Stretching Moore's law: quantum design of materials and devices for classical computation

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Cornell University Founded A.D. 1865
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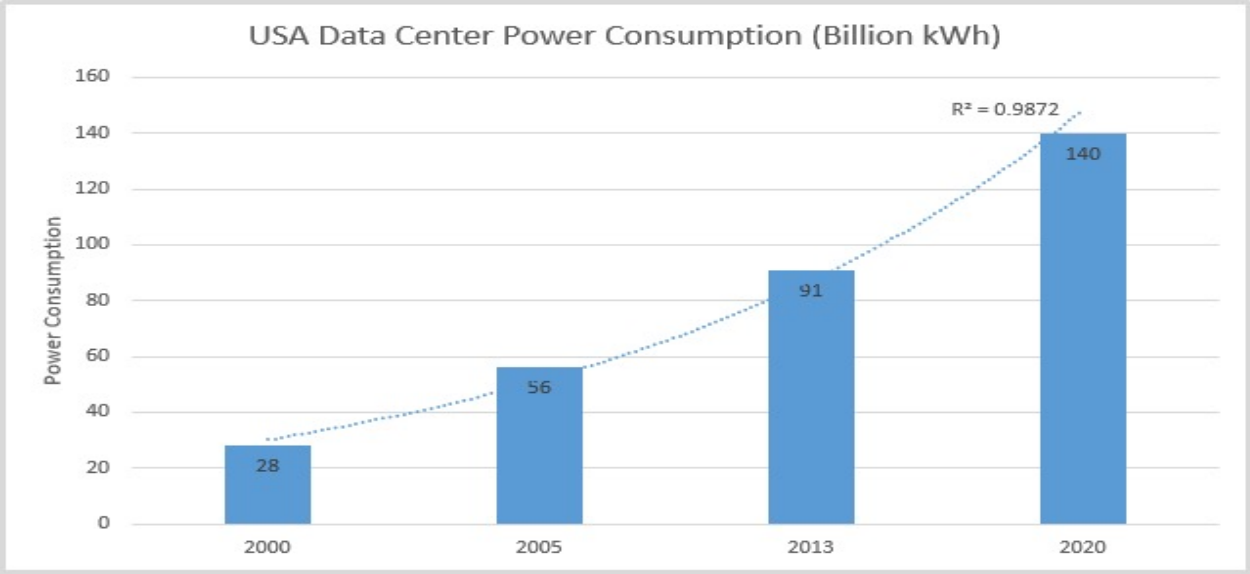
Computing contributes a considerable amount to energy grid



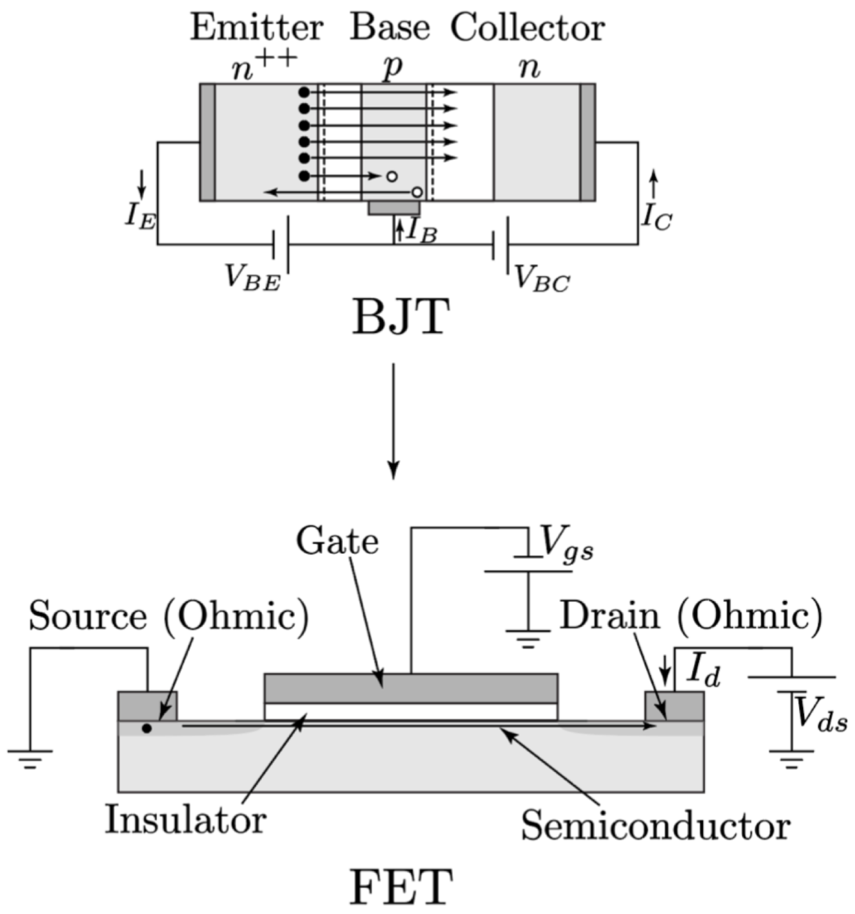
Microelectronics are growing in demand

IOT

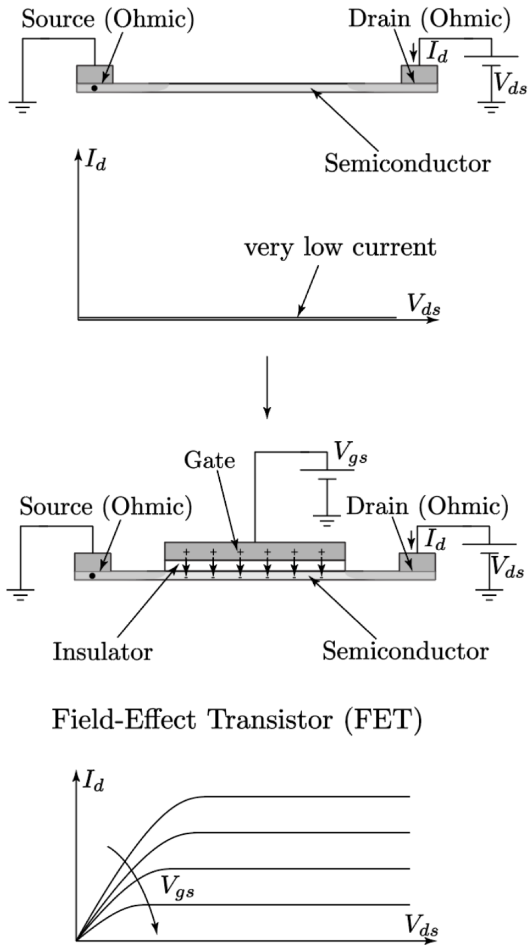
Machine Learning

Cloud storage

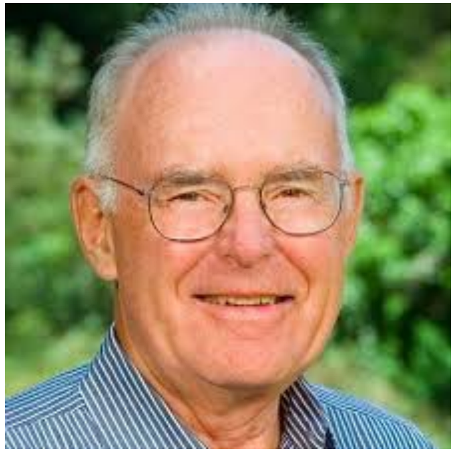
The current paradigm of microelectronics



