Strain Engineering Valleytronics for State Coherence

Exploring novel quantum degrees of freedom for next-generation computation!

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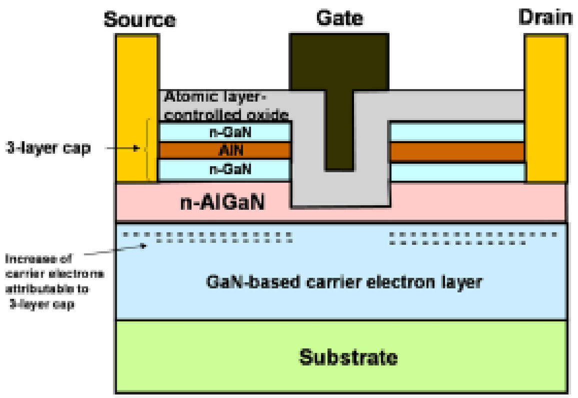
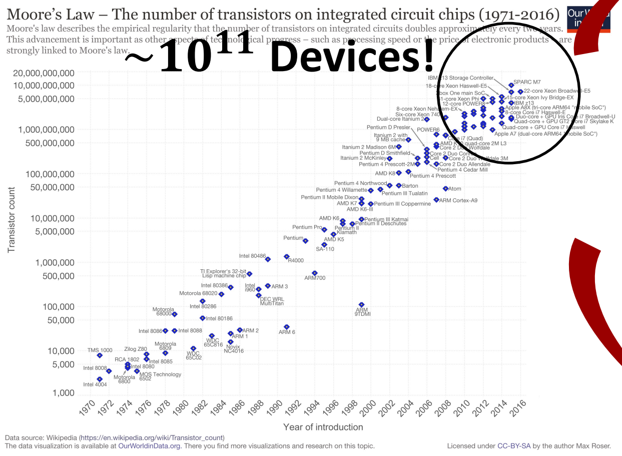
Coming to the End of Moore's Law?

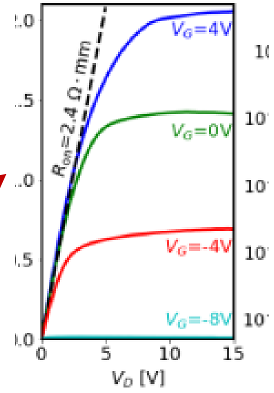
- -IC transistor density scales linear with time
- -Power loss scaling quadratic
- -Major effort to reduced subthreshold voltage swing ➔ 60 mV/Dec





$\sim 10^{11}$ Devices!

Low V_s



Heat Loss

III-V CMOS Design Concepts Dominant (HEMT) [Cornell Group Proposal]

Let's forget voltage? Think light. Think valleys.

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Valleytronics: Moving Electrons with Light for Computation

Time-reversal symmetry → Valley index corresponding to K/K' points in momentum space couple to right and left polarized light → NO GATE VOLTAGE = NO HEATING

Control of valley polarization in monolayer MoS_2 by optical helicity

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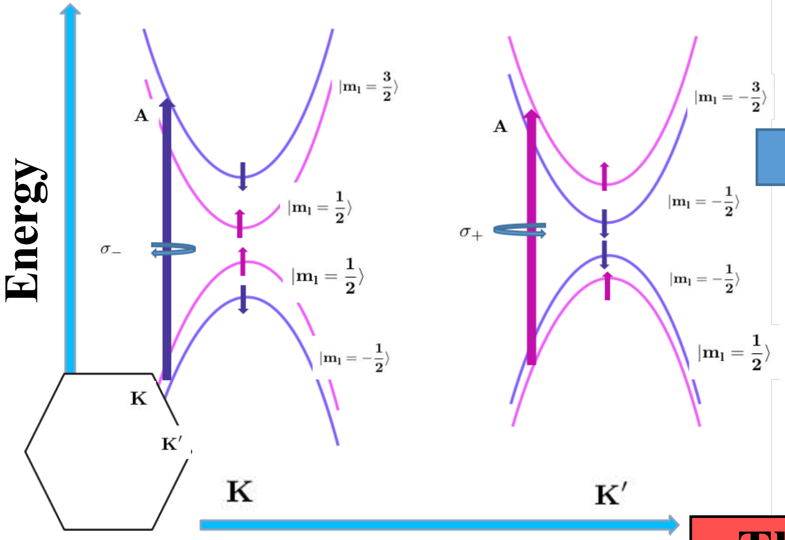

