SAND2015-4959C

Exceptional service in the national interest

Sandia National Laboratories

The Low Voltage TFET Demands Higher Perfection than Previously Required in Electronics

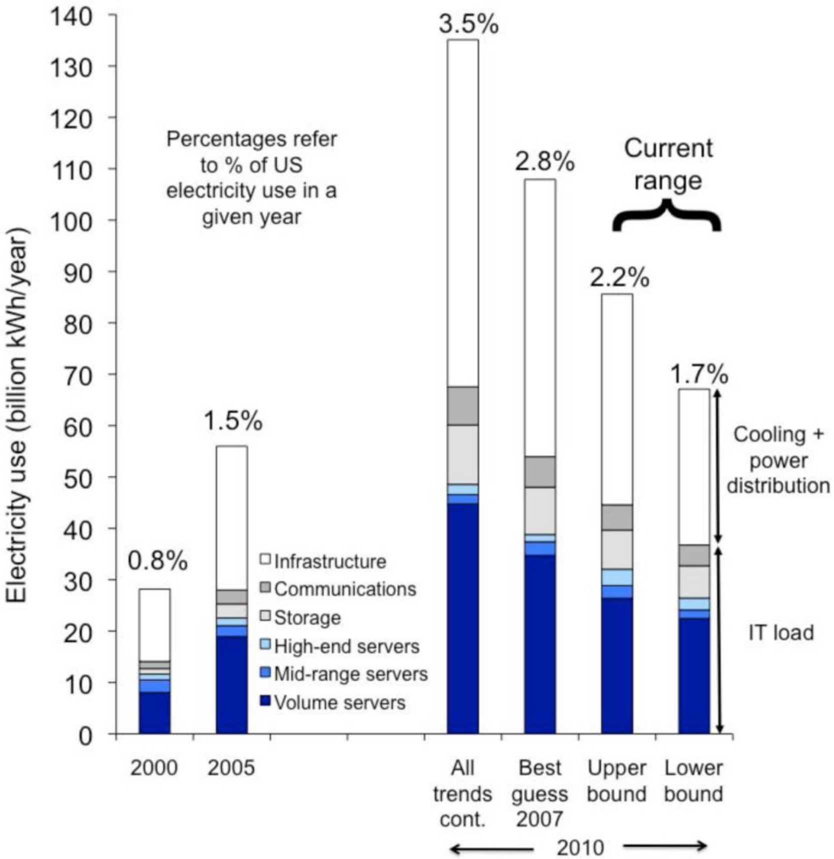
Sapan Agarwal, Eli Yablonovitch

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND NO. 2011-XXXXP

Data Center Electricity Usage



- In 2010, data centers accounted for ~1.3% of all electricity use worldwide, ~2% of all electricity use in the U.S.

