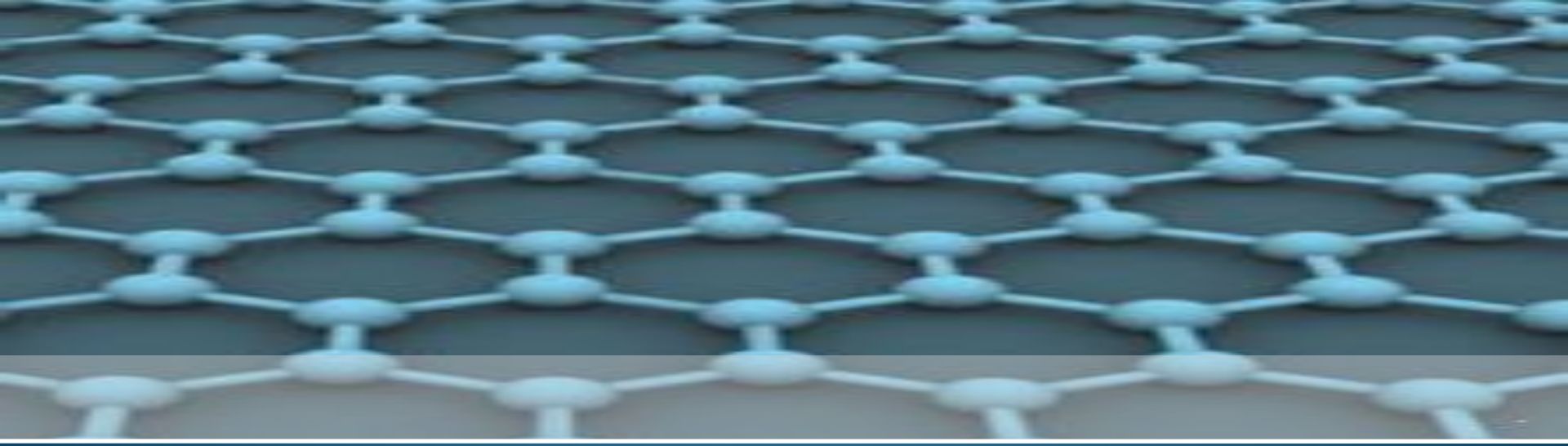

What could we do with layered structures of materials with just the right layers? -Feynman

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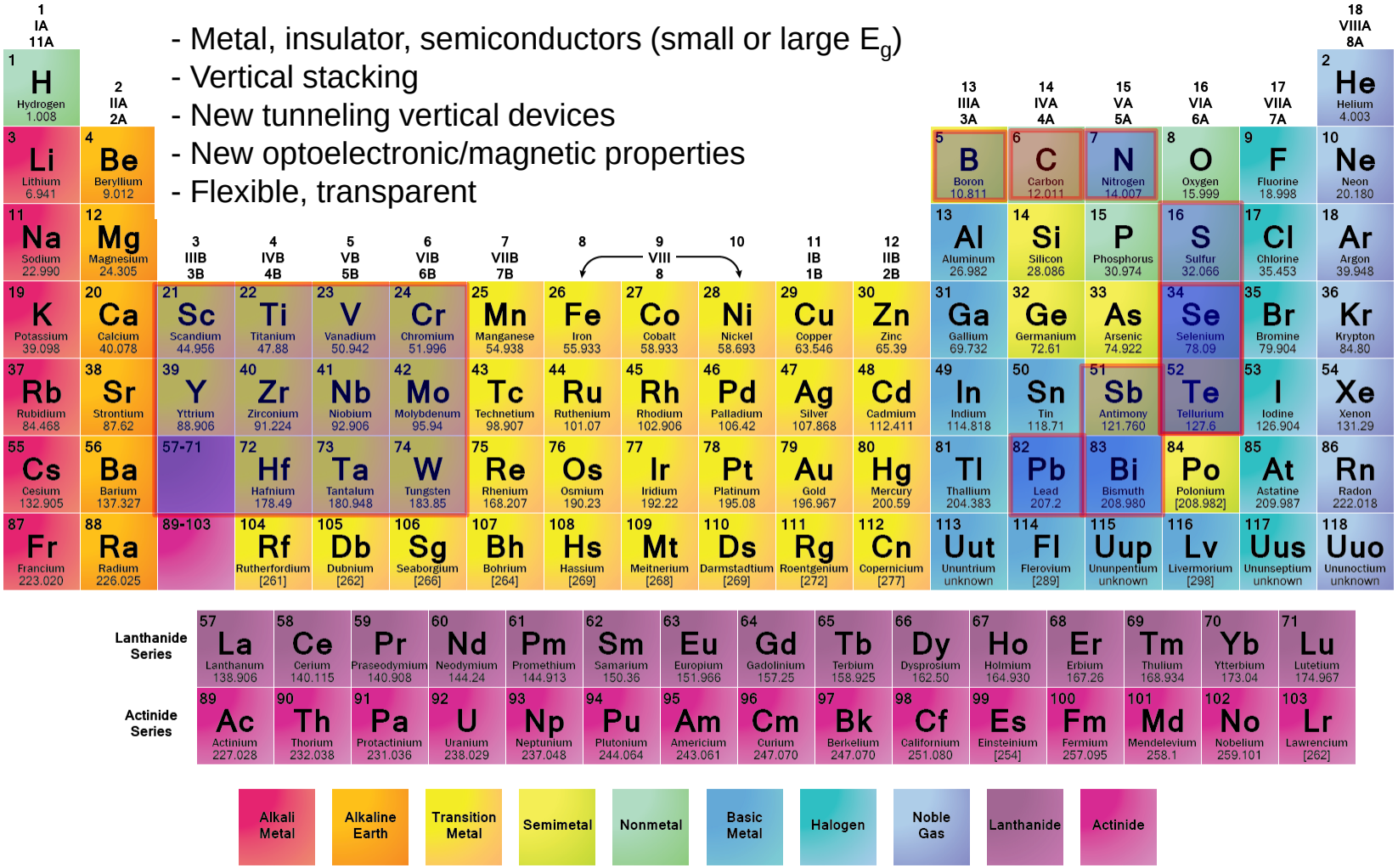
Periodic table: 2D layered materials

CINAP

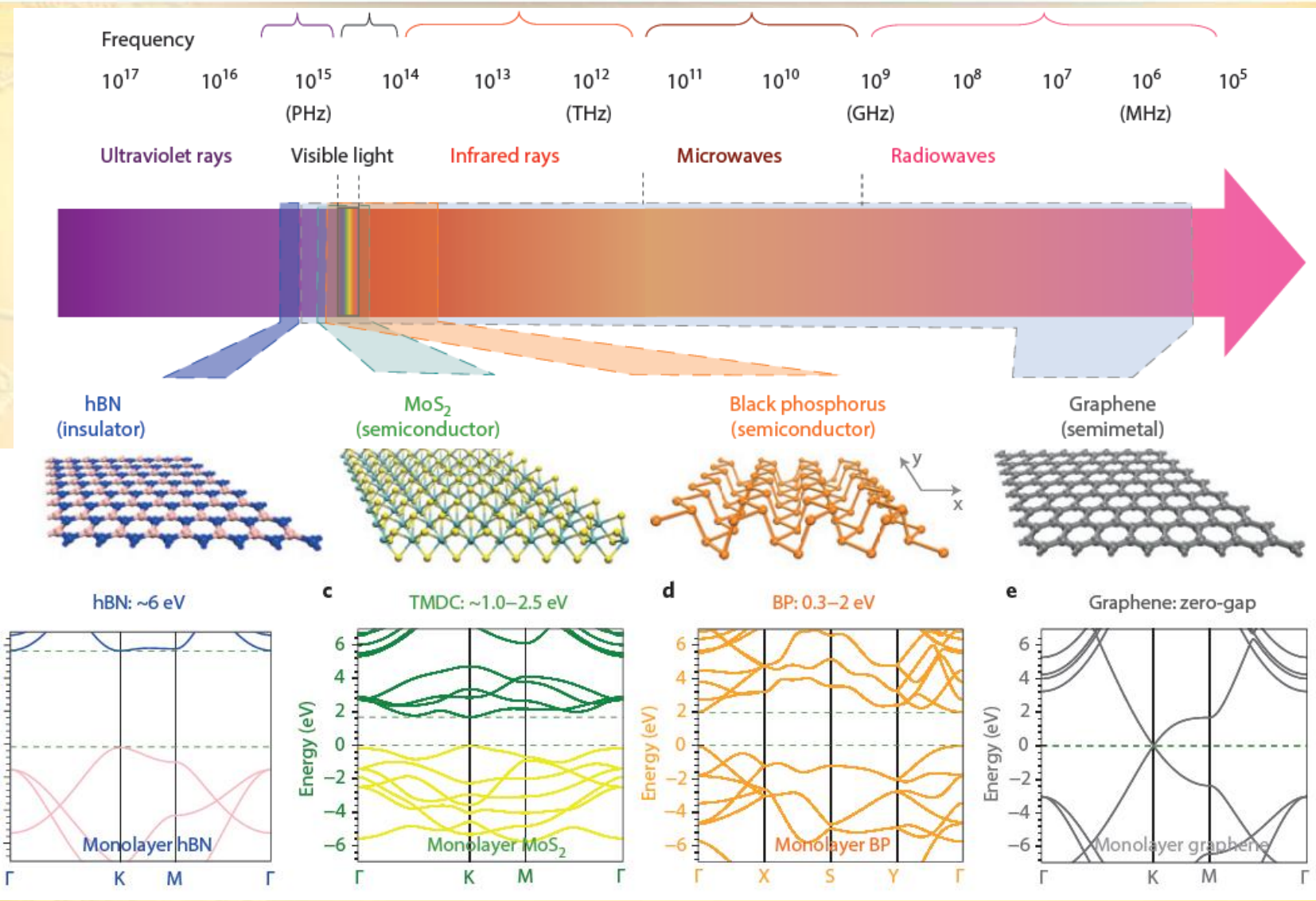
What could we do with layered structures of materials with just the right layers? -Feynman

- Metal, insulator, semiconductors (small or large E_g)
- Vertical stacking
- New tunneling vertical devices
- New optoelectronic/magnetic properties
- Flexible, transparent



New material and physics world in 2D !!!!

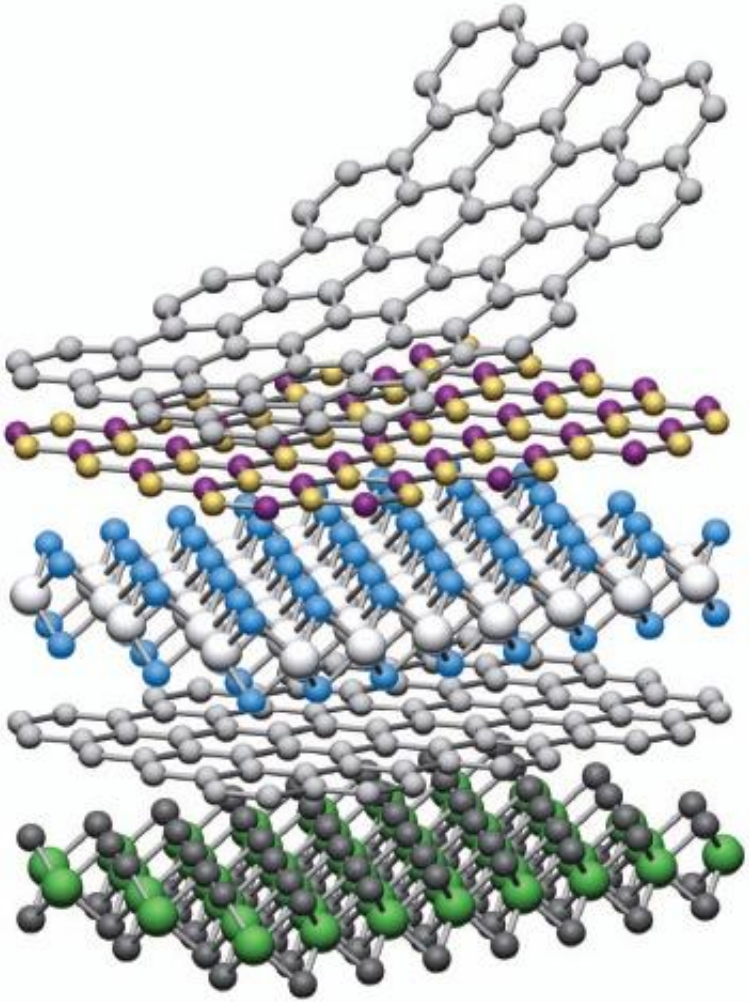
Atomic layered materials

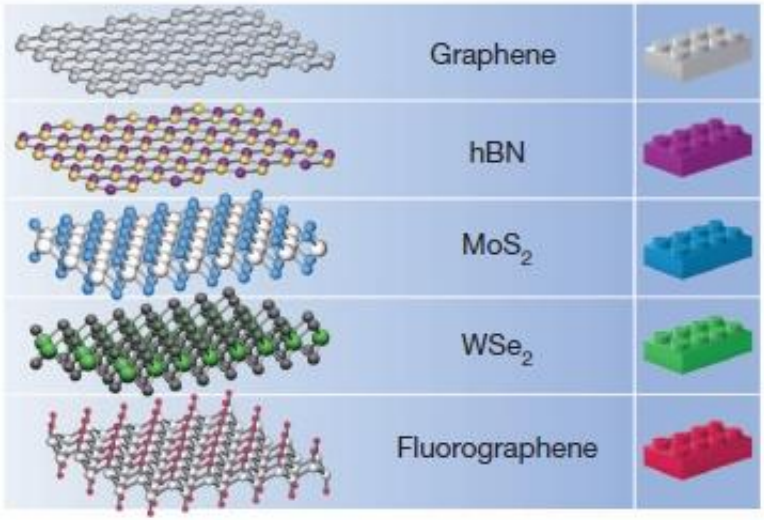


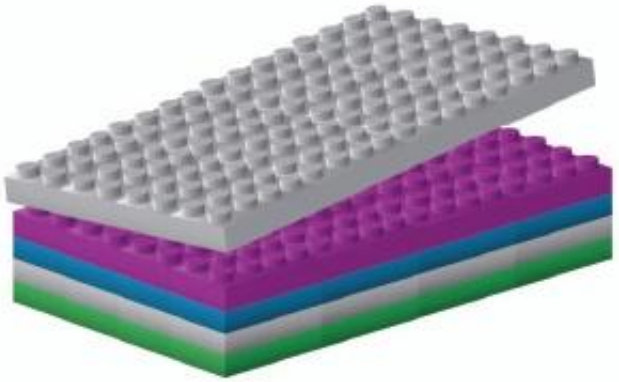
Nat. Photon. 8, 899-907 (2014)

