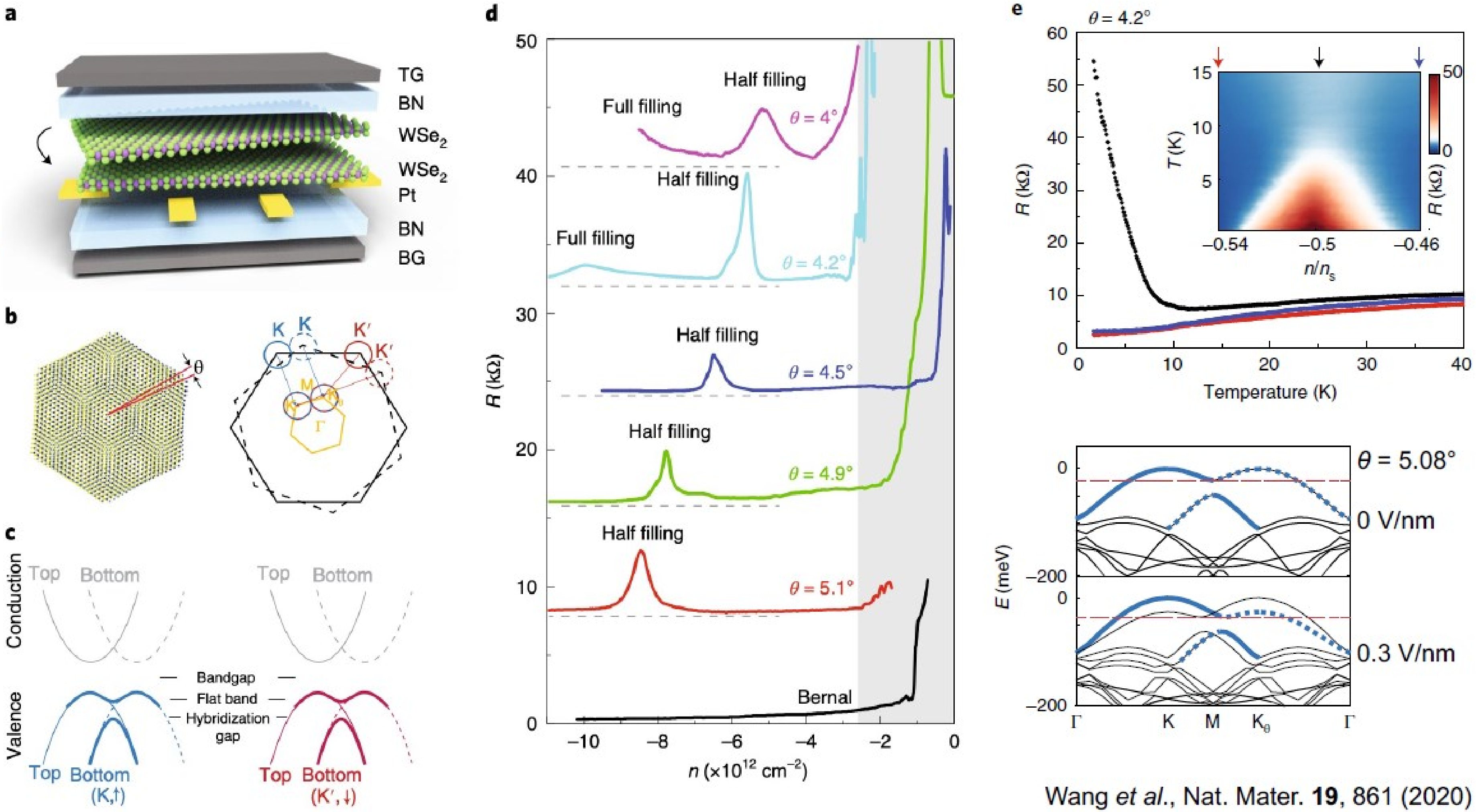
Twistronics

Twisted bilayer WSe_2

Bandwidth control (via **twist** angle & gate voltages) Carrier density control (via gate voltages)