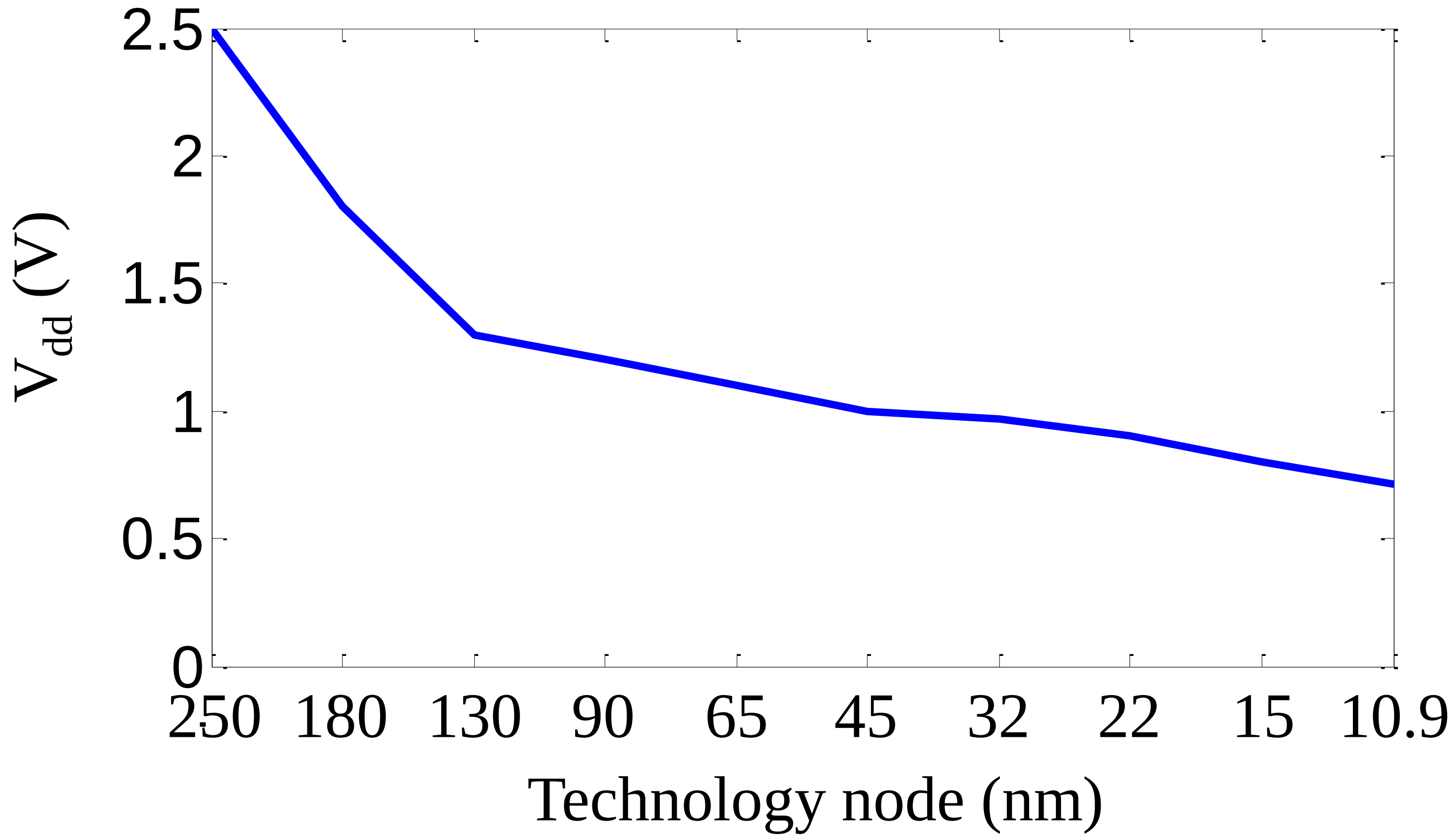

Google

Google's new data center in Hamina, Finland, has an energy-efficient cooling system that uses seawater from a nearby bay.