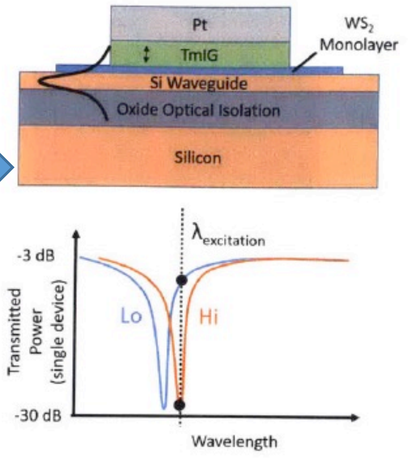

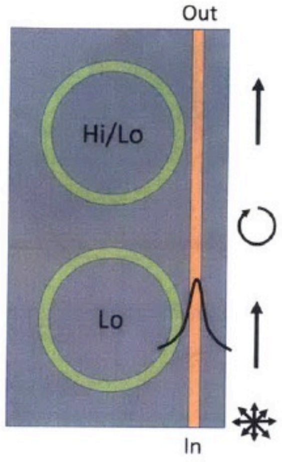

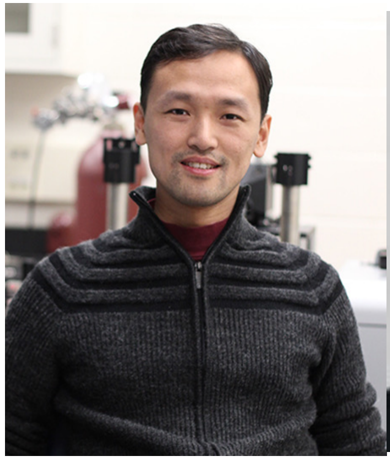

Kin Fai Mak (Cornell)

Tony Heinz (Columbia)

The grand physical challenge: Maintain state coherence to be robust to lattice vibrations. So heat doesn't matter?

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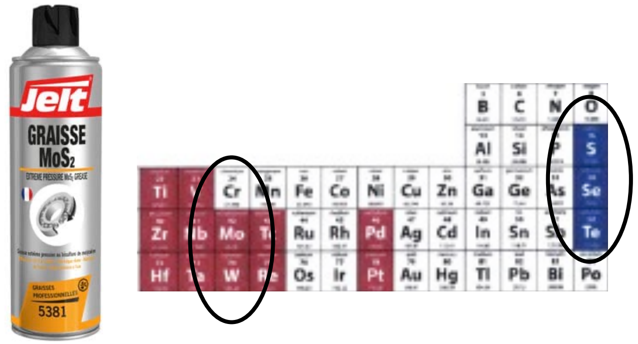
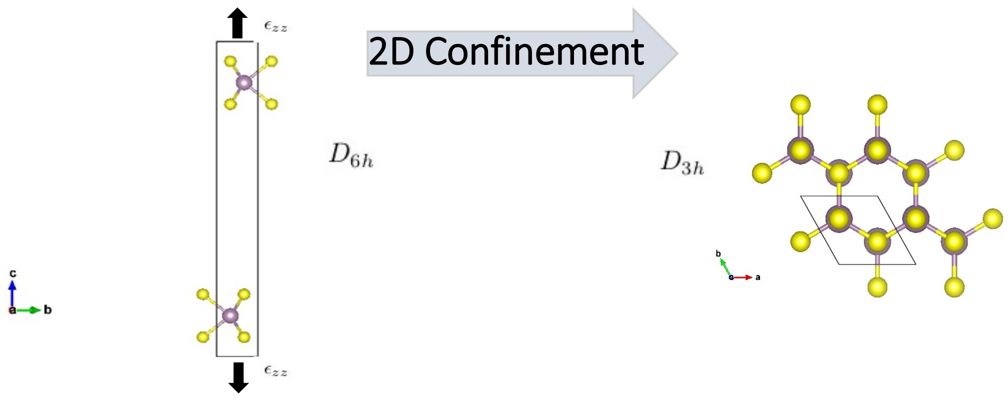
A Brief Introduction to 2D Transition Metal Dichacolgenides