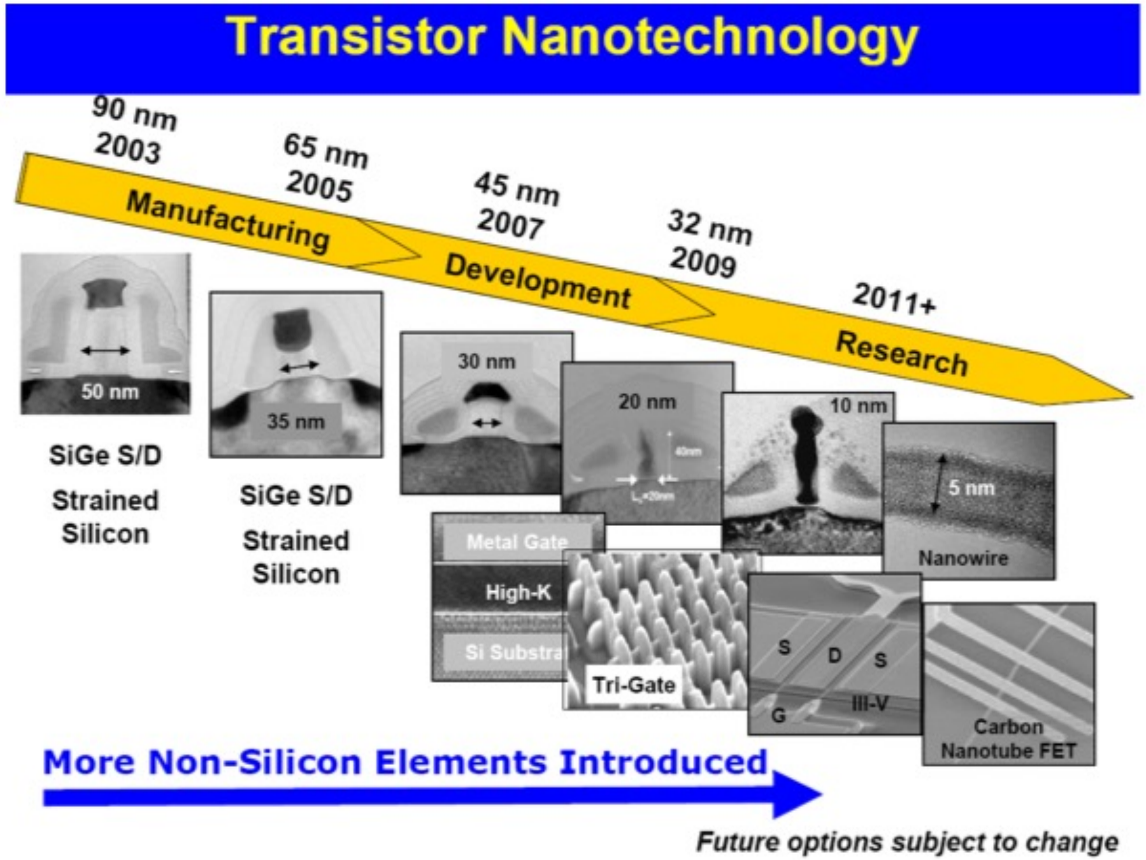
$$I_{DS} \approx I_{D0} \exp\left(\frac{qV_{GS}}{\eta kT}\right)$$



Moore’s law is dying

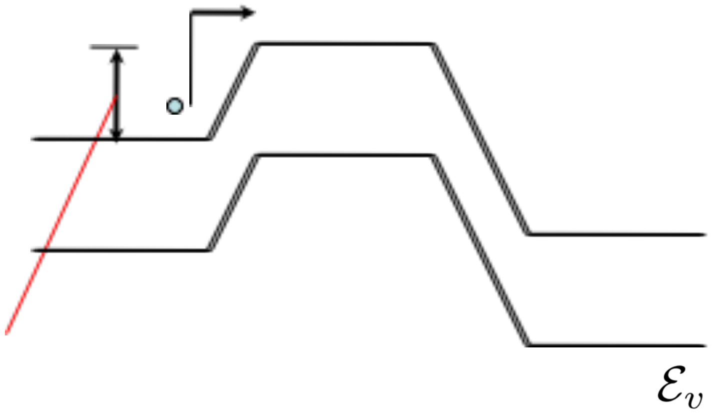


Gordon Moore

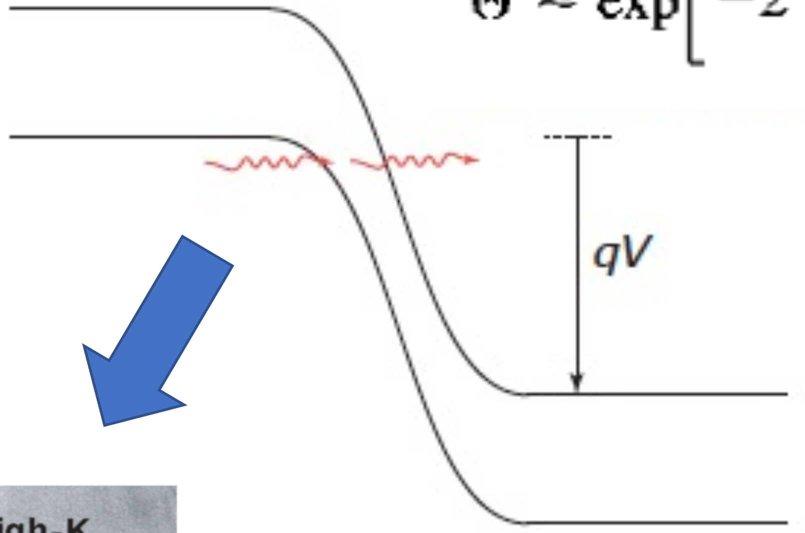


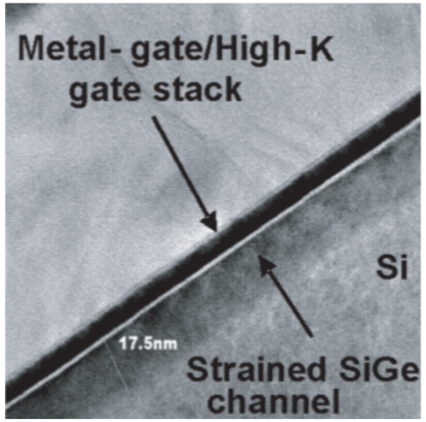
Today's microelectronics not sufficient to sustain Moore's law

$$q\phi_B = q(\phi_{bi} - \phi_S)$$



$$\Theta \approx \exp\left[-2\int_0^L \sqrt{\frac{2m^* E_B}{\hbar^2}}\, dx\right]$$





QM to engineer next-generation microelectronics

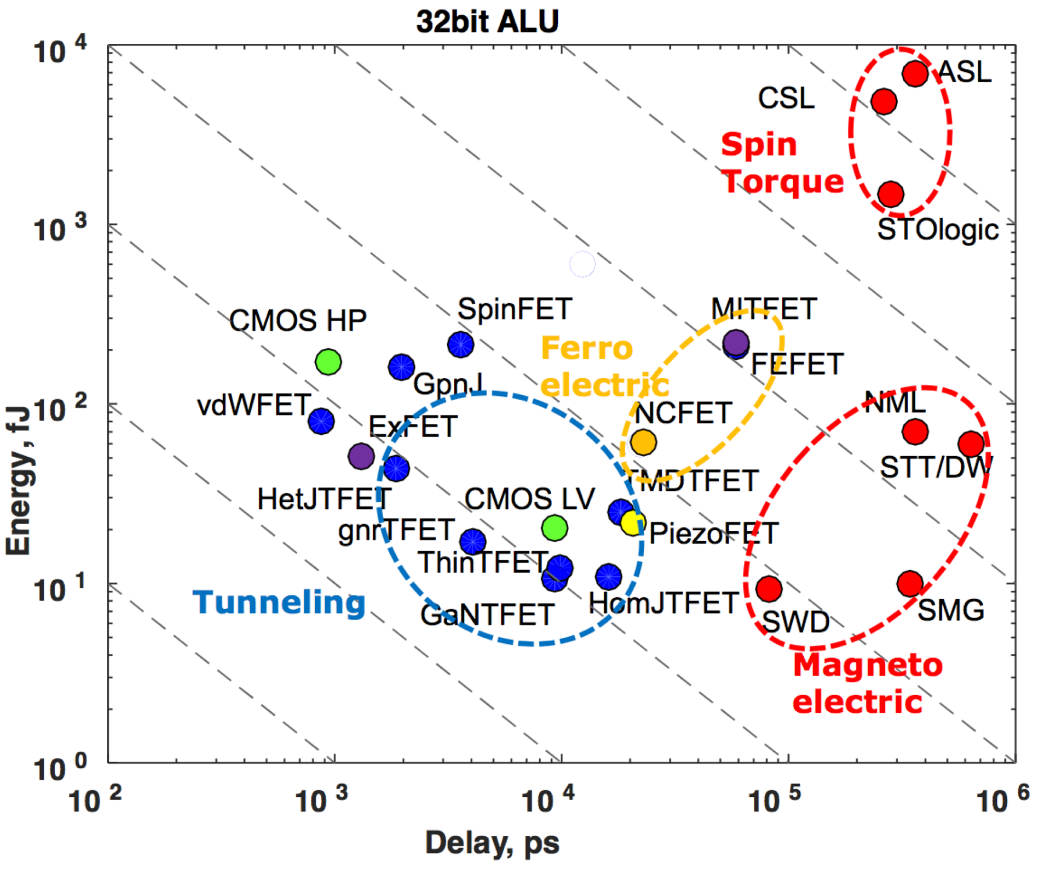
Is quantum mechanics useful?