Vertical structure

New device structures by van der Waals stacking





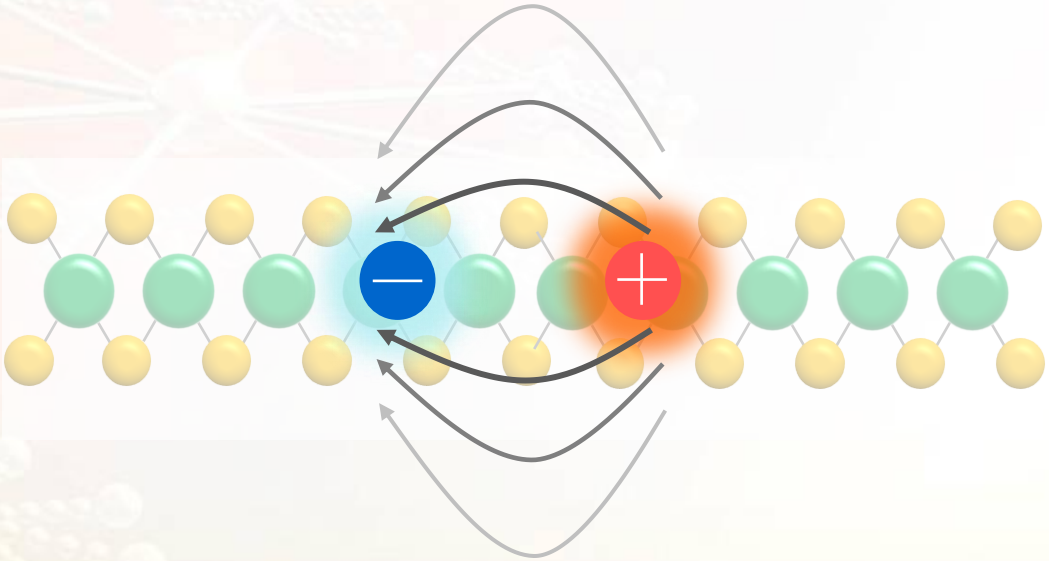


A. K. Geim et al. Nature 499, 419 (2013)

What is new in 2D?

Strong Coulomb interaction or less charge screening

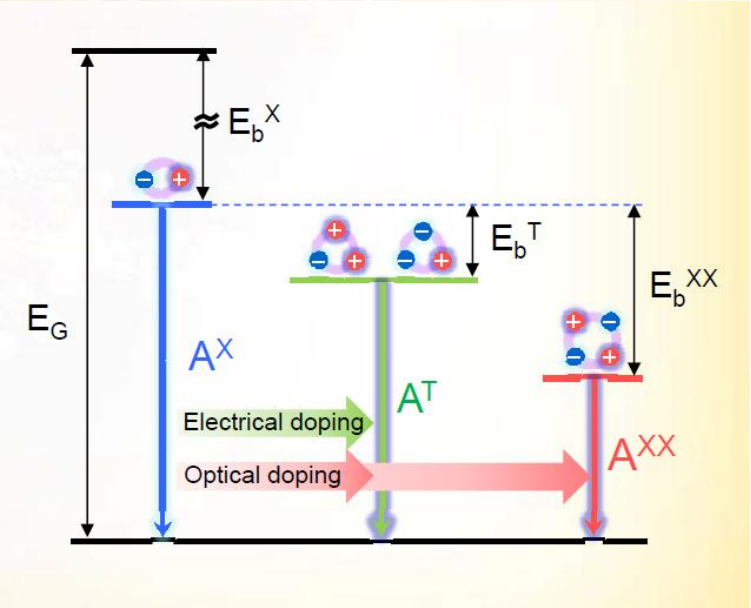
Coulomb interaction

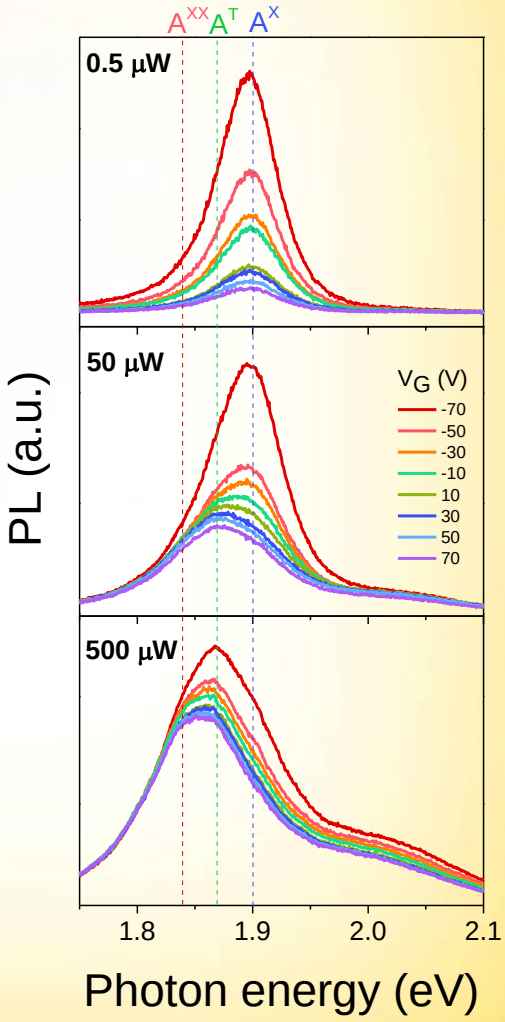


Excitons at room temperature

Large exciton binding energy

H. S. Lee et al. PRL, ASAP



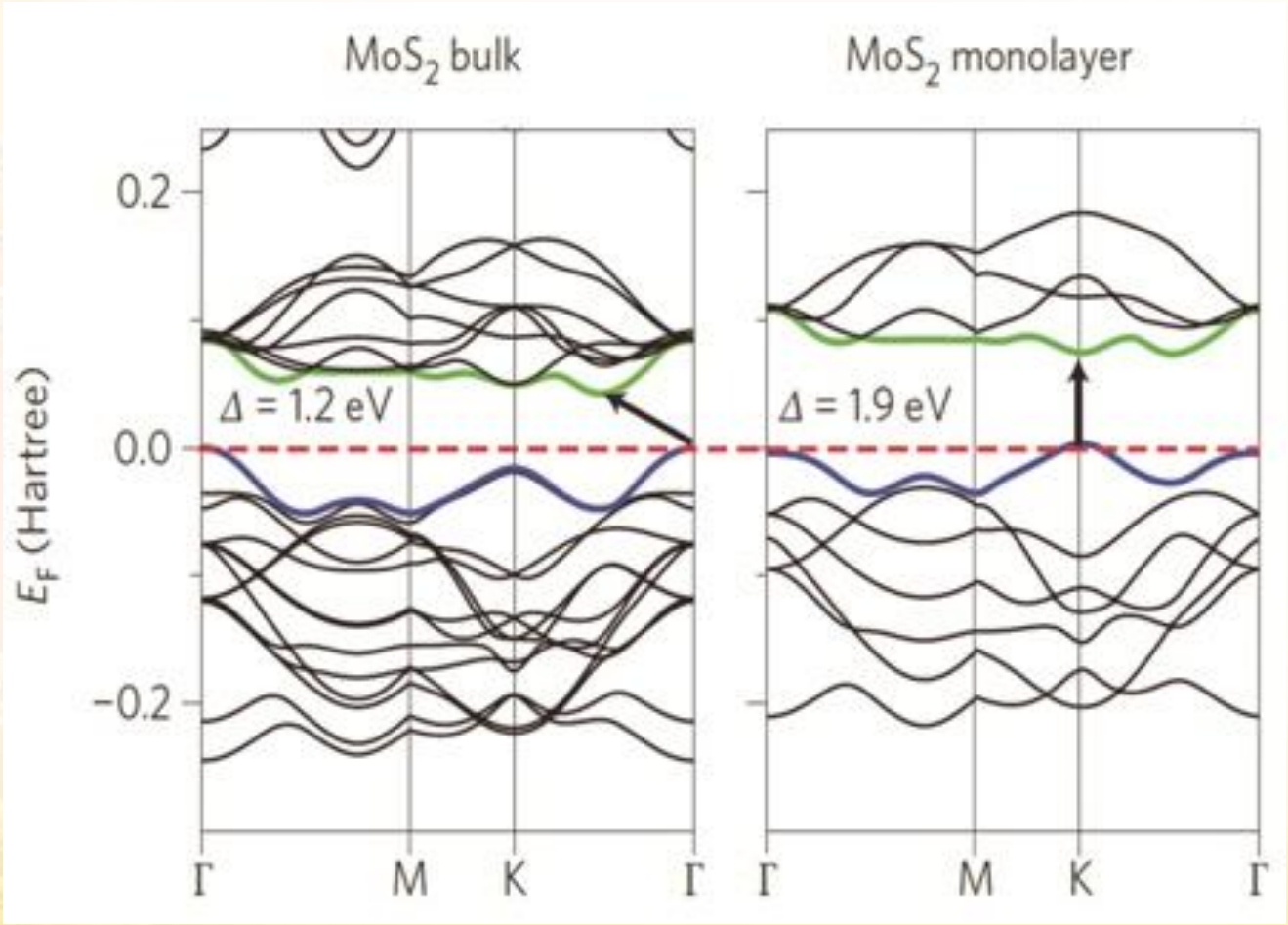


- Emergence of excitons at room temperature
  : $E_b^x \sim 1$ eV

- Emergence of multiexcitons at room temperature
  : trions, $E_b^{tri} \sim E_b^x + 30 \sim 40$ meV
  : biexcitons, $E_b^{bi} \sim E_b^{tri} + 30$ meV

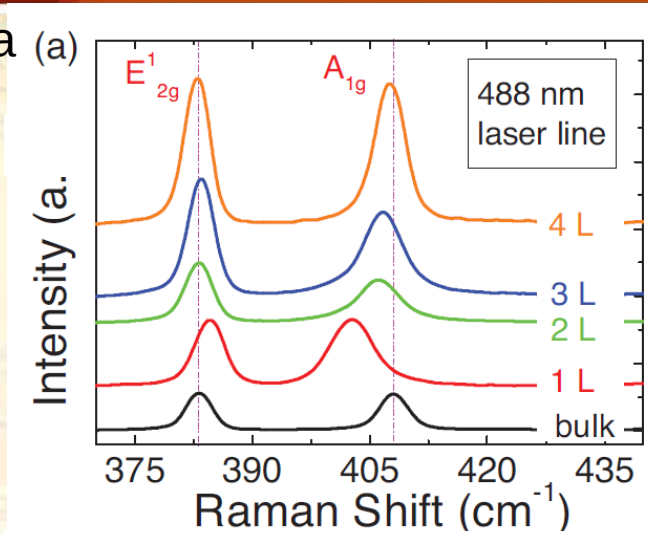
Layer dependence

Band structures: Indirect bandgap (ML) => direct bandgap (1L)