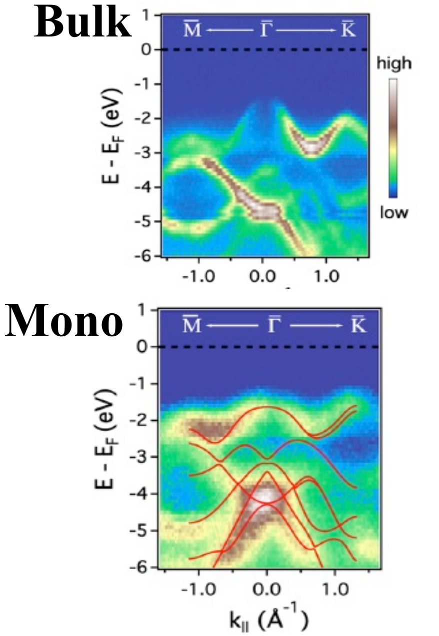
TMDs
Mo/W + S/Se
-Earth abundant
-Used in lubricants

2D Confinement of MoS_2 with Uniaxial Strain



Break Inversion Symmetry

Direct Band Gap Transition



ARPES MoS_2
[Cornell]

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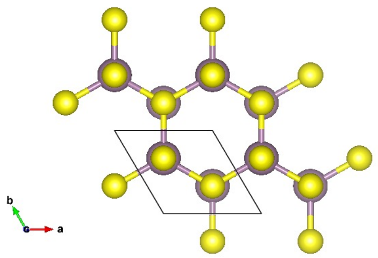
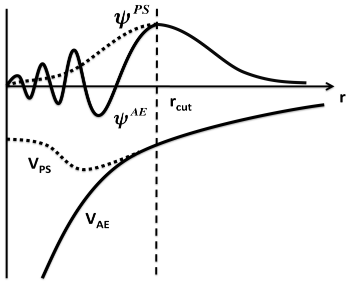
Engineering Electronic Materials with Quantum Mechanics

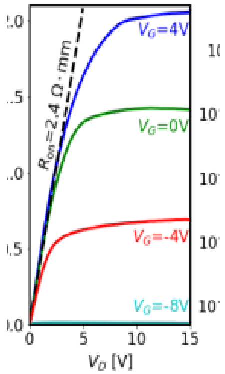




Hypothesize/tune structure and pseudo-interactions

$$(H_{KS}(\mathbf{k}) - \epsilon_n(\mathbf{k}))|\phi^{KS}_{n,\mathbf{k}}\rangle = 0$$

Solve SE for material in super computer ➔ use DFT ➔ obtain wavefucntions



$$\frac{1}{\tau_{n\mathbf{k}}} = \frac{2\pi}{\hbar}\sum_{m\nu}\int\frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}}|g_{nm\nu}(\mathbf{k},\mathbf{q})|^2$$
$$\times\left[(1 - f_{m\mathbf{k}+\mathbf{q}} + n_{\mathbf{q}\nu})\delta(\varepsilon_{n\mathbf{k}} - \hbar\omega_{\mathbf{q}\nu} - \varepsilon_{m\mathbf{k}+\mathbf{q}})\right.$$
$$\left.+ (f_{m\mathbf{k}+\mathbf{q}} + n_{\mathbf{q}\nu})\delta(\varepsilon_{n\mathbf{k}} + \hbar\omega_{\mathbf{q}\nu} - \varepsilon_{m\mathbf{k}+\mathbf{q}})\right].$$