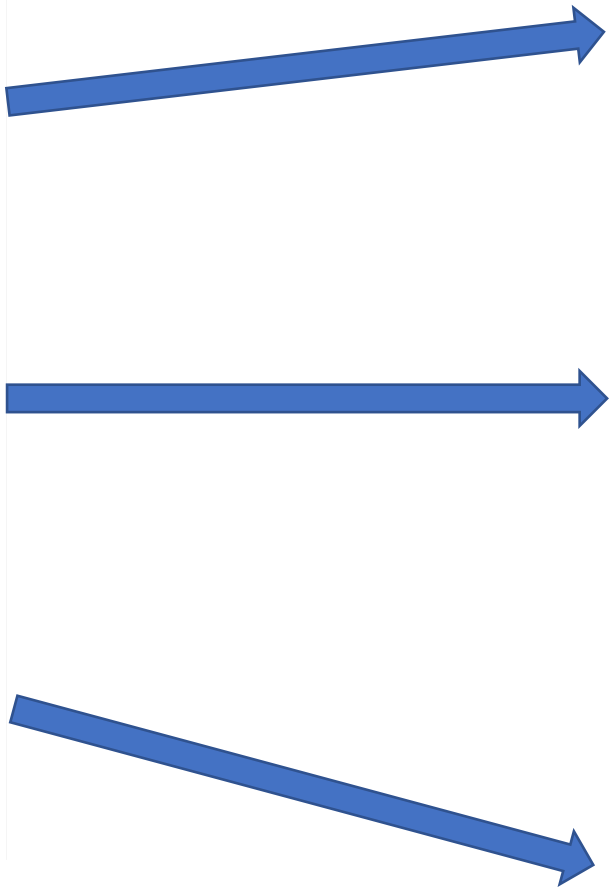
By Rolf Landauer

IBM Thomas J. Watson Research Center, PO Box 218, Yorktown Heights, New York, NY 10598, USA

friction are determined by quantum mechanical interatomic forces. But we do not need to understand those to design, make or use a screw driver. The transistor is a modern device based on the motion of holes and electrons in energy bands. But it really isn't that different from a screw driver; once we know about holes and electrons and mobilities, we do not need to go back to the Schrödinger equation. The overall behaviour of the transistor does not exhibit quantum mechanical coherence; the

Smaller and lower energy needs to go beyond charge





q

Photonics, superconductors, new semiconductors?

$|\uparrow\rangle$

$|K\rangle$

First principles techniques to guide materials design

Define engineering figure of merit (i.e. coherence time) → **Identify material properties most responsible for FOM** → **Obtain mapping from wavefunction/energy to property**

→ **Compute wavefunctions/energy and properties for max FOM** → **Vary experimental parameters predicted from theory**

Quantum approach to device/material design

(a) Material design in conjunction for better information storage/processing [materials for RSFQ devices]

(a) Material design for reliable communication [suppression of low-frequency noise mechanisms]

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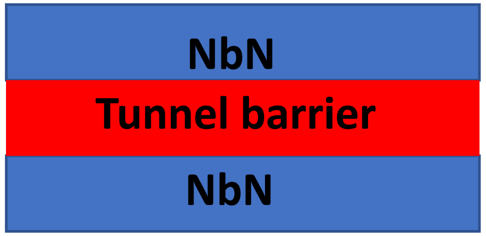
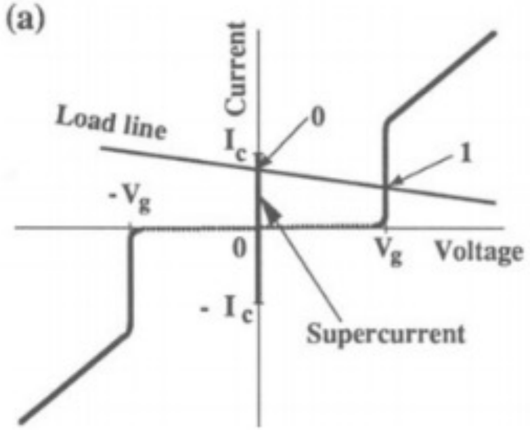
Rapid single flux quantum logic (RSFQ)

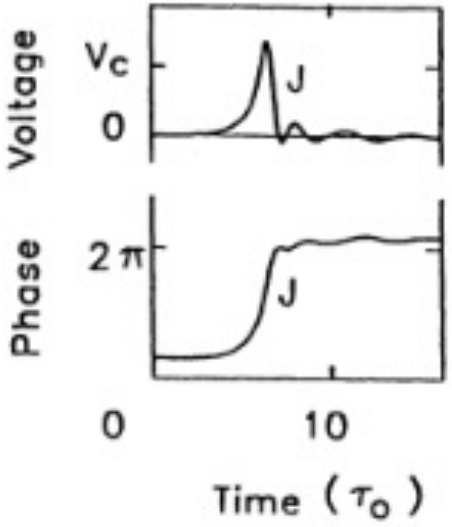


Josephson Junction

"the simplest basic components of the RSFQ family … were demonstrated to work at clock frequencies in excess of 100 GHz"[Weinstock]

$$J = J_c \sin[\phi]$$





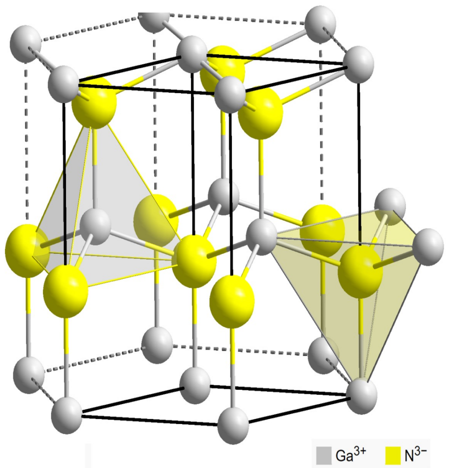
Objective: explore new materials demonstrating high clock speeds, high critical current, and long coherence times

Material platforms for III-V based JJs

Superconducting Transition Metal Nitrides	
NbN	$T_c \cong 17.0K$
HfN	$T_c \cong 8.7K$
ZrN	$T_c \cong 10.0K$
TaN	$T_c \cong 10.9K$

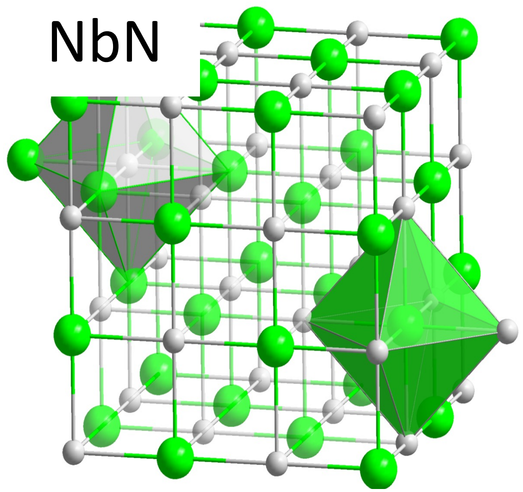
Lengauer, W., Surf. and Int. An 15 (6), 1990