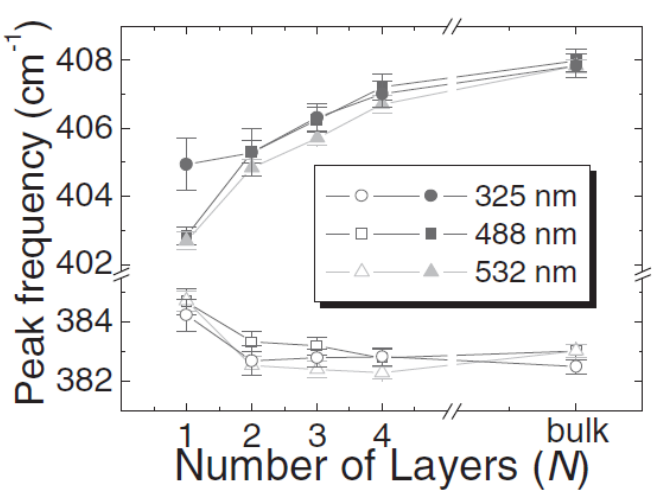


Optical properties

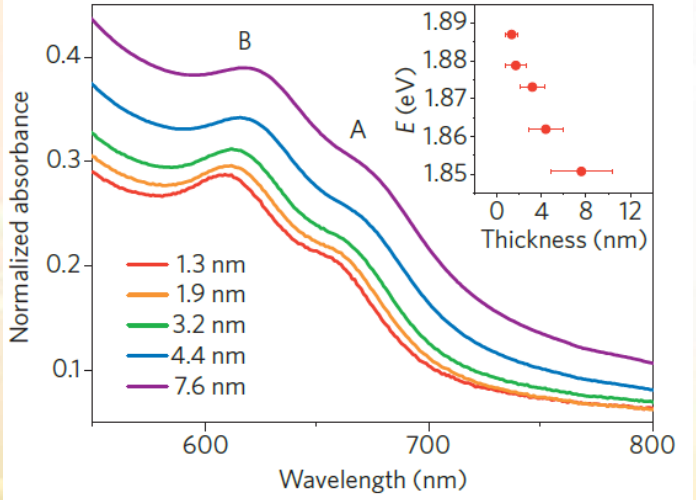
a



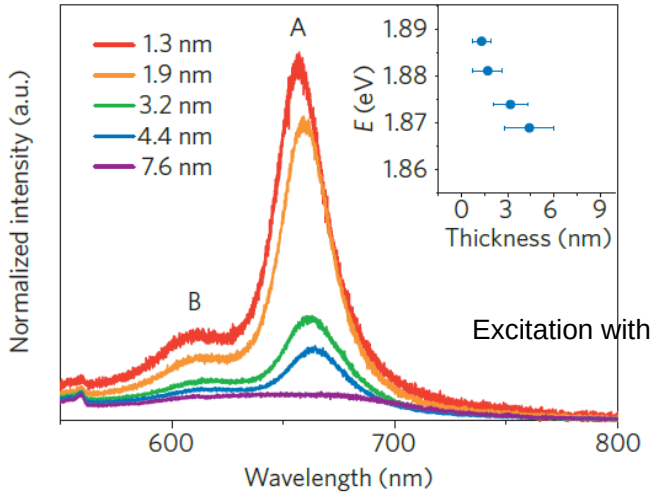
b



c



d



Excitation with 514 nm laser

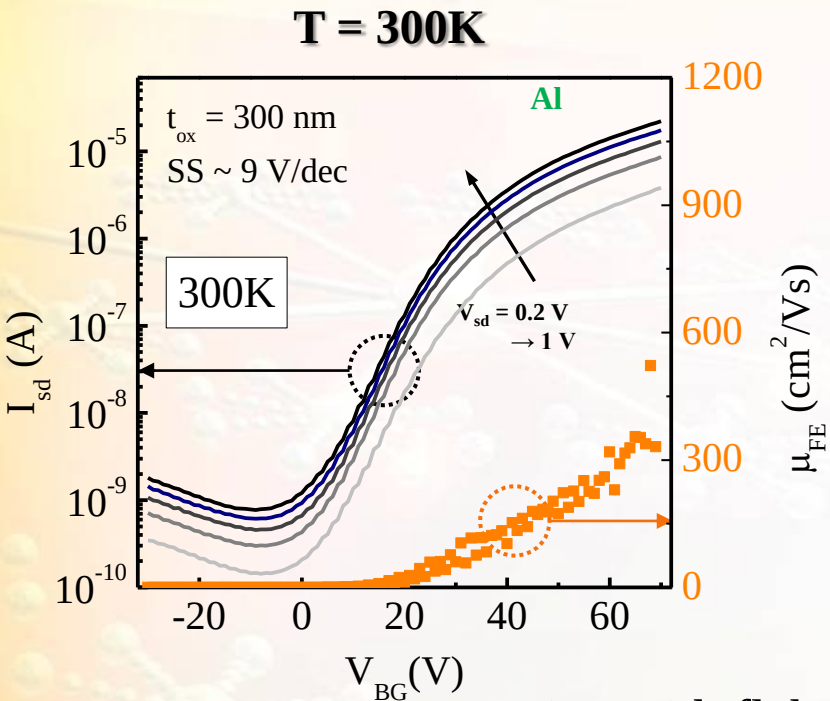
(a,b) Li, H. et al. Adv. Funct. Mater. **2012**, *22*, 1385–1390
(c,d) Eda, G. et al. Nano Lett. **2011**, *11*, 5111–5116

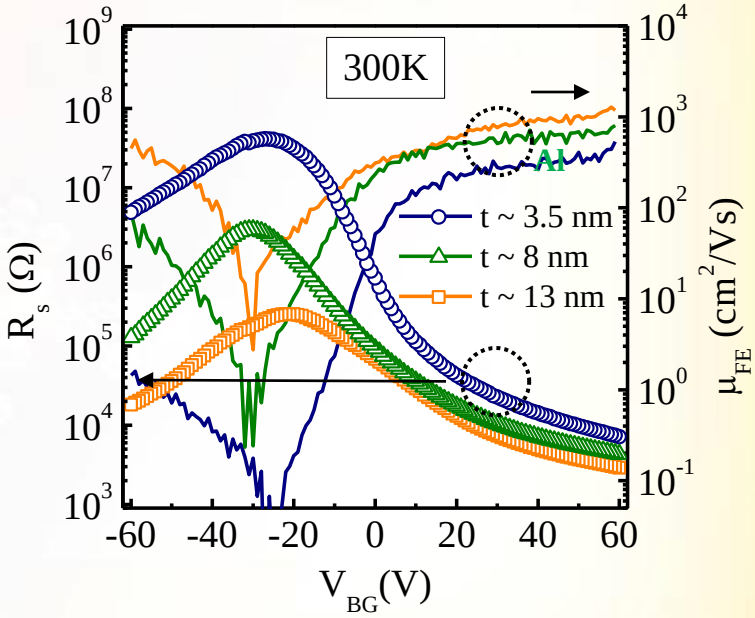
Layer dependence

Transport properties

Al contact for n-type Tr

D. Perrelo et al., Nature Comm. 6, 1-8 (2015)





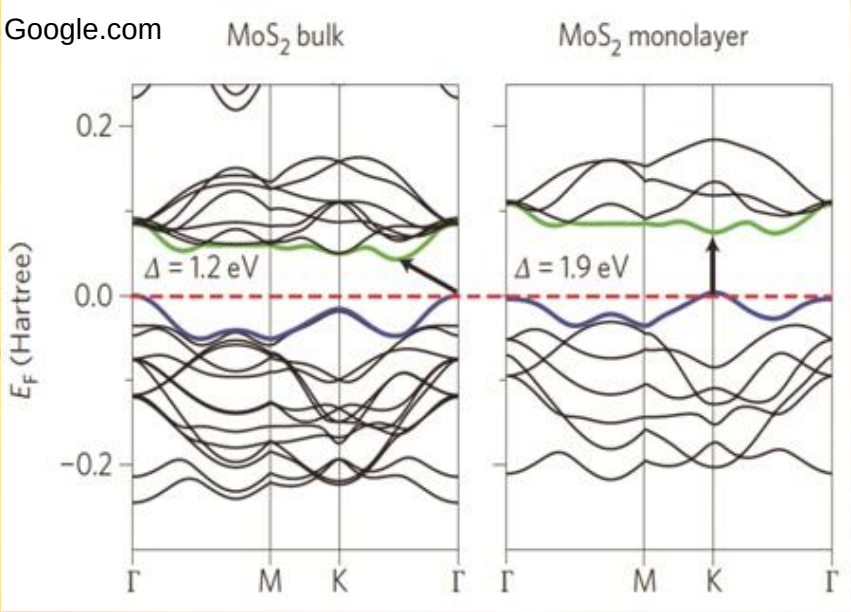
- Type conversion with flake thickness: n-type to ambipolar
  - Graphene-like electron and hole mobilities
- Mobility increases in proportion to film thickness
  - Bandgap shrinkage and surface scattering reduction

Layer dependence

Structural phase transition

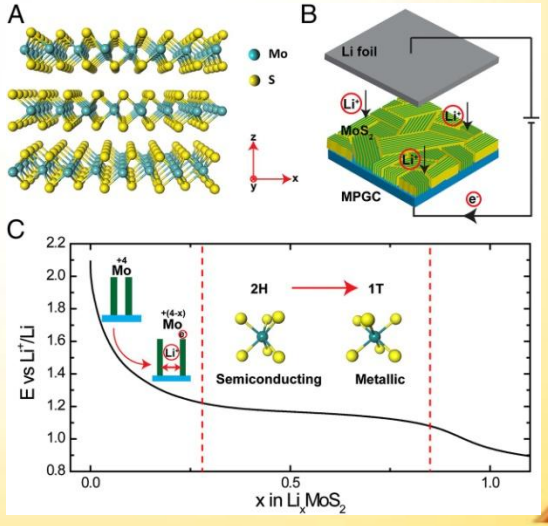
Why MoS_2?

Google.com

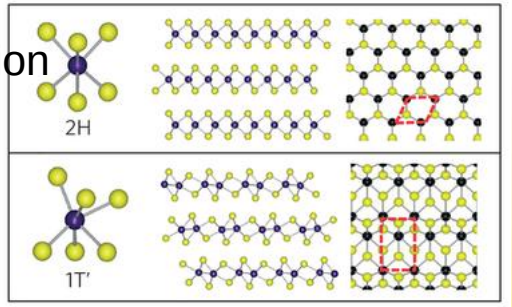


- Reduced charge screening
- High mobility ~200 $cm^2\ V^{-1}s^{-1}$ (MoS_2)
- Optical properties:
  Indirect bandgap (bulk) => direct bandgap (1L)
  Wide range of bandgap (1.0 ~ 2.5 eV)

H. Wang et al., PNAS 11, 19701 (2013)



- Various phases exist
- Tailoring such phases is a big challenge
- MoS_2 phase transition:
  2H (semicond) => 1T (metal)
  by Li intercalation
- Difficult to realize
- Severe lattice distortion
- Local phenomena



Why $MoTe_2$?

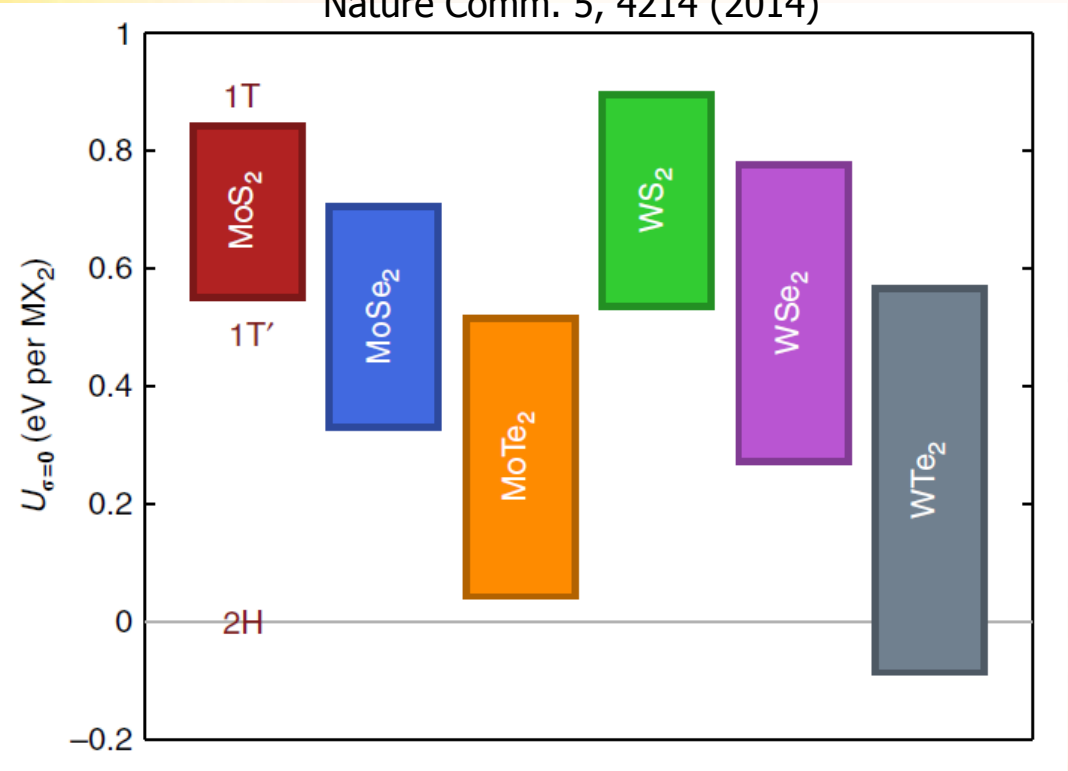
Similar to MoS_2 but…..