Predict electronic properties ➔ device behavior, carrier lifetimes

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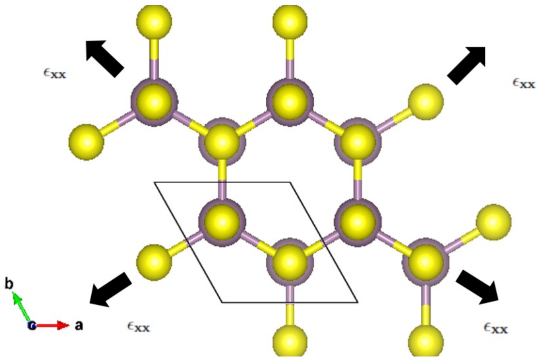
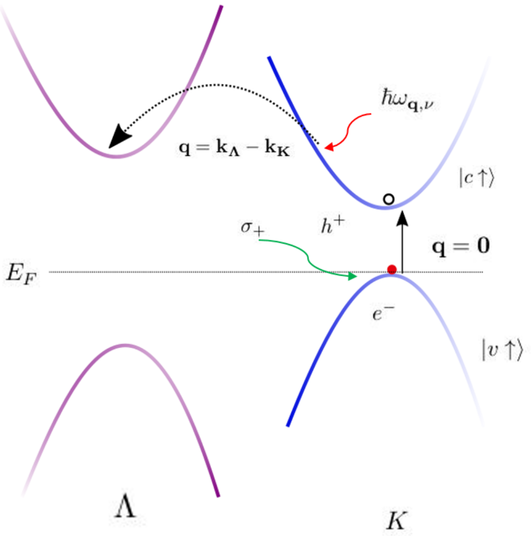
Engineering Coherence by Stretching Atomic Layers

Proposal= Apply biaxial strain to 2D TMD material

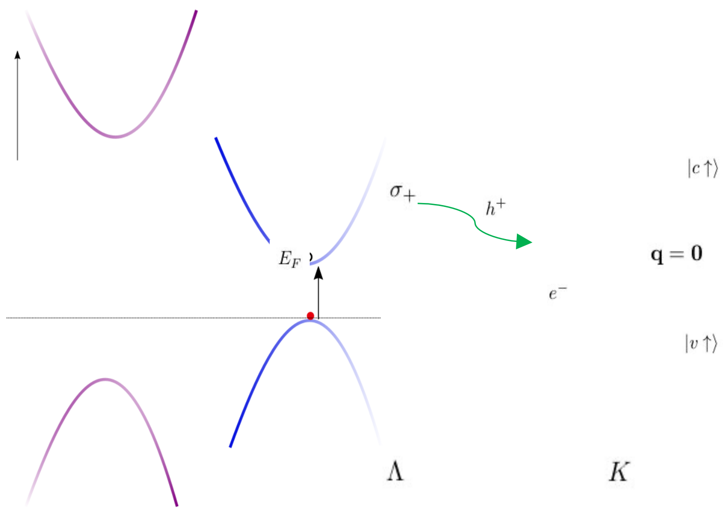
-Spatially separate K-Λ valleys == > fewer intervalley scattering events ➔ thermal vibrations don't interfere coherence ➔ longer exciton lifetime