GaN, AlN



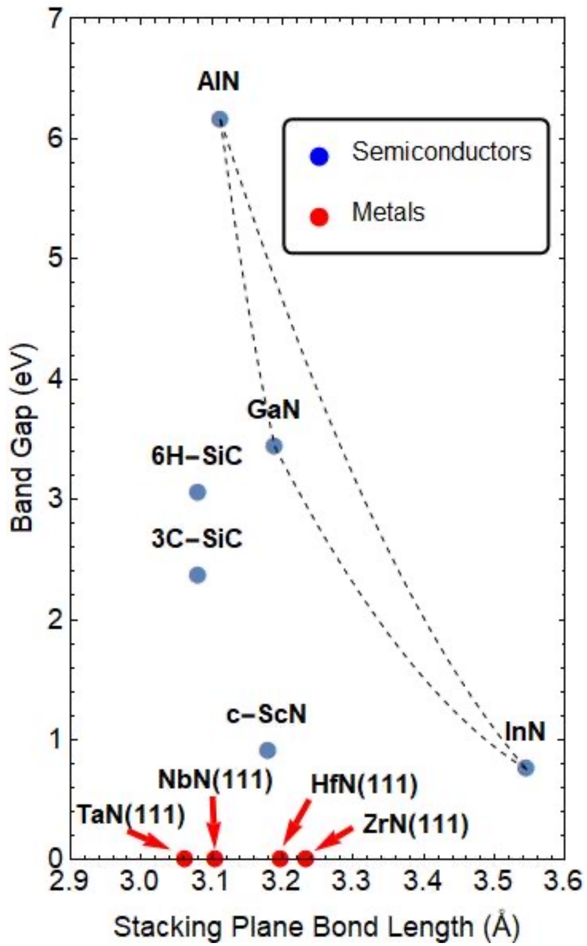
en.wikipedia.org/wiki/File:Wurtzite_polyhedra.png

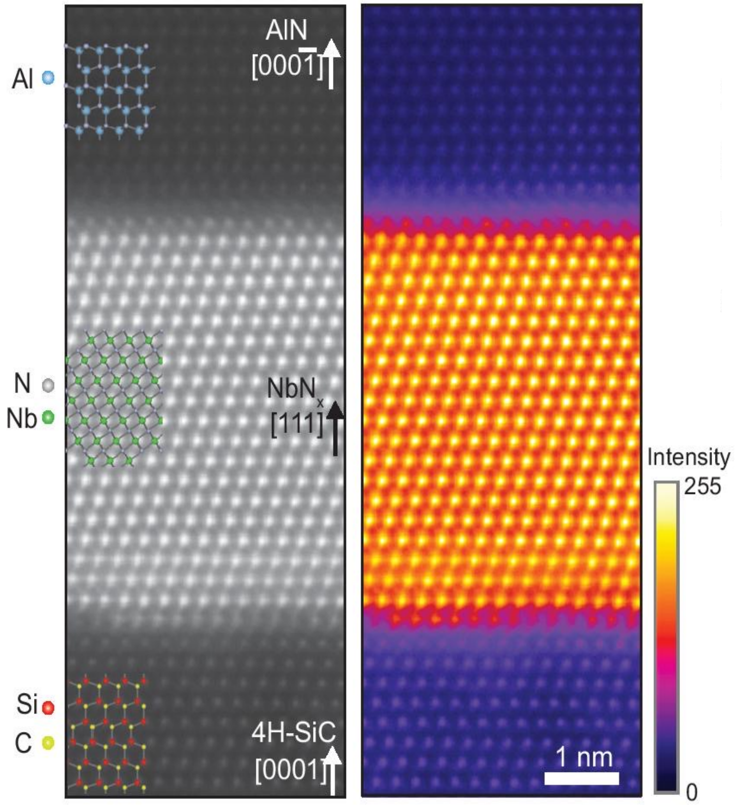
NbN



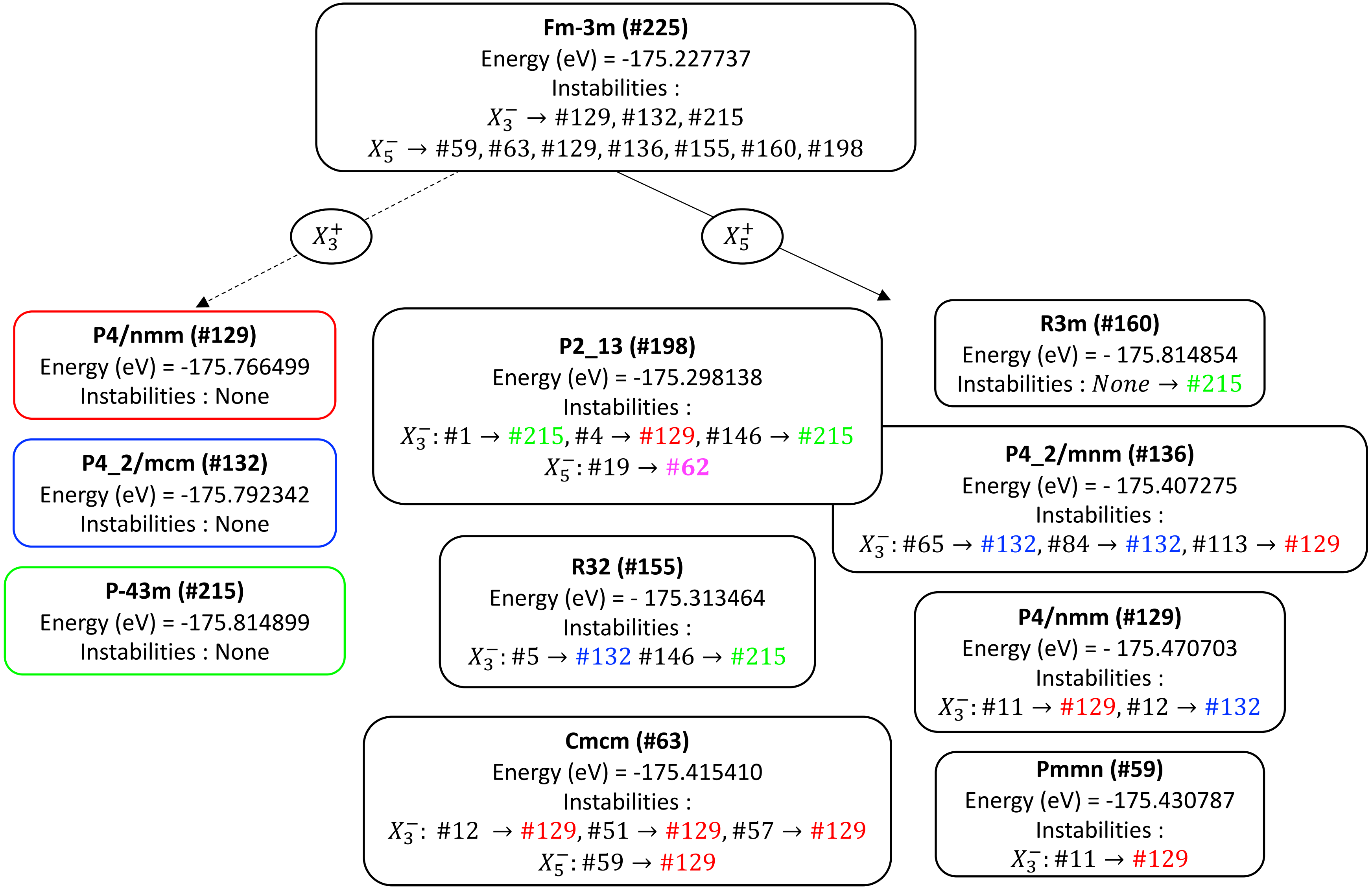
commons.wikimedia.org/wiki/File:NaCl_polyhedra.png

Compatibility of NbN superconductor with GaN (and AlN)