J. Koomey, *Growth in Data center electricity use 2005 to 2010* (Analytics Press, Oakland, CA), 2011

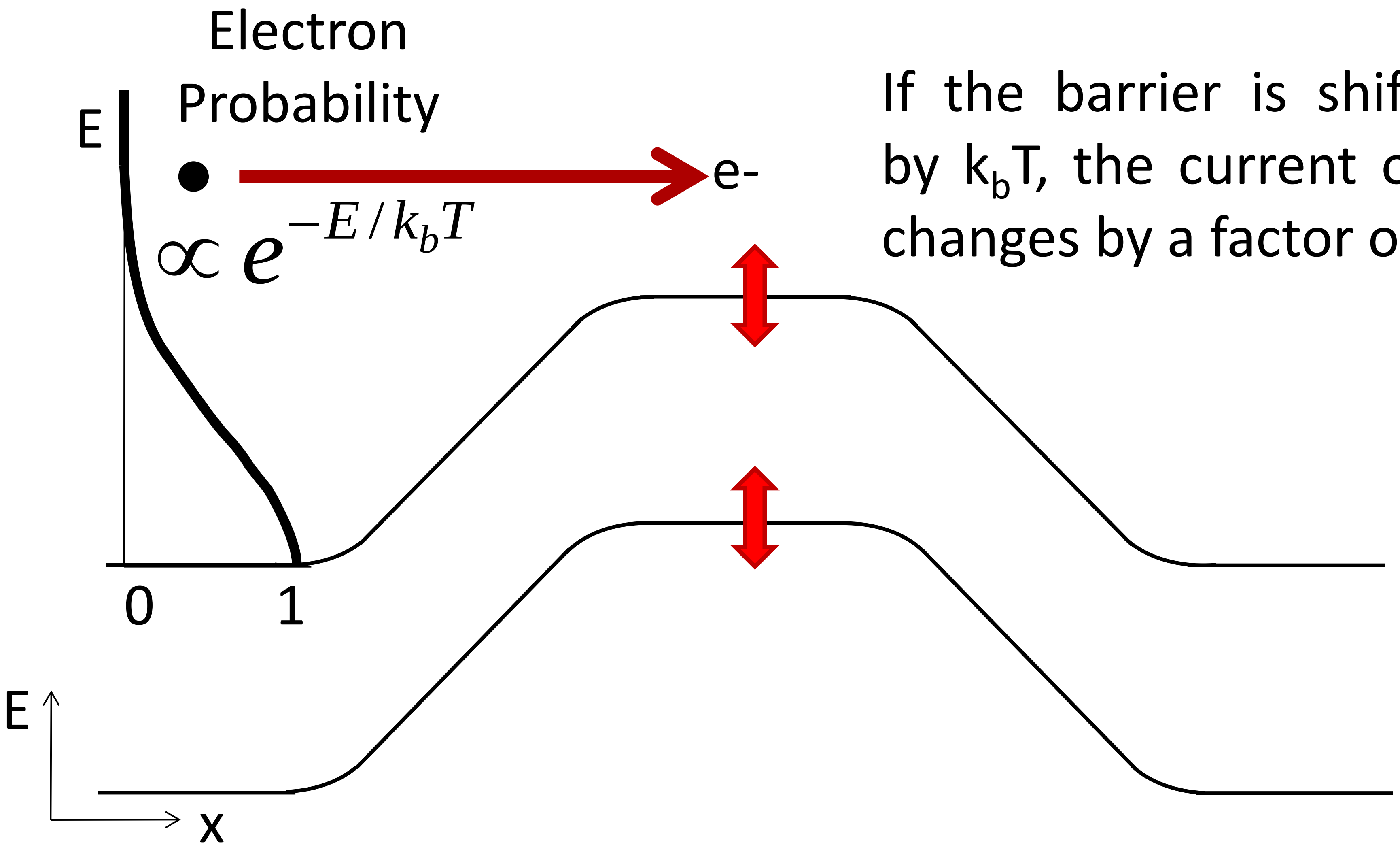
Power Usage Rising

- Power consumption is $\propto V_{dd}^2$ and V_{dd} (operation voltage) scaling has slowed.



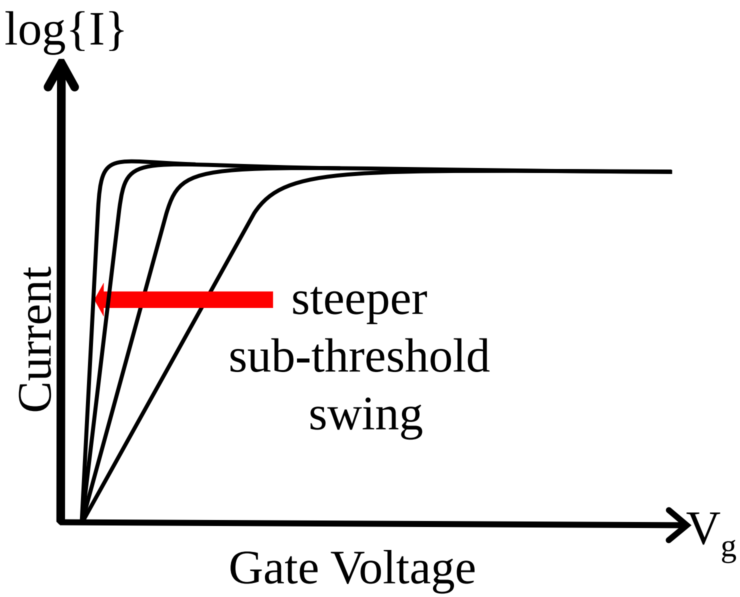
High Performance ITRS Roadmap

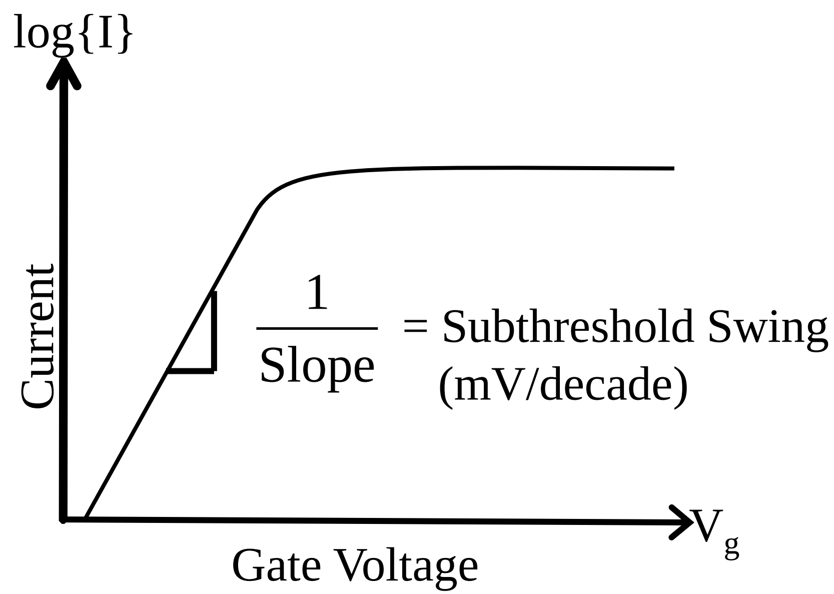
What's Wrong With Current Transistors?