-Energetically separate K-Λ valleys ➔ only desire direct transitions for valley logic coherence





$$\epsilon_{xx} = 0$$



$$1.0\% < \epsilon_{\mathbf{xx}} < 2.0\%$$

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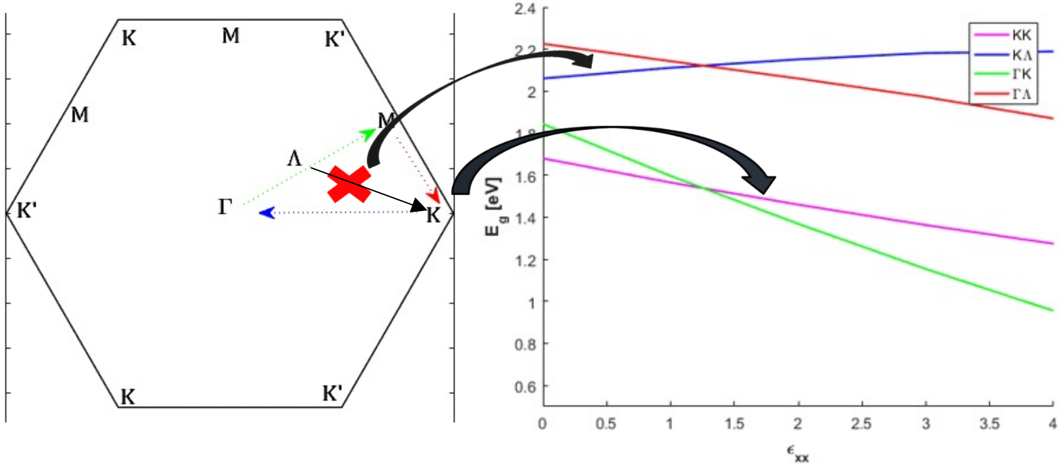
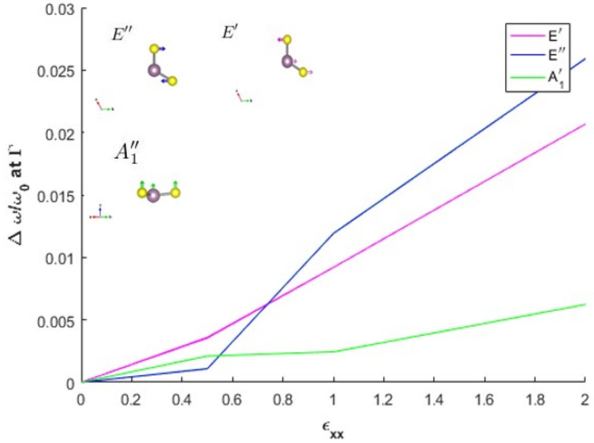
Theoretical Results of Strain Engineering Valleytronics

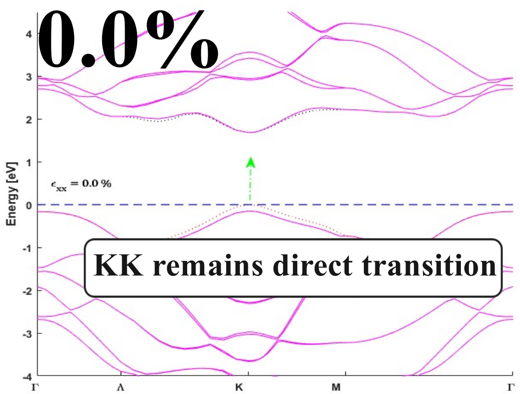
Energetics ➔ energetic contribution to coherence improves with strain

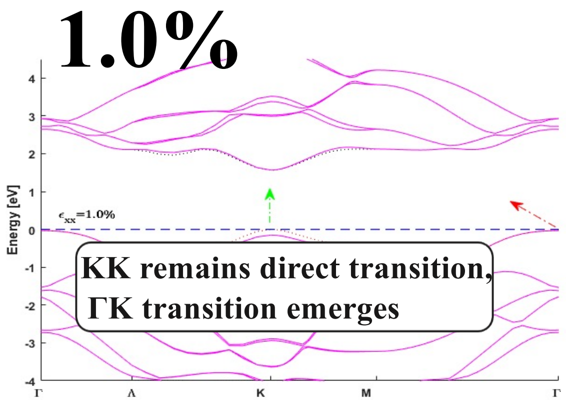


K-space transition ➔ energetic contribution to coherence improves with strain



Upper bound on strain = 1.0 % ➔ stay between 0-1.0%





Take away ➔ we can now engineer valley coherence of deviceswith application of biaxial strain on 2D materials