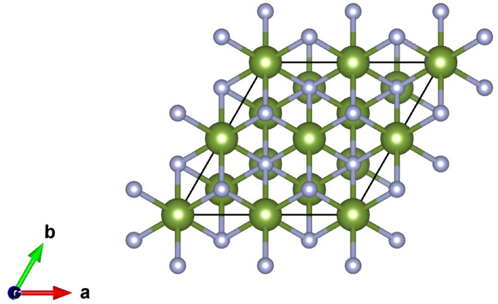


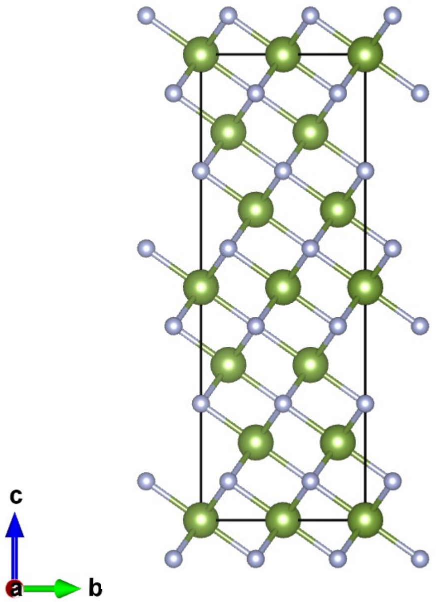


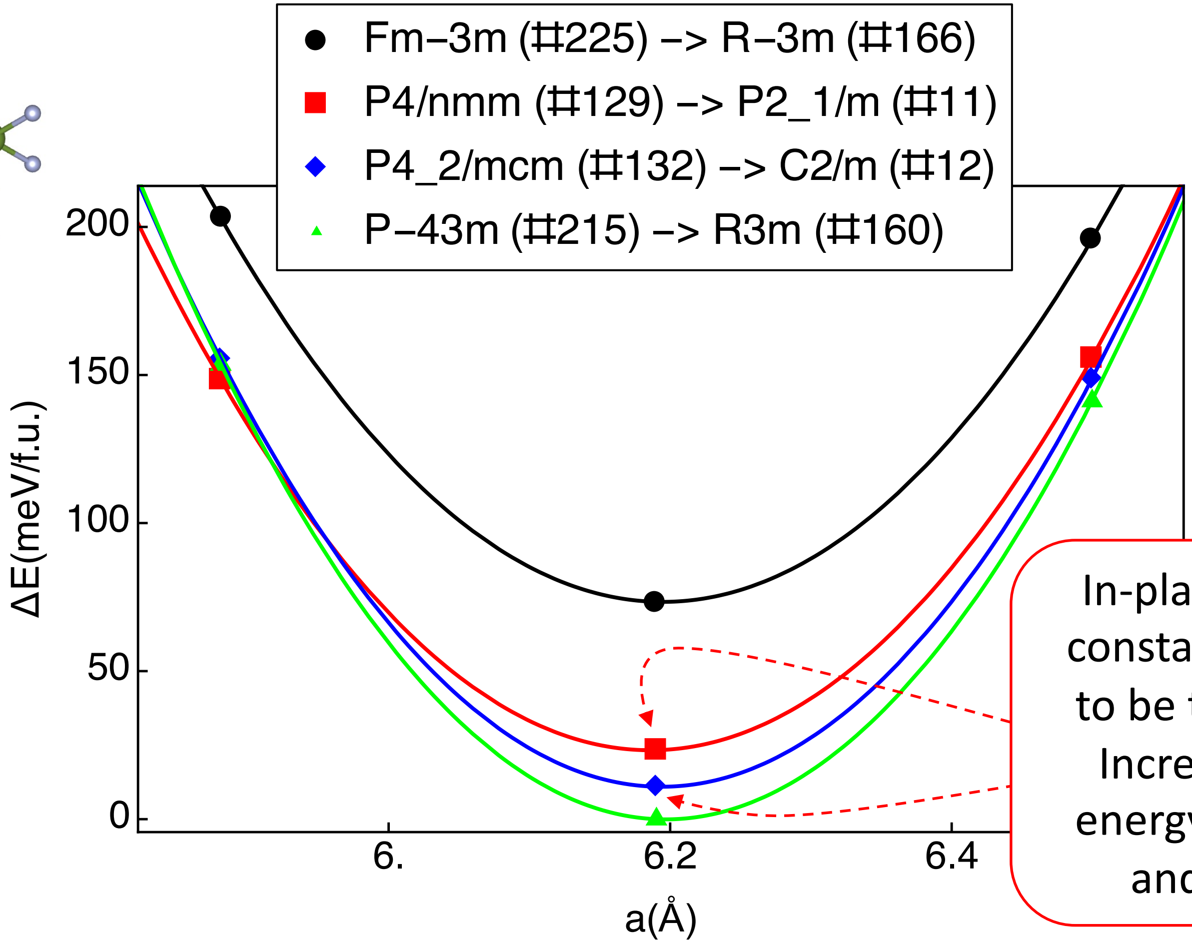
Exploring phase space for epitaxial growth



Exploring phase space for epitaxial growth cont’d







In-plane lattice constants forced to be the same. Increases the energy of #129 and #136

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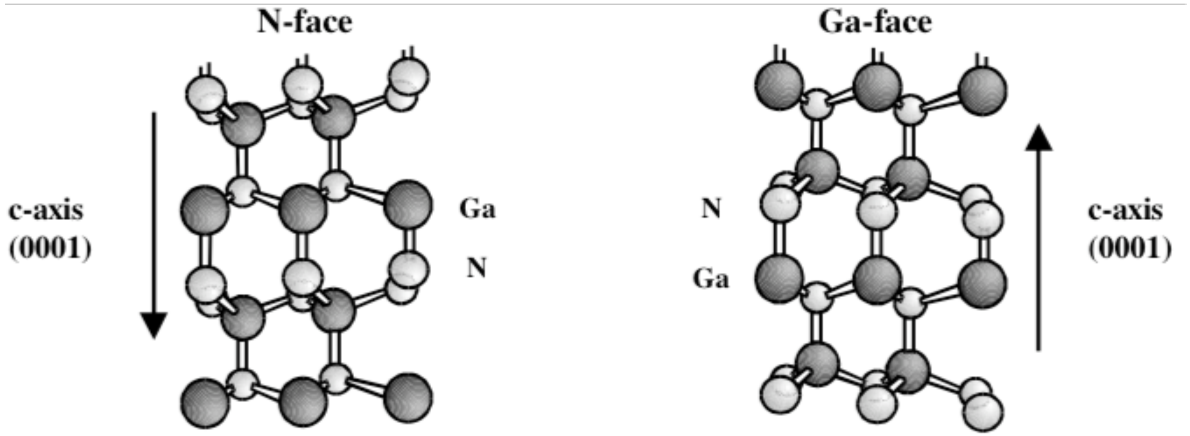
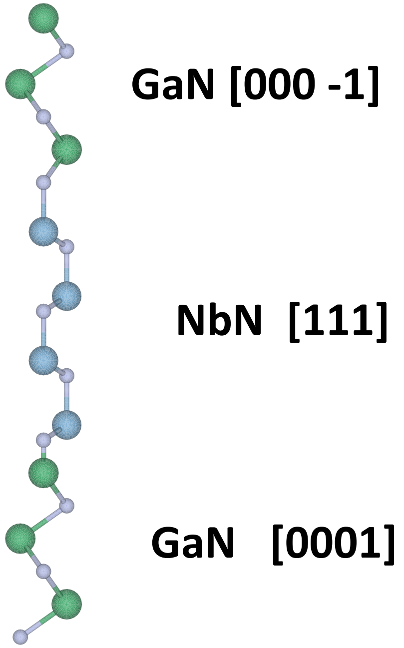
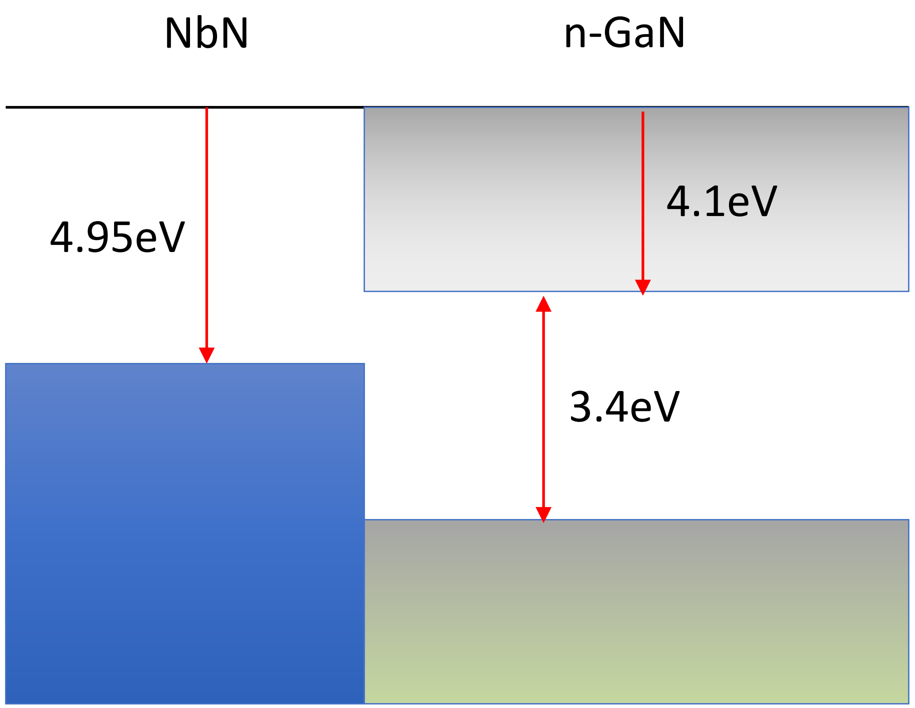
Polarity engineering for better transport