- Bandgap : ~ 1 eV, similar to Si
  - good for energy harvesting
  - good for TFET
- Cohesive energy difference between 2H and 1T is smaller than that of MoS_2
- Rich physics: CDW, superconductivity…

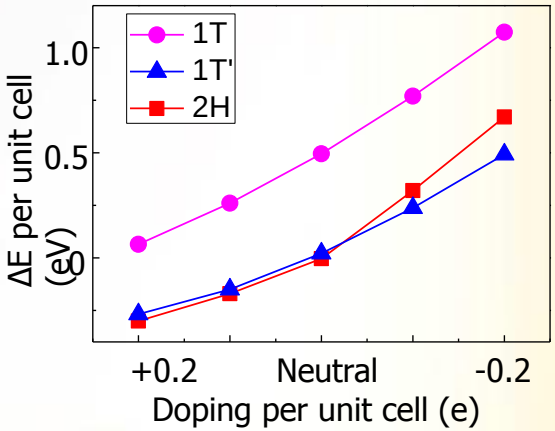
Polymorph engineering of $MoTe_2$

Phase stability

Nature Comm. 5, 4214 (2014)



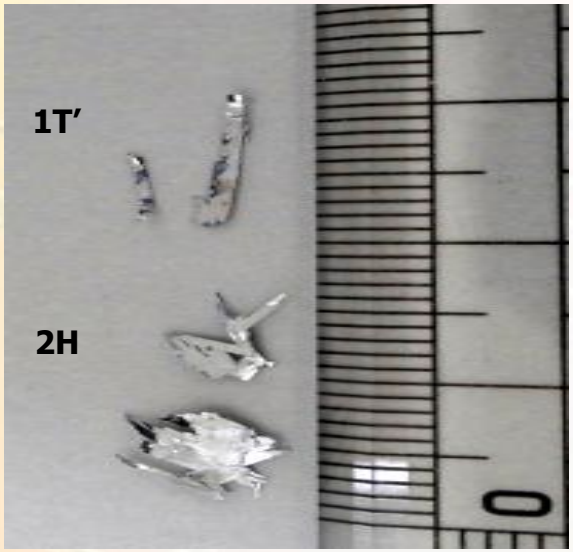
Cohesive energy of $MOTe_2$



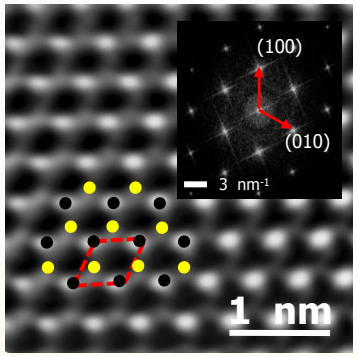
-> Polymorph engineering is easier in $MoTe_2$

Single crystal $MoTe_2$ by flux method

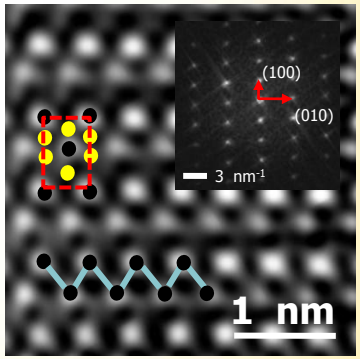
Single crystal growth (flux method): mix Mo and Te powder with sodium flux & sintering



TEM comparison



2H-$MoTe_2$



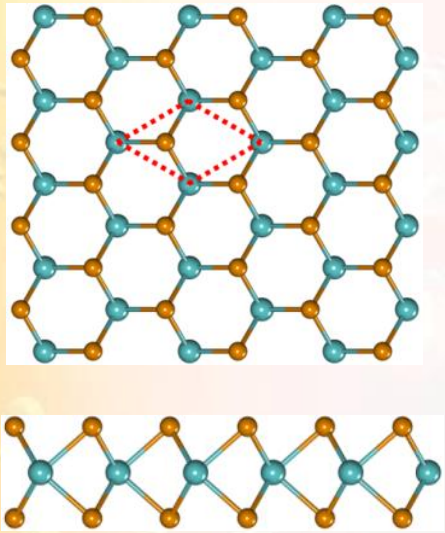
1T′-$MoTe_2$

Structures of $MoTe_2$

D. H. Keum & S. Y. Cho et al., Nature Phys. 11, 482 (2015)

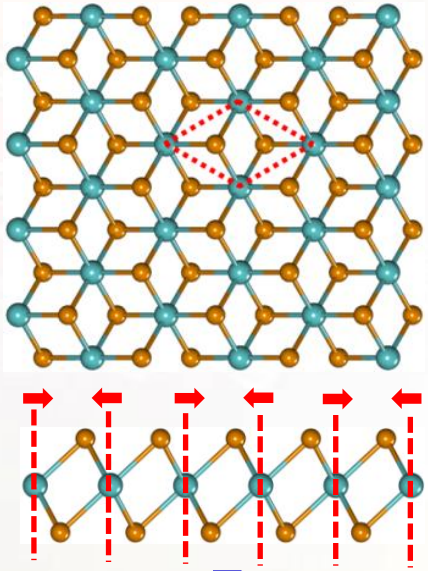
Semiconductor 2H

Hexagonal



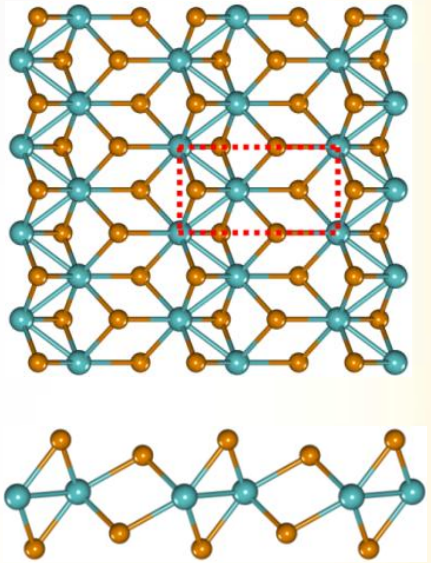
Metal 1T

Octahedral



Small bandgap metal 1T'

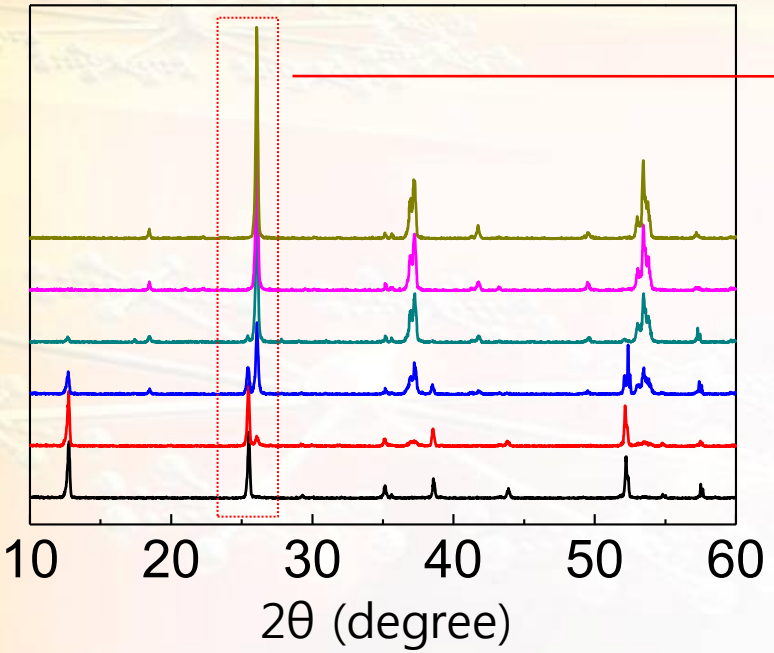
Distorted octahedral

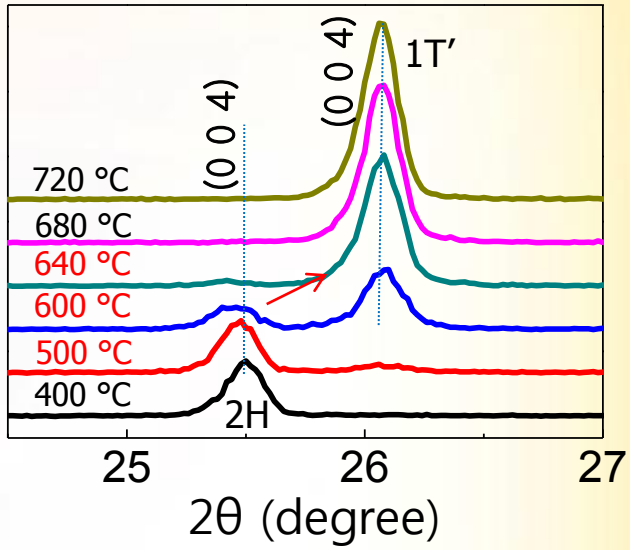


Peierls distortion
->Band inversion

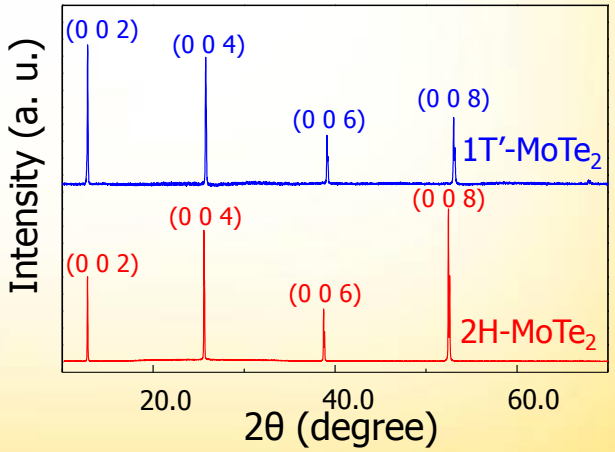
1T' phase is more stable than 1T phase!

Temperature-dependent XRD





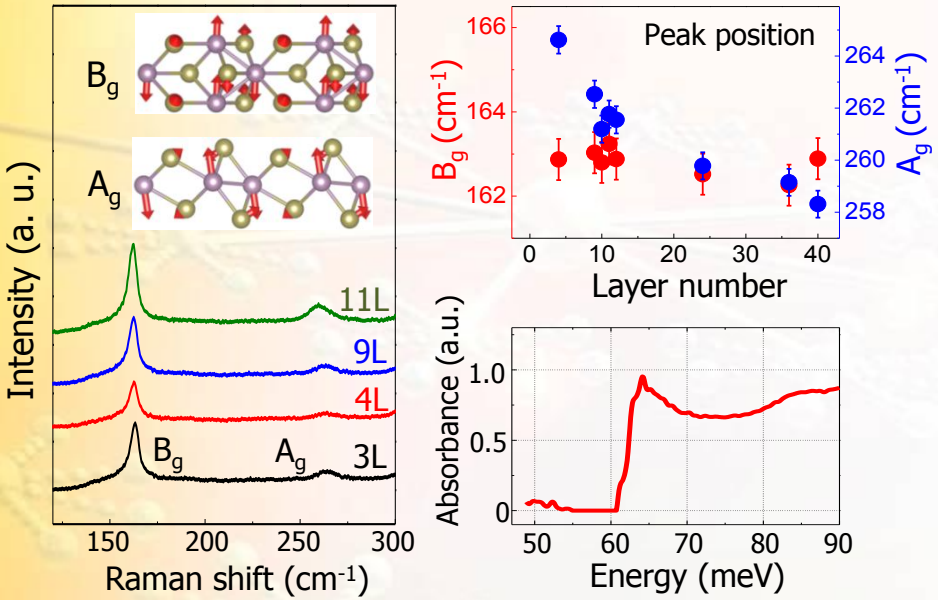
Structural phase transition by temperature
-> absence of Te deficiency
-> reversible phase transition