If the barrier is shifted by k_bT, the current only changes by a factor of e

Need a New, More Sensitive Switch





The New Switch has to Satisfy Three Specifications

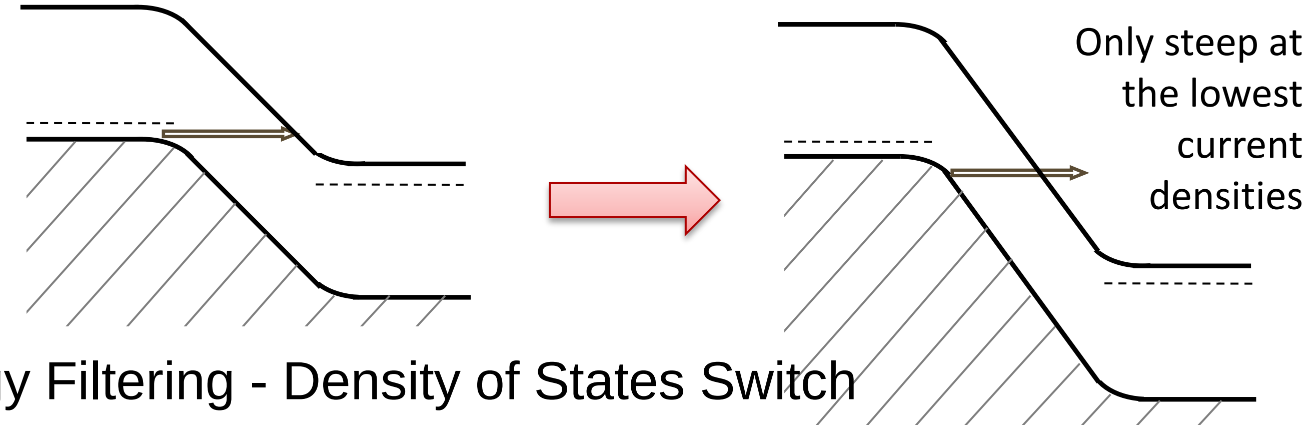
1. Steepness (or sensitivity)
   switches with only a few milli-volts
   60mV/decade $\Rightarrow$ **1mV/decade**

2. On/Off ratio. $10^6 : 1$

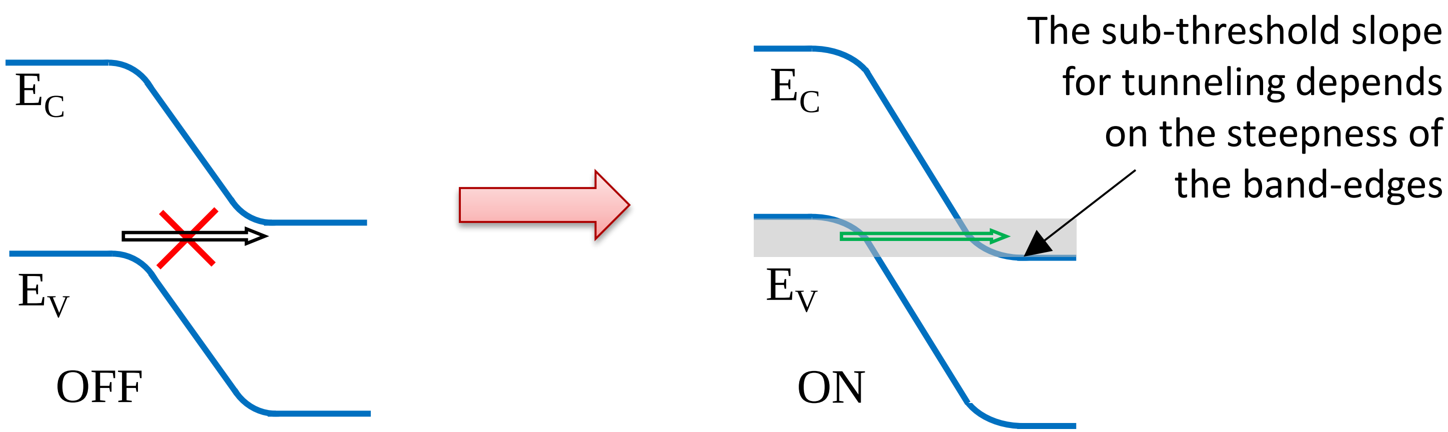
3. Current Density or Conductance Density
   (for miniaturization)
   old spec at 1Volt: 1 mAmp/micron
   our spec: **1 milli-Siemen/micron**