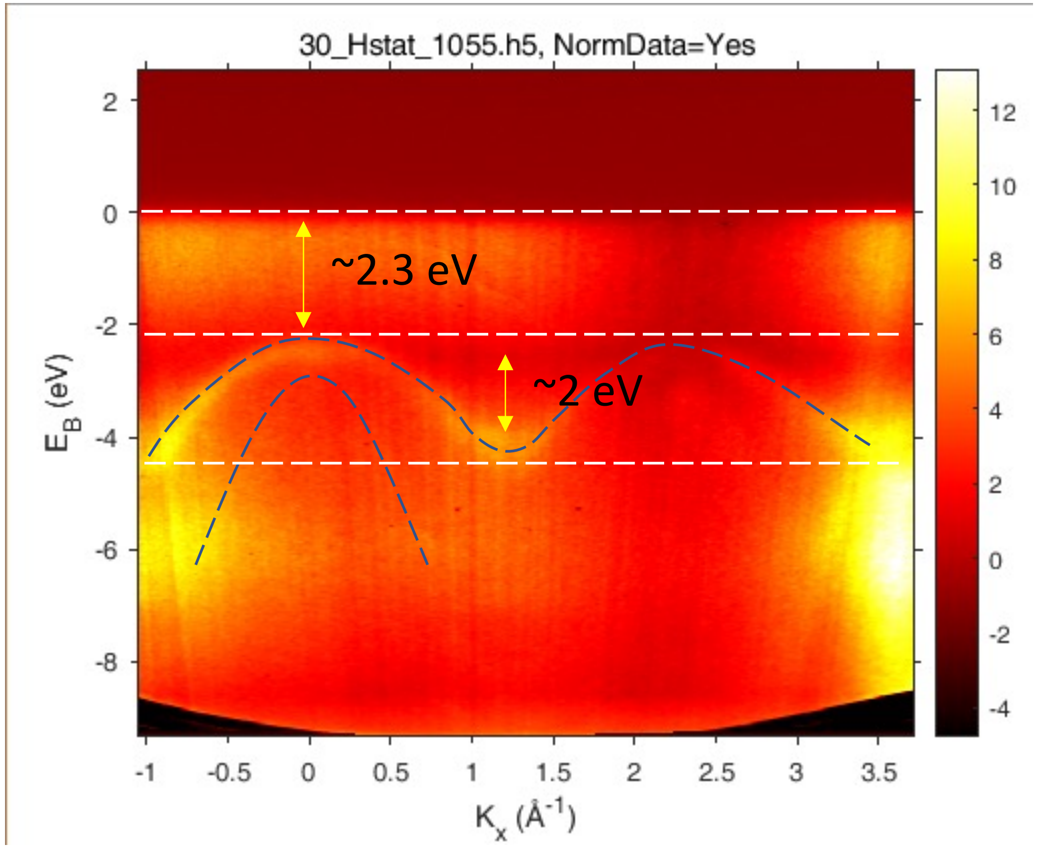




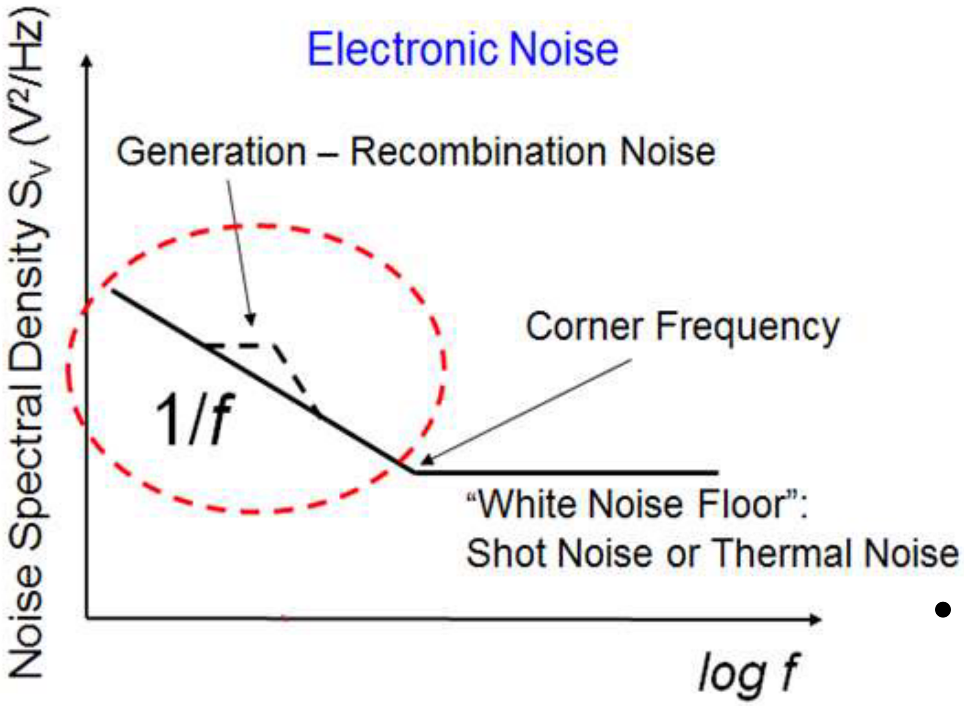
Improving transport (maximize tunneling probability)

$$\Theta \approx \exp\left[-2\int_0^L \sqrt{\frac{2m^*E_B}{\hbar^2}}\,dx\right]$$