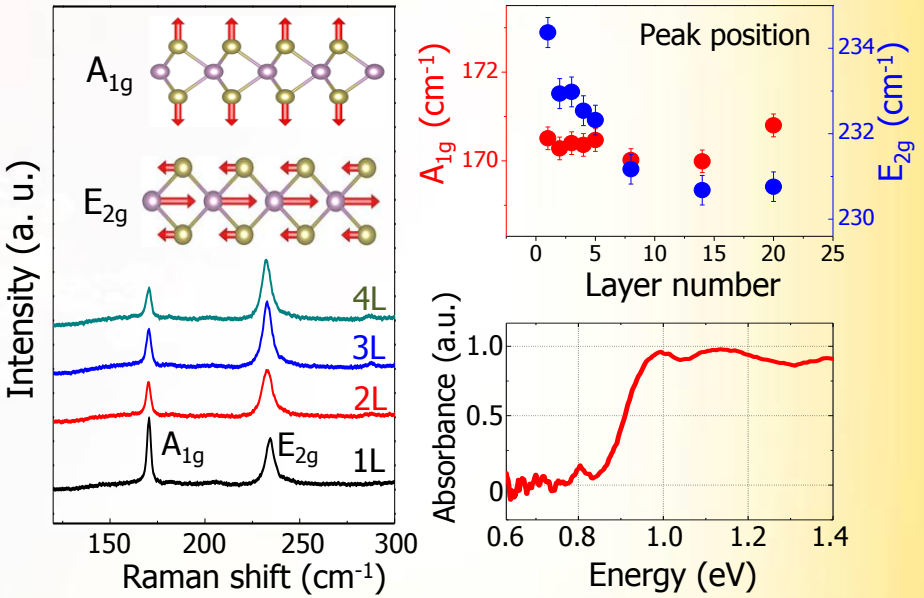
Raman & absorption spectroscopy

D. H. Keum & S. Y. Cho et al., Nature Phys. 11, 482 (2015)

1T′-$MoTe_2$



2H-$MoTe_2$



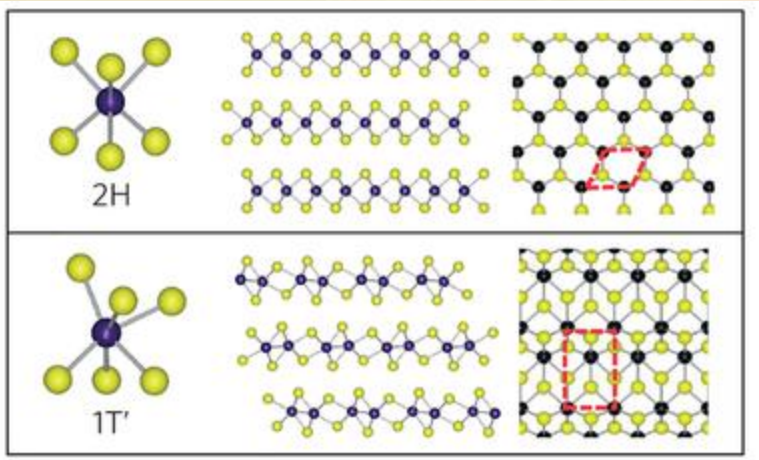
Few-layer $MoTe_2$

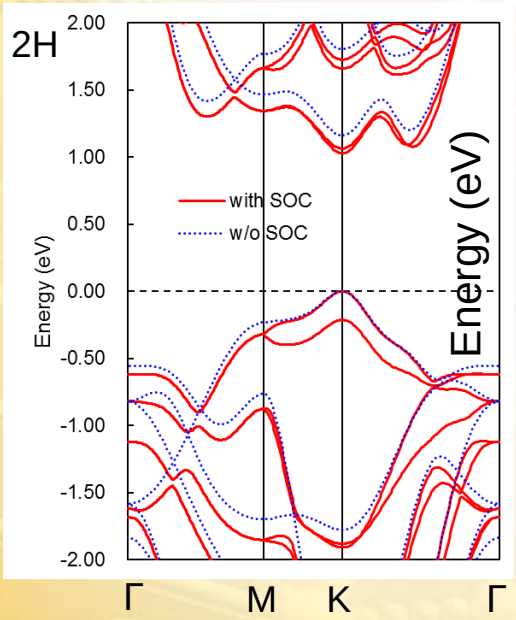
-> Sign of small bandgap in monoclinic TMDs

-> New results on Raman and absorption spectroscopy in 1T′-$MoTe_2$

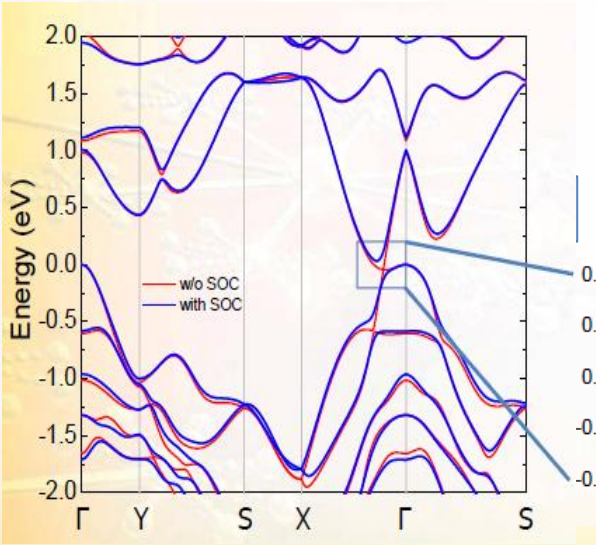
Large spin-orbit coupling

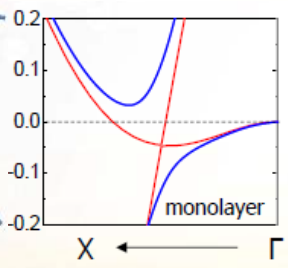
band splitting in VBM at K
- SOC effect

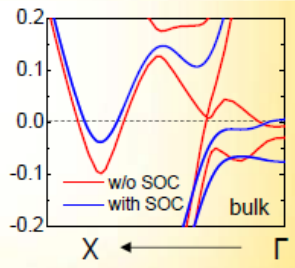




1T'

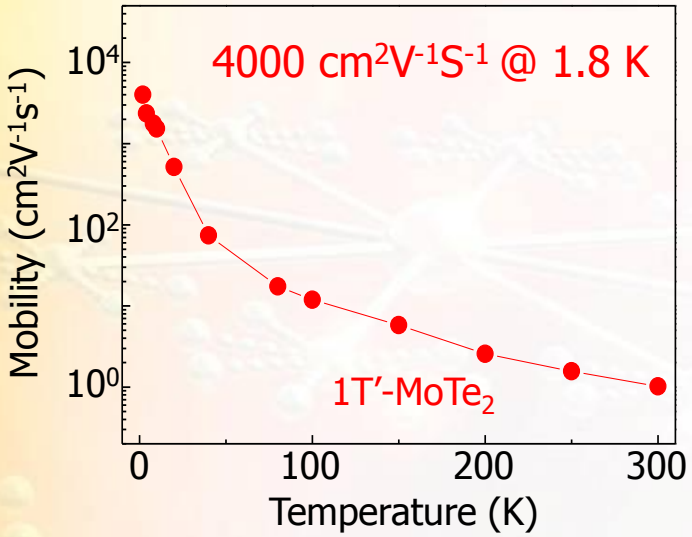




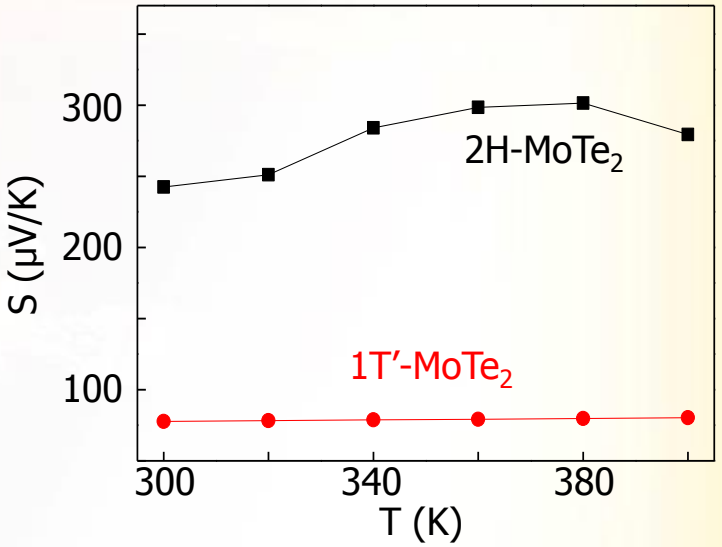


Electrical properties

Carrier mobility of 1T′-$MoTe_2$



Seebeck constants of $MoTe_2$



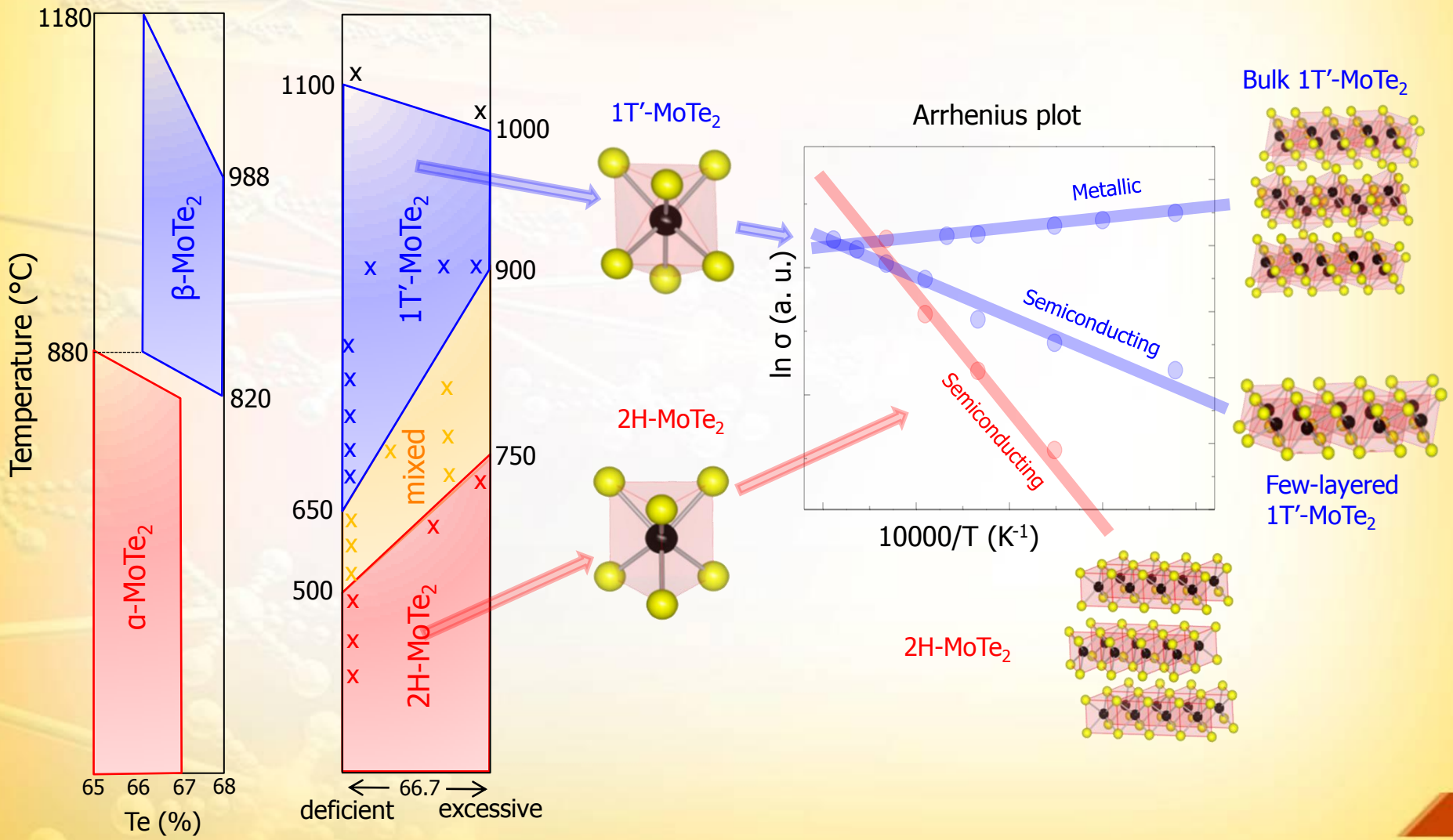
-> High carrier mobility at low temperature

-> High power factor : 0.04 ~ 11 mW/mK^2

(4 mW/mK^2 : state-of-the-art thermoelectric materials)

Electronic phase transition in $MoTe_2$

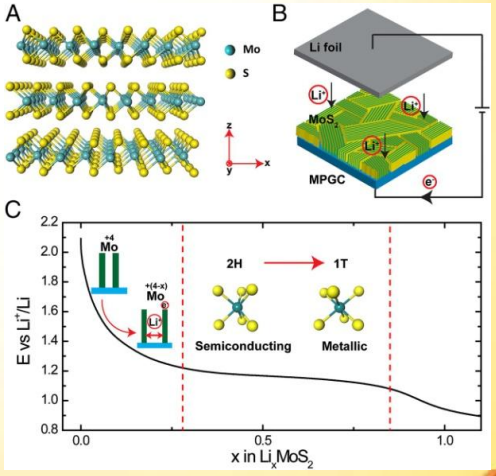
D. H. Keum & S. Y. Cho et al., Nature Phys. 11, 482 (2015)



Ohmic contact in 2D??