Moiré superlattice

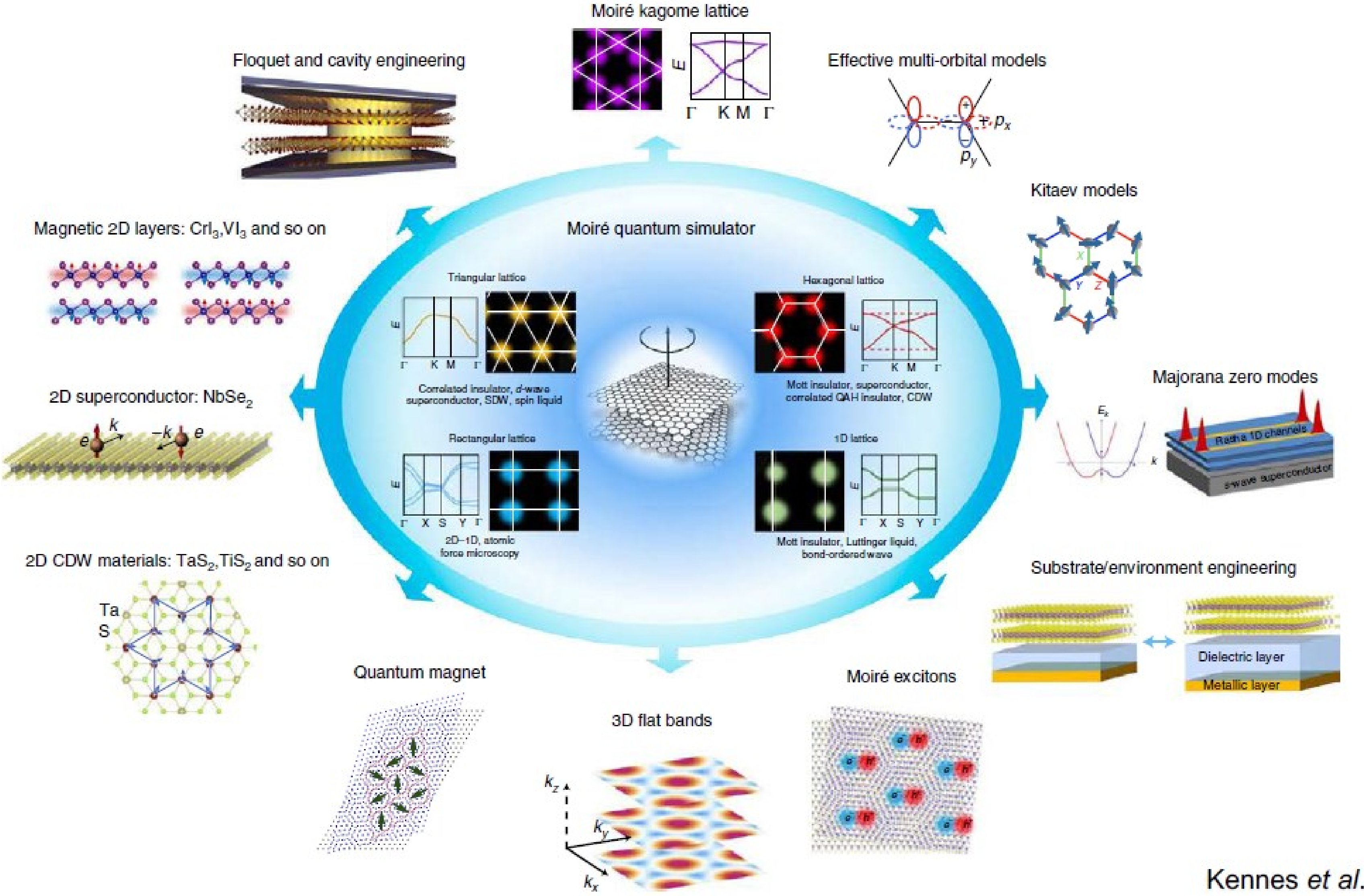
Flat band (pseudo-spin degenerate, 2e- per 126⋯205 W atoms)



Wang *et al.*, Nat. Mater. **19**, 861 (2020)

Moiré quantum simulator

Controllable quantum Hamiltonians realized by twisted van der Waals heterostructures



Kennes *et al.*, Nat. Phys. **17**, 155 (2021)