Noise is frequency dependent: draw focus to 1/f noise

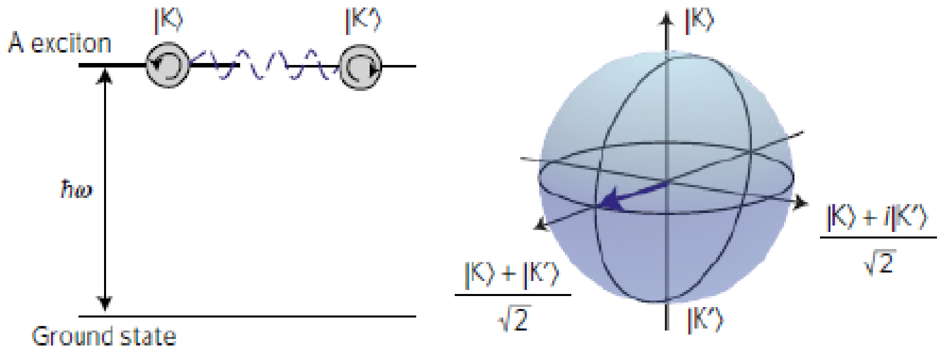


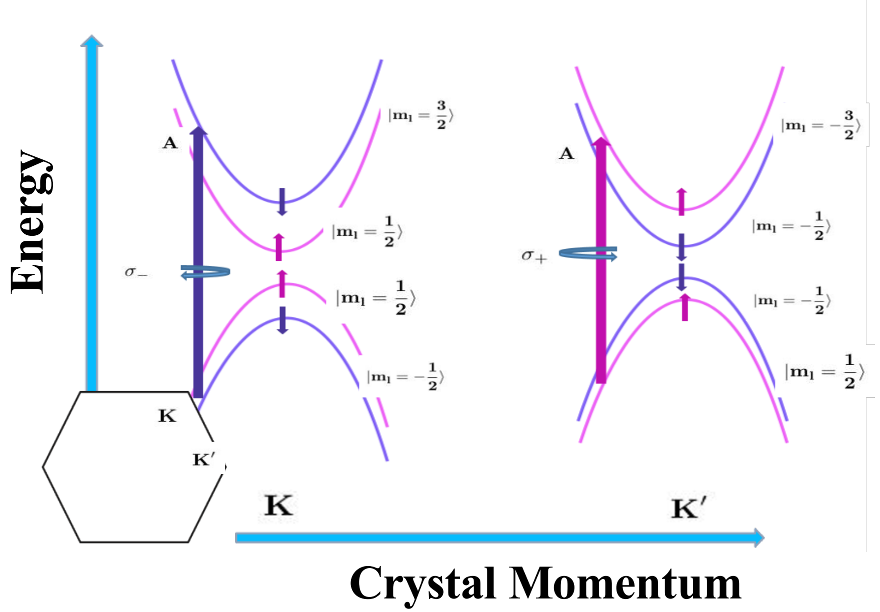
$$I \sim qN\mu$$

$$\delta I \sim q(\delta N \mu + N \delta \mu)$$

- 1/f noise due to generation-recombination effects, acoustic phonon scattering, impurity scattering, etc.
- Observed in frequency range of 0 – 1 MHz
- Large device-to-device variation in noise spectrum

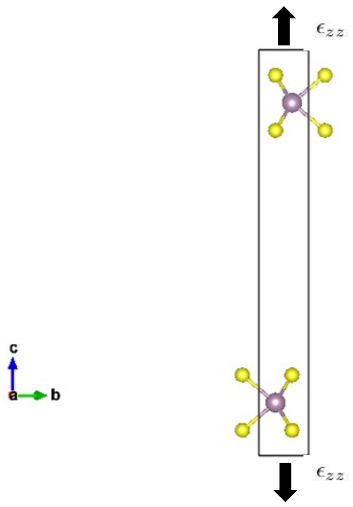
Valleytronics: an overview





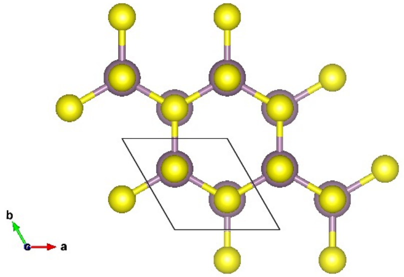
Material platform for valleytronics: 2D TMDs

Bulk MoS_2:



2D Confinement →

Monolayer MoS_2:



D_{6h}

$$\Gamma = A_{1g} + 2A_{2u} + 2B_{2g} + B_{1u} + 2E_{1u} + 2E_{2g} + E_{2u}$$

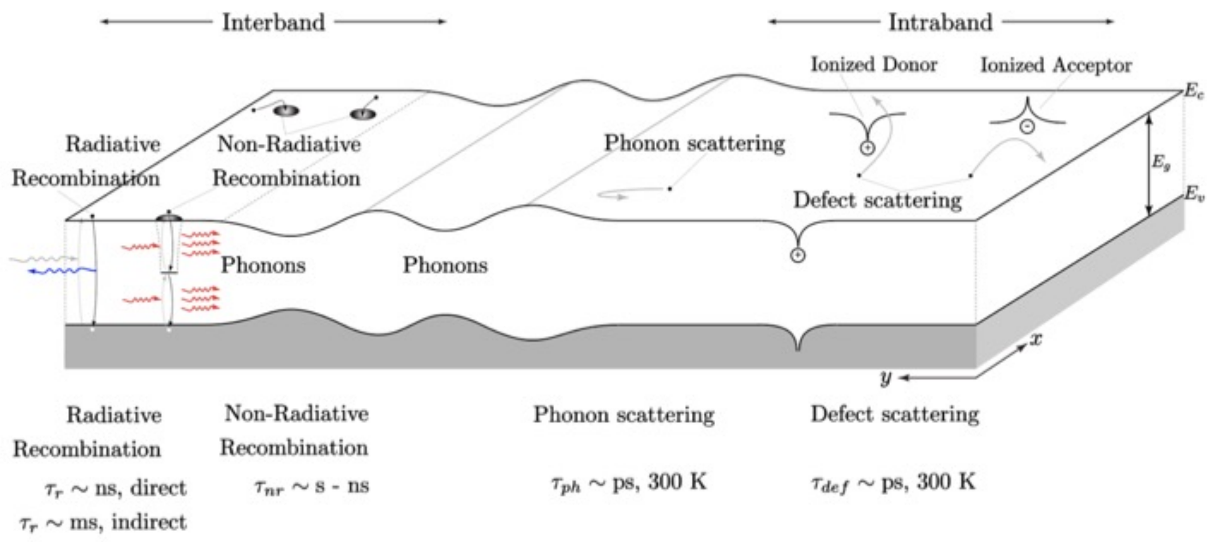
Indirect gap, possesses 18 phonon modes, inversion symmetry present.

D_{3h}

$$\Gamma = 2A_1'' + A_1' + 2E' + E''$$

Emergence of direct gap, degeneracies at K/K' points, piezoelectricity, possesses 3 etc.

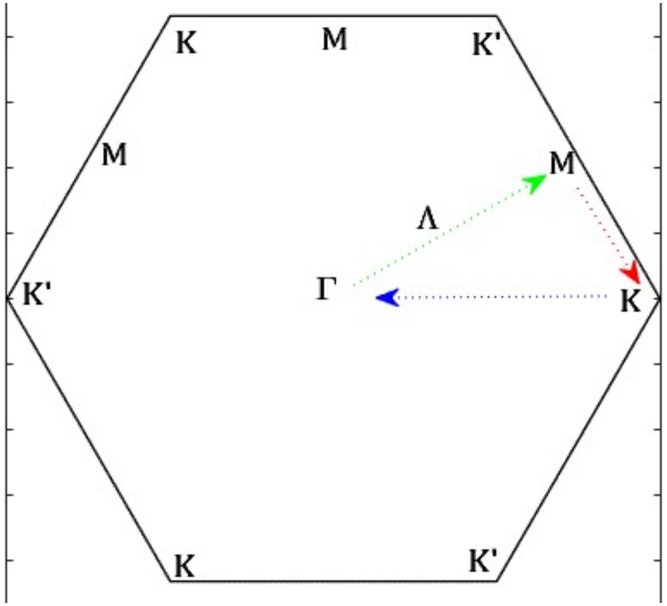
Scattering is a problem

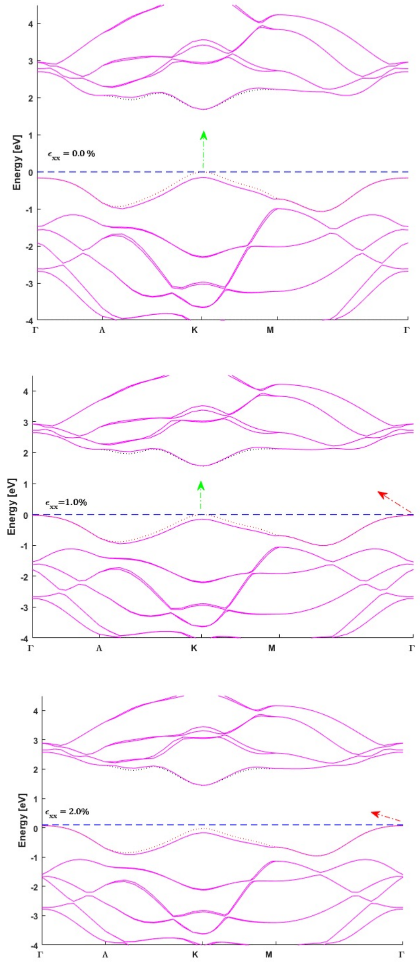


$$\frac{1}{\tau_{n\mathbf{k}}} = \frac{2\pi}{\hbar} \sum_{m\nu} \int \frac{d\mathbf{q}}{\Omega_{\mathrm{BZ}}} |g_{nm\nu}(\mathbf{k},\mathbf{q})|^2 \times [(1 - f_{m\mathbf{k}+\mathbf{q}} + n_{\mathbf{q}\nu})\delta(\varepsilon_{n\mathbf{k}} - \hbar\omega_{\mathbf{q}\nu} - \varepsilon_{m\mathbf{k}+\mathbf{q}})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