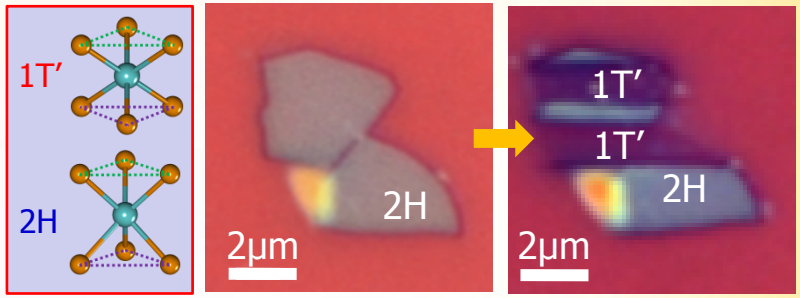
- Ohmic contact in Si: Ion implantation
- Ohmic contact in 2D?
  - ion implantation damages 2D layer
  - metal/2D: weak van der Waals interface
    => side contact to provoke covalent bonds?
  - phase transition from 2H to 1T
    by Li intercalation in MoS_2
  - phase transition by light irradiation
  - BN to modulate Schottky barrier??

H. Wang et al., PNAS 11, 19701 (2013)



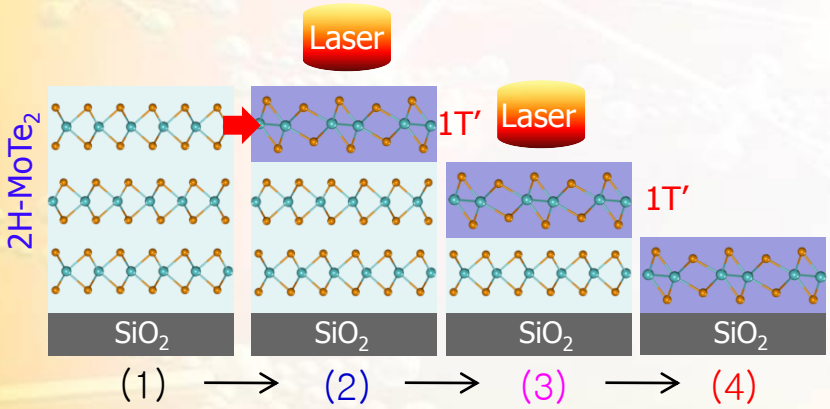
Light-induced phase transition in $MoTe_2$

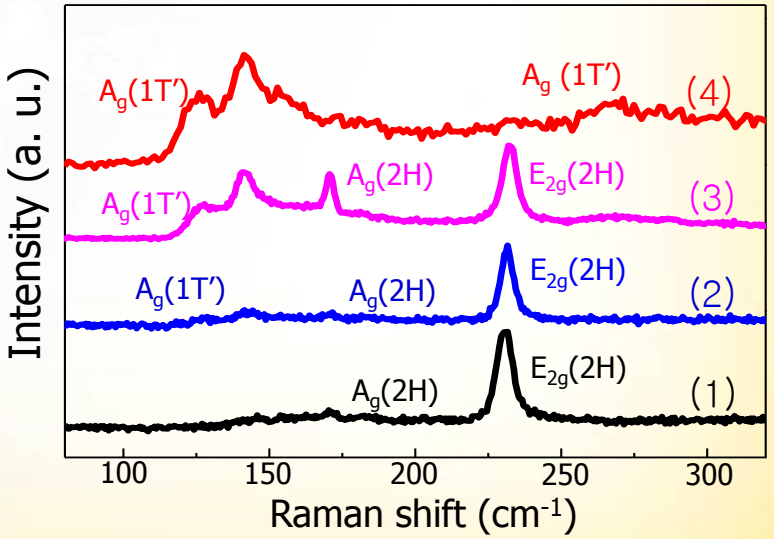
S. Cho et al., Science 349, 625 (2015)



Light illumination!!

Laser irradiation at a chosen local area
=> Phase control with 1 μm spatial resolution

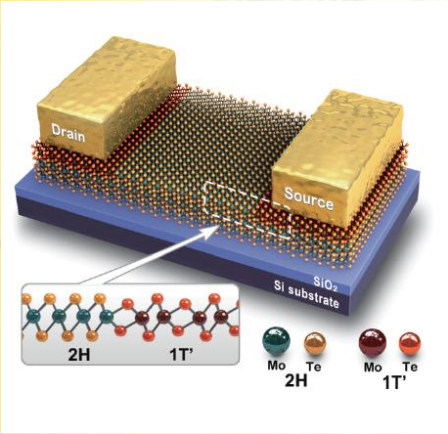


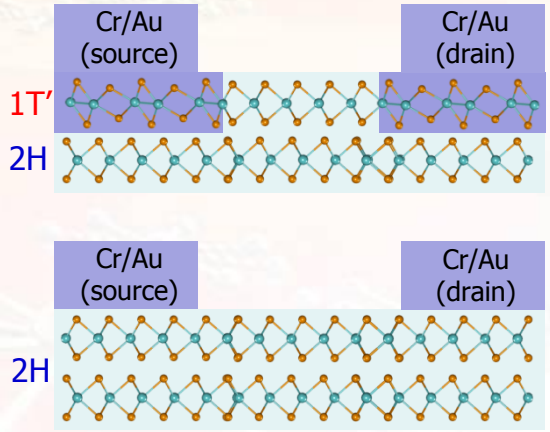


- Laser thinning
- Phase conversion to 1T'

Laser-patterned Ohmic junction in $MoTe_2$

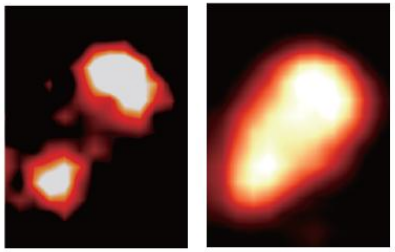
Laser patterning on transistor
(only at source/drain area)





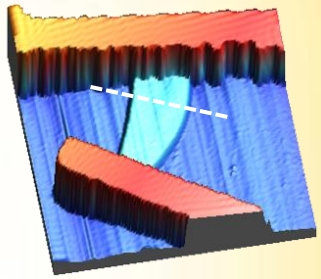
S. Cho et al., Science 349, 625 (2015)

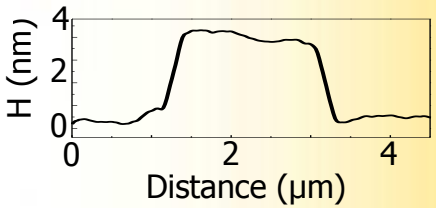
Local 1T' at S & D

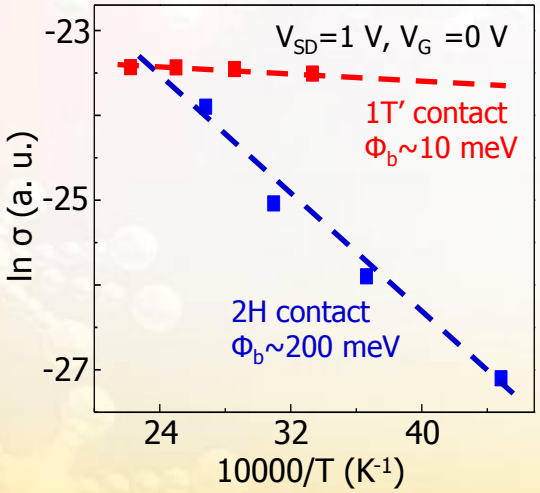


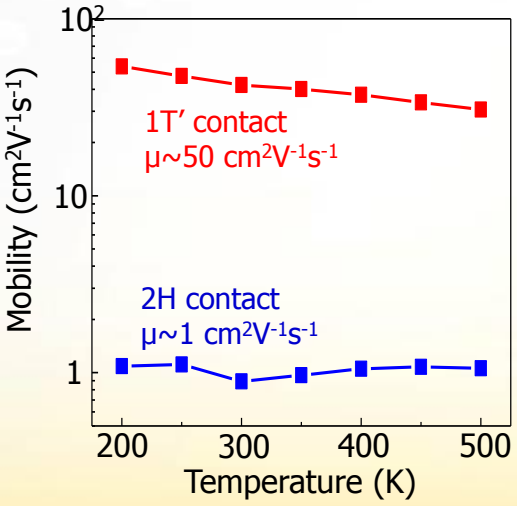
Raman of 1T' Raman of 2H

Laser thinning









-> New ohmic contact formed at the junction

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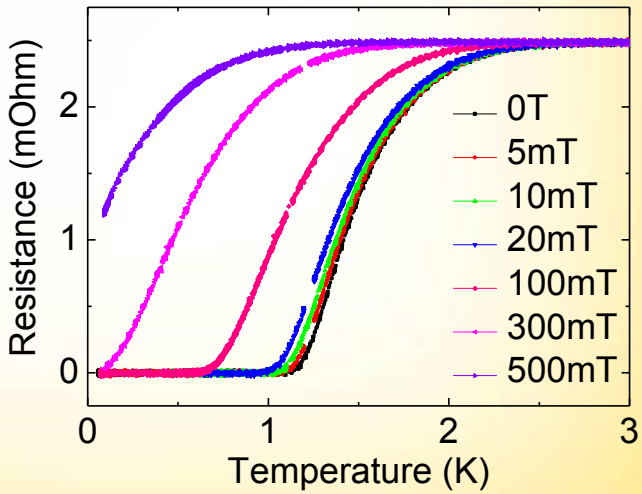
Summary & Future works

Key findings

- Reversible Structural Phase Transition
- Bandgap Opening in 1T'-$MoTe_2$ by 'Spin-Orbit Coupling'
- Local Phase Transition -> Ohmic contact in 2D
- Room-Temperature Phase Transition by Small Strain

Future projects

- Superconductivity in $MoTe_2$
- Bandgap ~ 1 eV
  => Photovoltaic, Optoelectronic devices
- Vertical tunneling device



Environmental susceptability

Physical and chemical properties can be easily modulated by environment

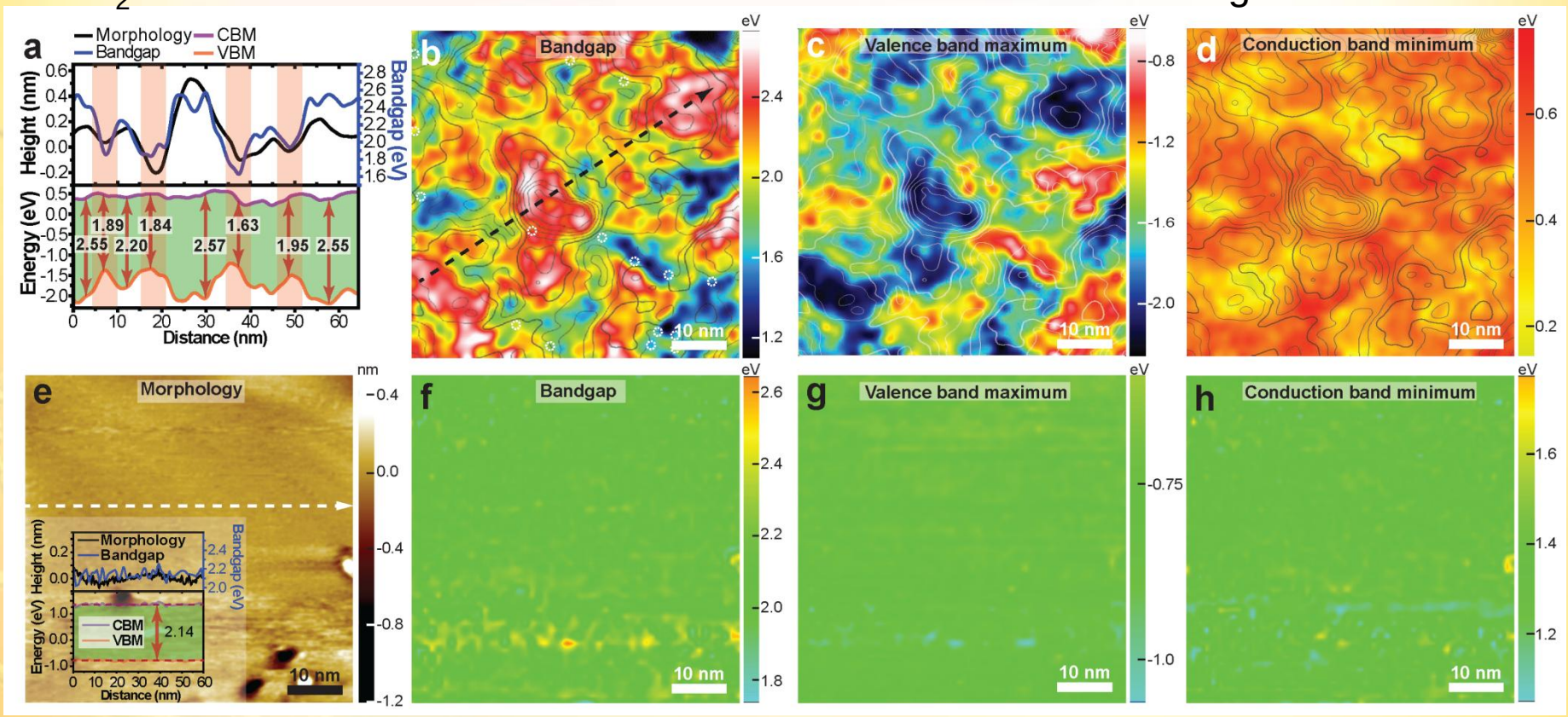
Strain effect

B. G. Shin et al., submitted!

Bandgap is strongly modulated with local strain in MoS_2 !