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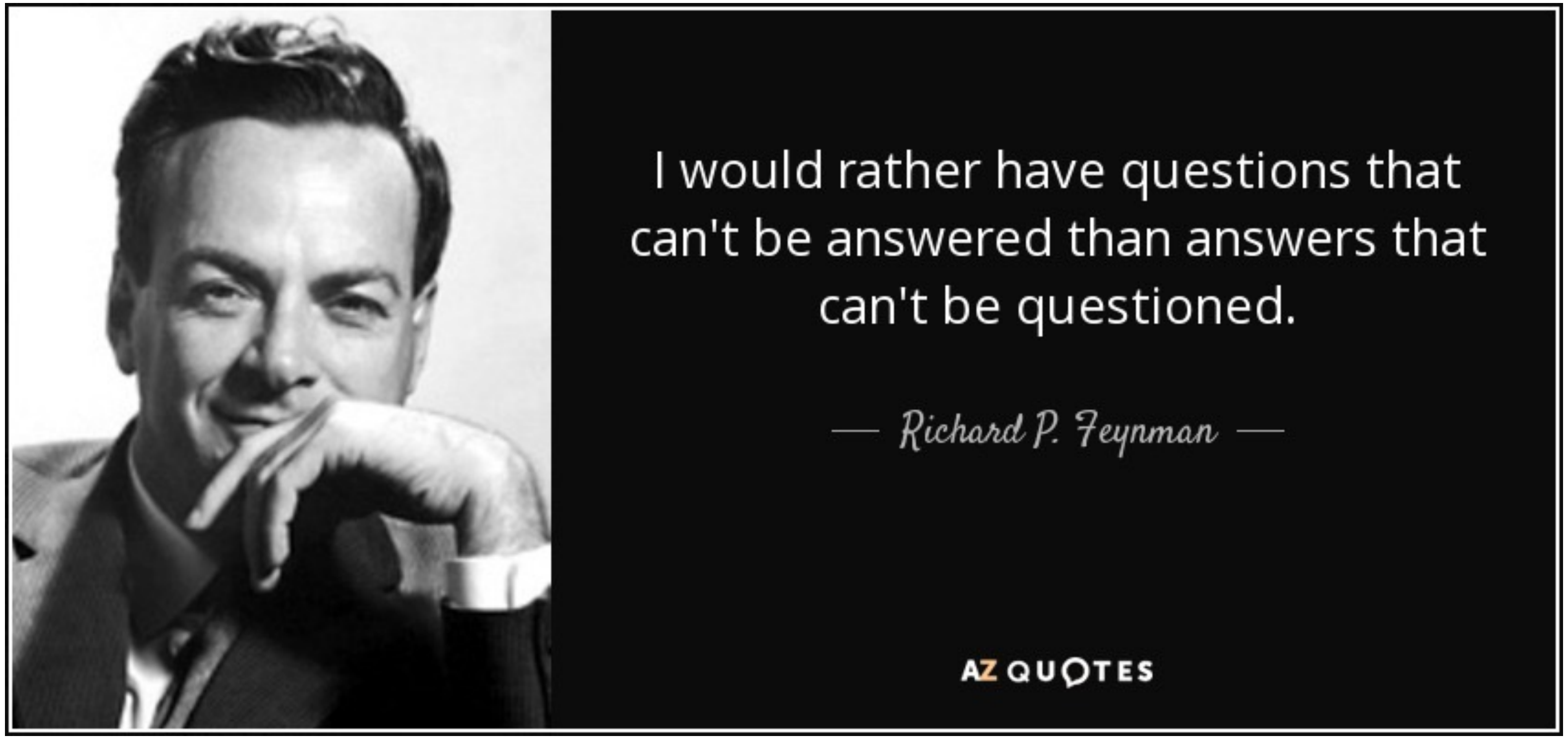
So just ask the right questions and think valleys…



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