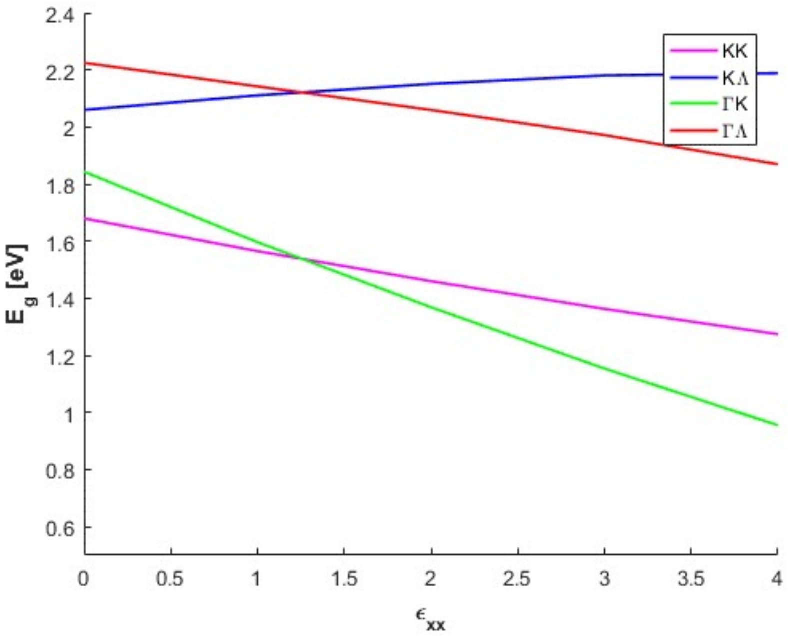
$$g_{mn\nu}(\mathrm{k},\mathrm{q}) = \langle u_{m\mathrm{k+q}} | \Delta_{\mathrm{q}\nu} v_{\mathrm{SCF}} | u_{n\mathrm{k}} \rangle_{\mathrm{uc}}$$

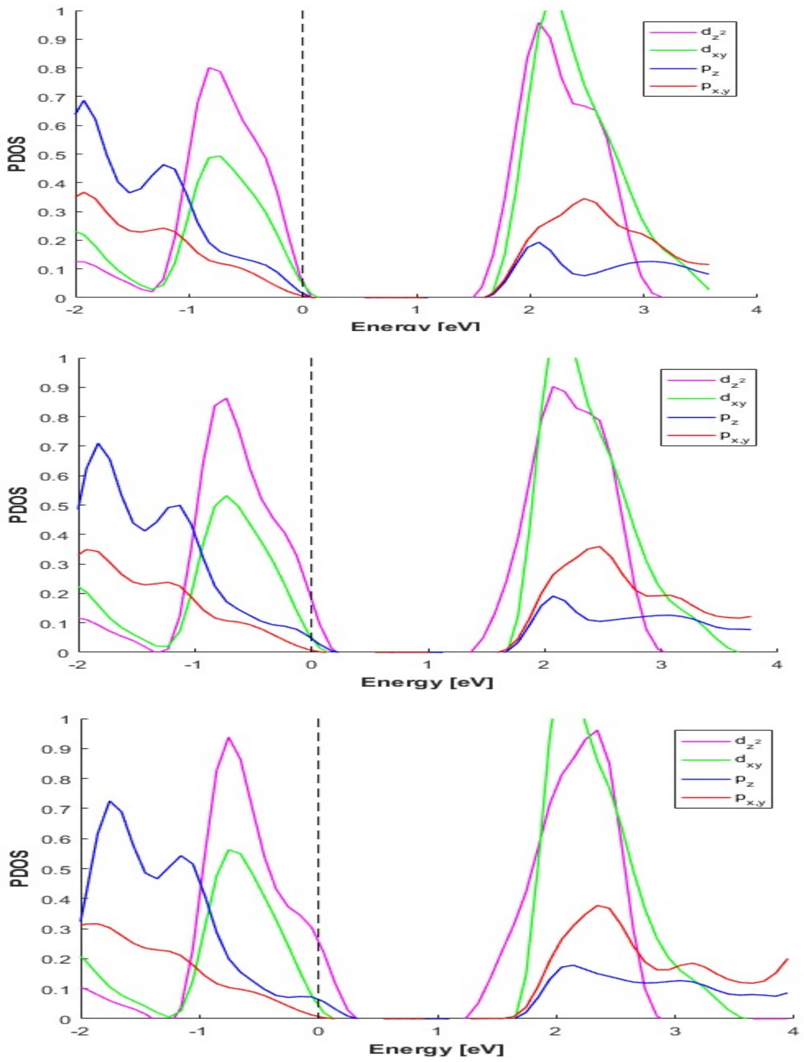
Using strain engineering to increase valley lifetime



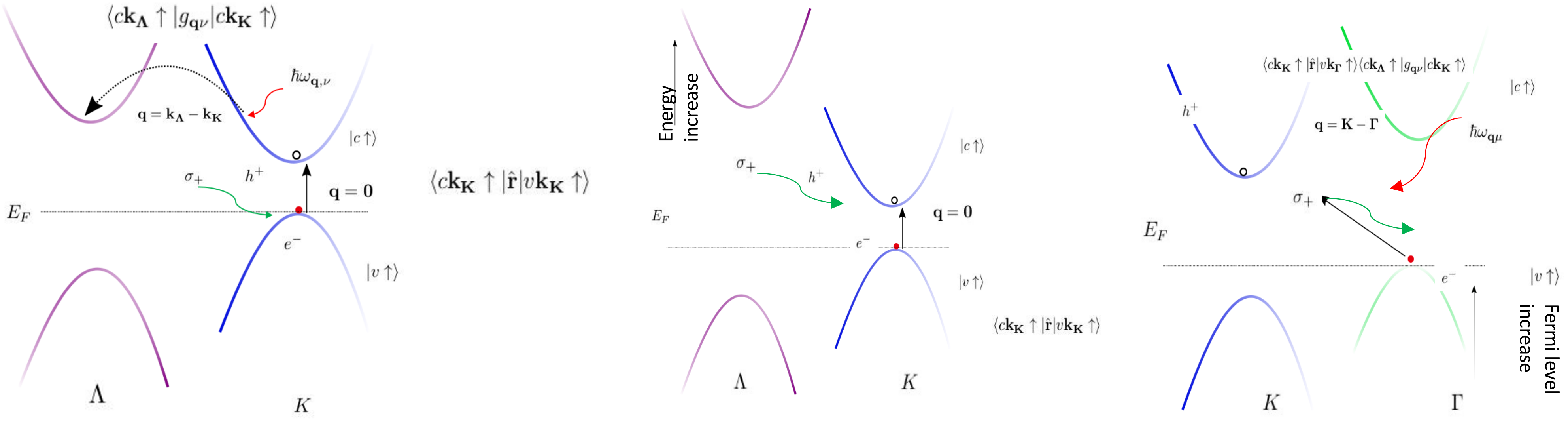


Using strain engineering to increase valley lifetime (cont'd)





Using strain engineering to increase valley lifetime (cont'd)



$\epsilon_{xx} = 0$ $1.0\% < \epsilon_{\mathbf{xx}} < 2.0\%$ $\epsilon_{\mathbf{xx}} \geq 2.0\%$

Next steps with this…

(a) Look at entire valley lifetime predictions with applied strain
(b) Experimental realization of strained TMDs → exciton lifetimes with strain

Going smaller and more energy efficient will require quantum

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