SiO_2

Roughness ~ 1 nm



HOPG

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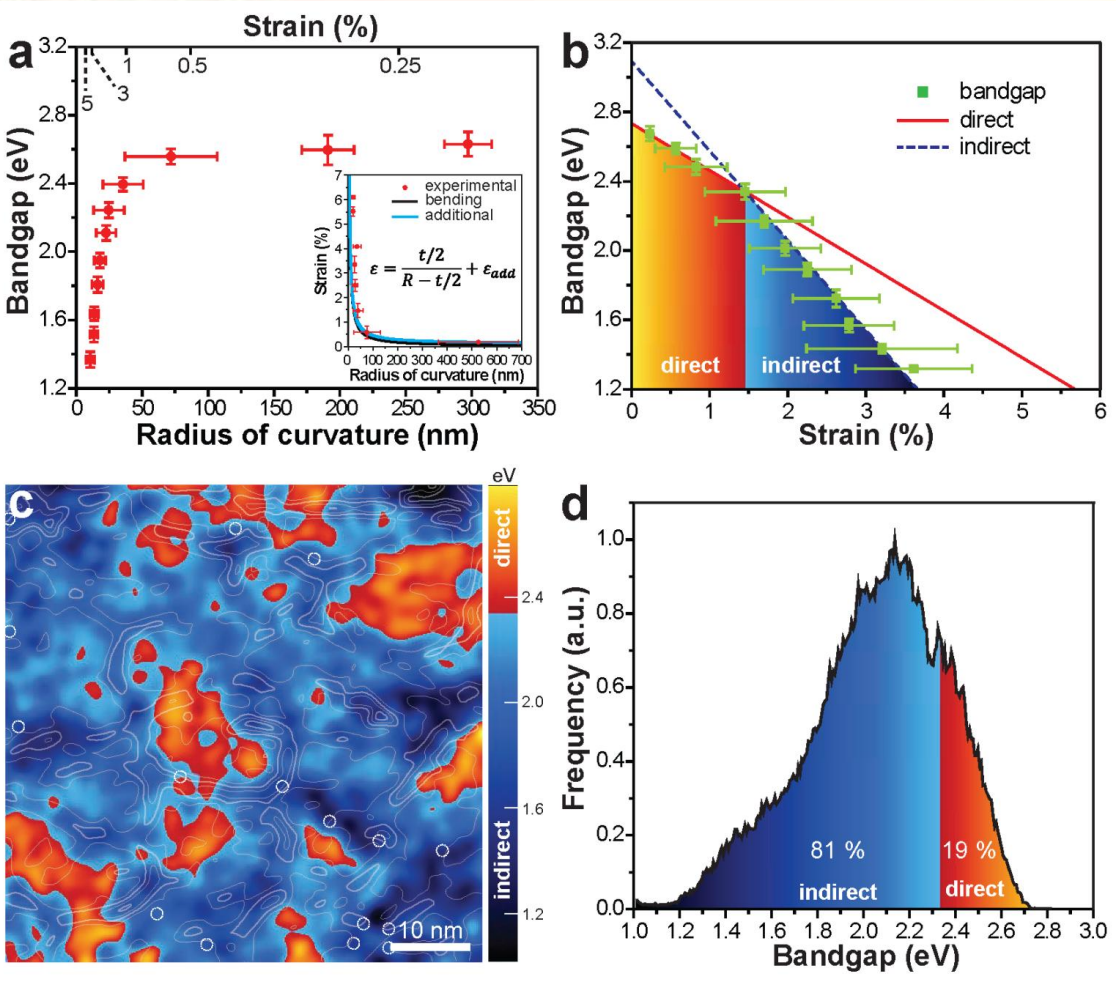
Cinap

B. G. Shin et al., submitted!

80% area is converted to indirect bandgap from direct bandgap!

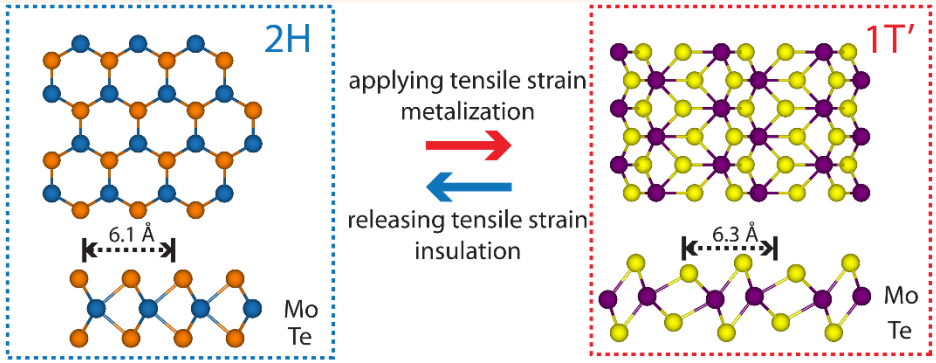


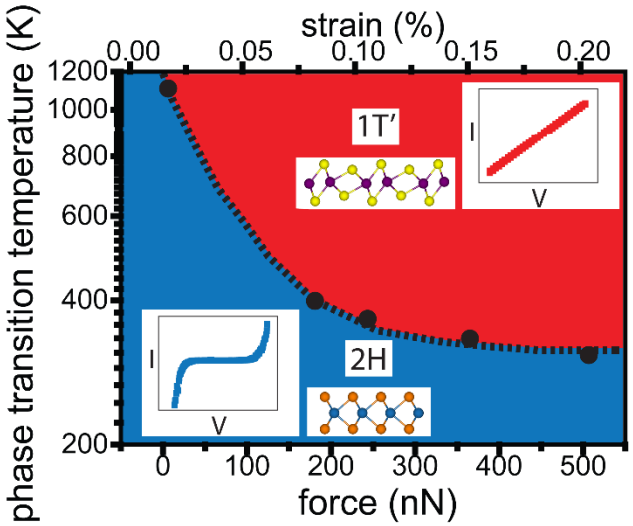
Room-temperature phase transition

High phase transition T to low phase transition T???

S. H. Song *et al.*, submitted

Tensile strain





Fully reversible upon release

1100 K at zero strain
=> 300 K at 0.2% tensile strain

First-order M-I transition at RT can be induced by small tensile strain (0.2%)

Dielectric constant modulation

Elias et al., Nature Physics 2011

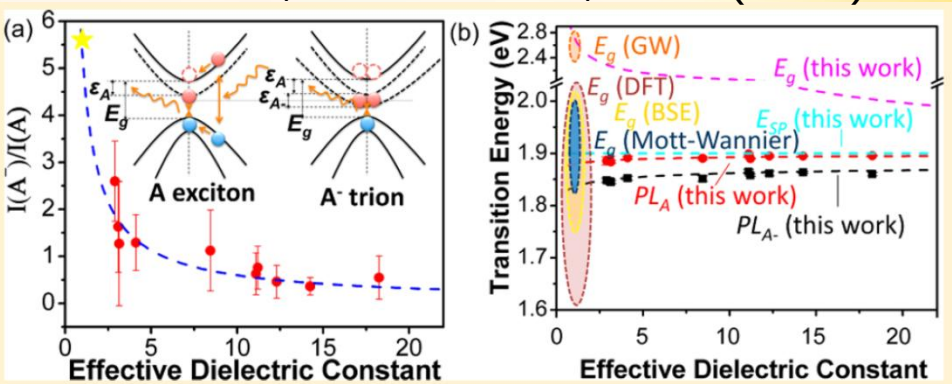
From the renormalization group theory:

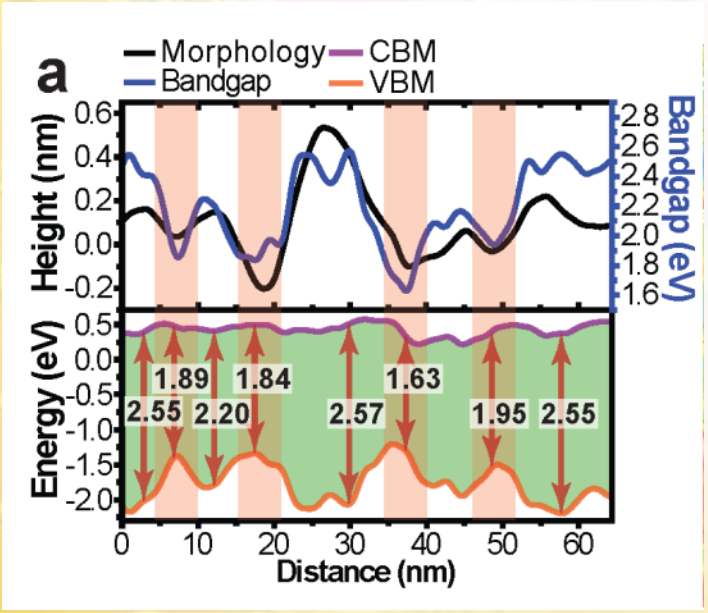
$$\frac{k}{v_F}\frac{\partial v_F}{\partial k} = -\frac{e^2}{4\varepsilon\hbar v_F}$$

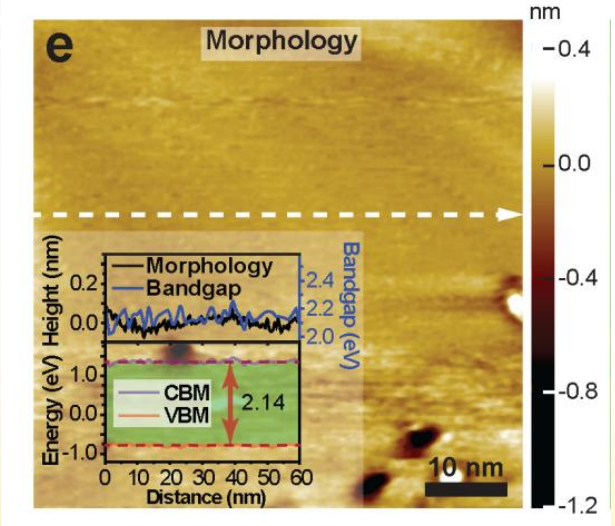
where $\varepsilon = (1+\varepsilon_s)/2$

$$\alpha = e^2/\varepsilon\hbar v_F$$

Lin et al., NanoLett. 14, 5569 (2014)





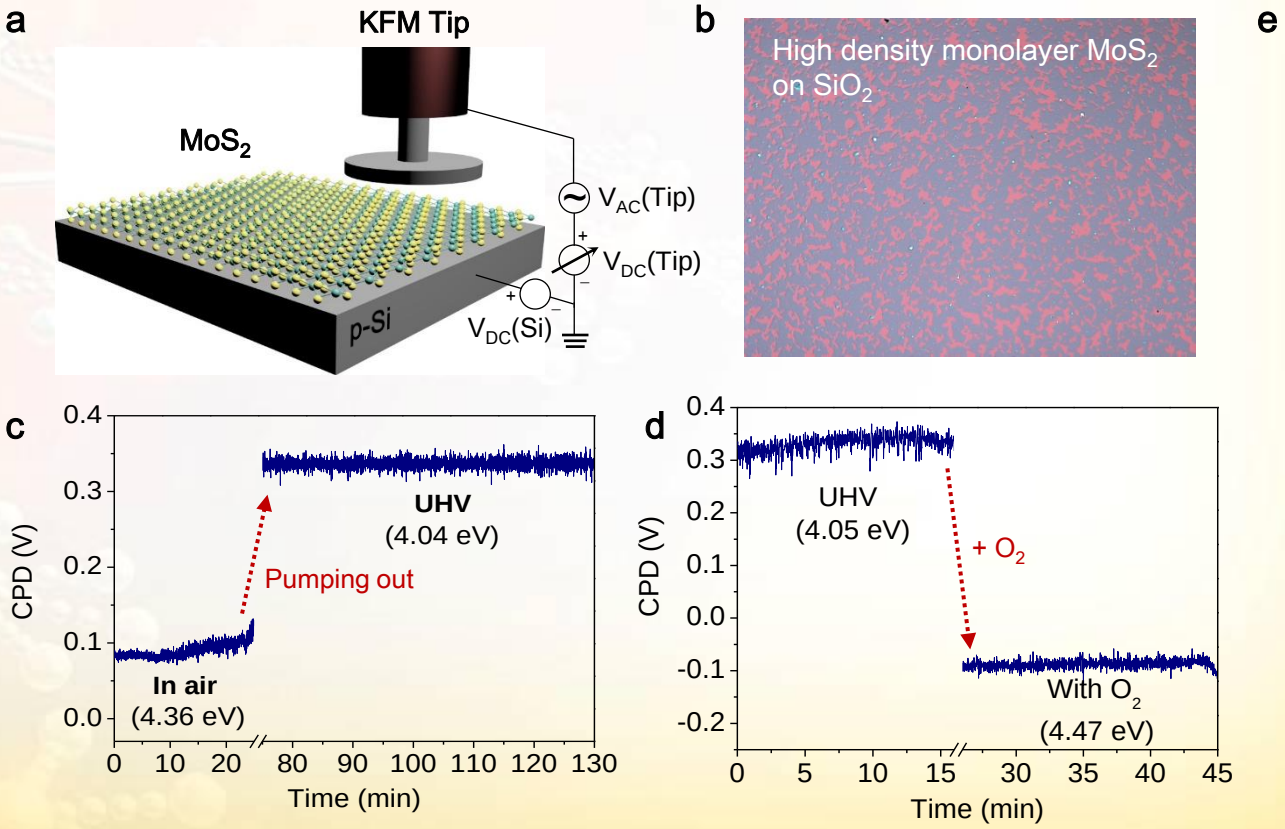


Work function modulation

S. Y. Lee et al., submitted

Work function of MoS_2 is modulated by O_2 adsorption/desorption!

: 0.4 eV, similar to graphene



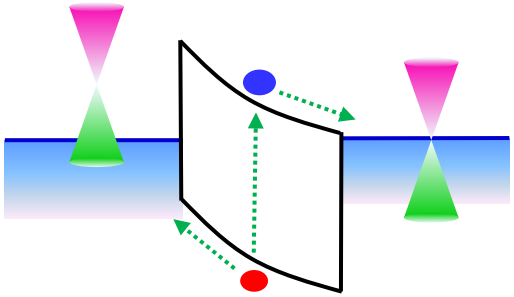
van der Waals stacking

Quantum mechanical phenomena

1L-MoS_2 vs 6L-MoS_2

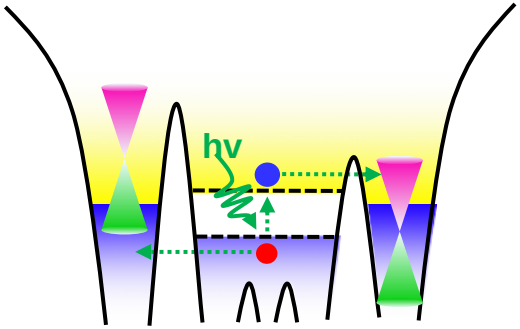
Multi-layer charge transport

Continuity equation $\frac{d}{dt}\delta n = D\frac{d^2}{dx^2}\delta n + \mu\xi\frac{d}{dx}\delta n - \frac{\delta n}{\tau} + g$

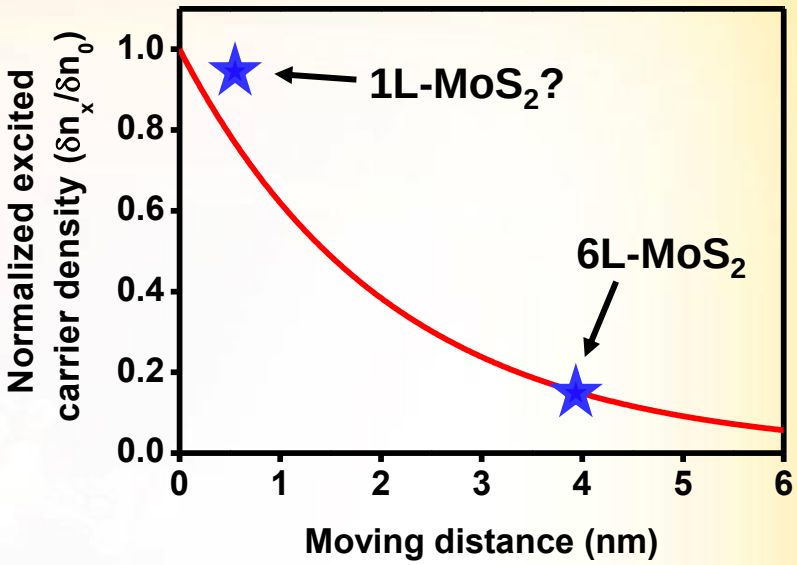


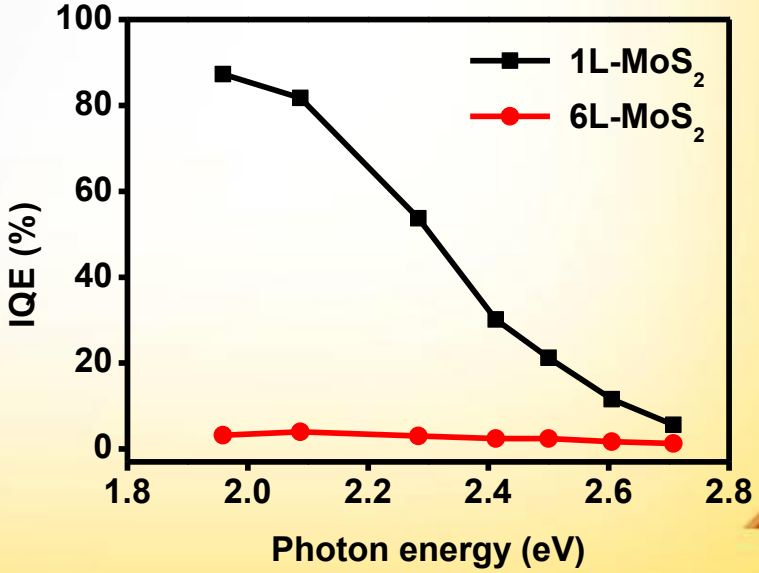
Monolayer charge transport

Tunneling probability $\overline{\Psi}\cdot\Psi = \overline{A}\cdot Ae^{-2\alpha x}$



W. J. Yu et al., submitted





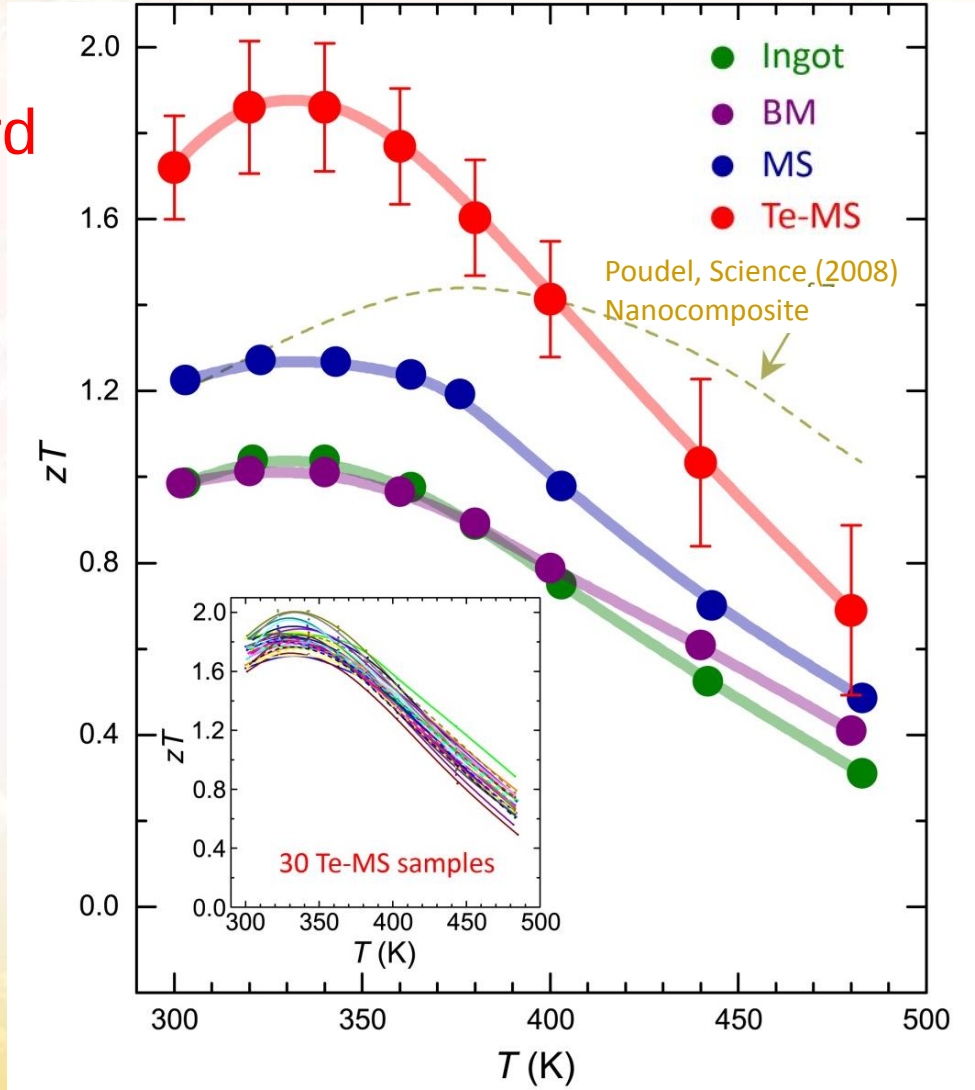
Thermoelectric Properties ($Bi_{0.5}Sb_{1.5}Te_3$)

Dimensionless Figure of Merit, *zT*

S. I. Kim et al., Science 348, 109-114 (2015)

World-best record for RT TE!

$$zT = S^2 \sigma / \kappa \; T$$

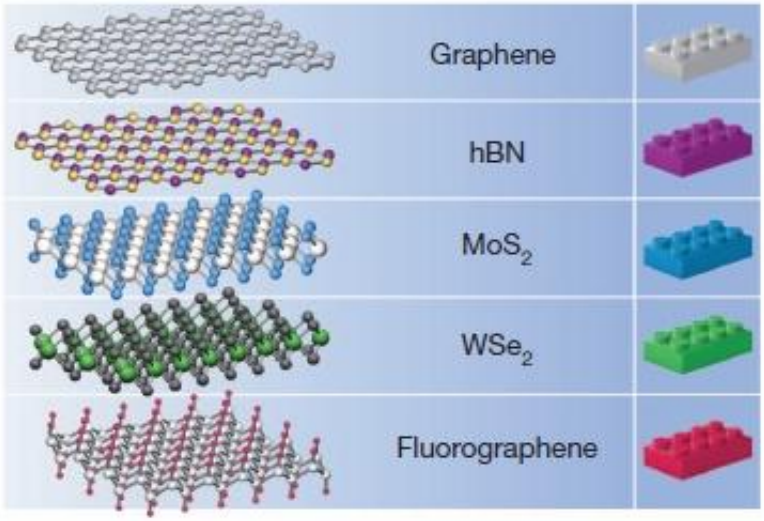


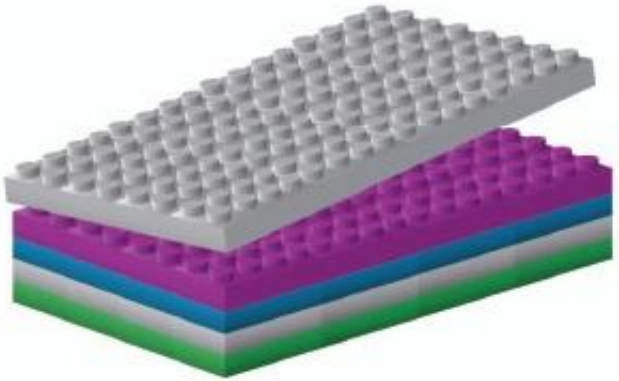
Synthesis of 2D materials

- Large-area, monolayer monocrystalline graphene
  (Adv. Mat. 27, 1376 (2015))
- Large-area, AB stacking bilayer graphene (unpublished)
- Large-area, monolayer MoS_2, seed growth by CVD
  (Nature Comm. (2015))
-Large-area monolayer WSe_2 on Au substrate by CVD
  (ACS Nano 9, 5510 (2015)
- Seed growth for MX_2 (M: Mo, W, X: S, Se) (unpublished)
- Thin $MoTe_2$ film from Mo metal
  (ACS Nano 9, 6548 (2015))
- Multilayer hBN is also available
  => on SiO_2/Si, unpublished
  => on Fe : Nature Comm., ASAP
- on Pt: Large area monolayer hBN, ACS NANO 8, 8520 (2014)
- on Au: mm-size monolayer singlecrystalline hBN, unpublished

Summary

van der Waals engineering!





There is a plenty of room for new phenomena in 2D materials!