2 Ways to Obtain Steepness

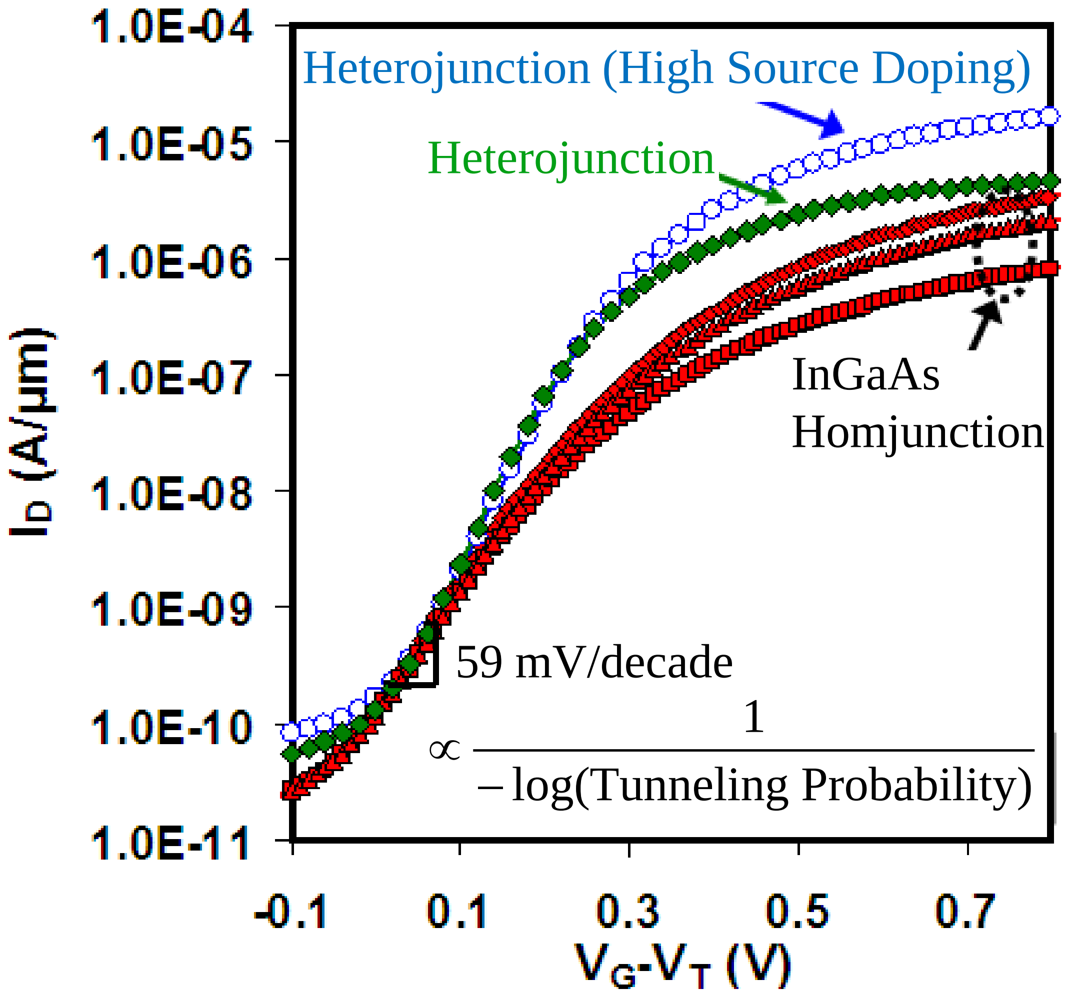
- Modulate the Tunneling Barrier Thickness



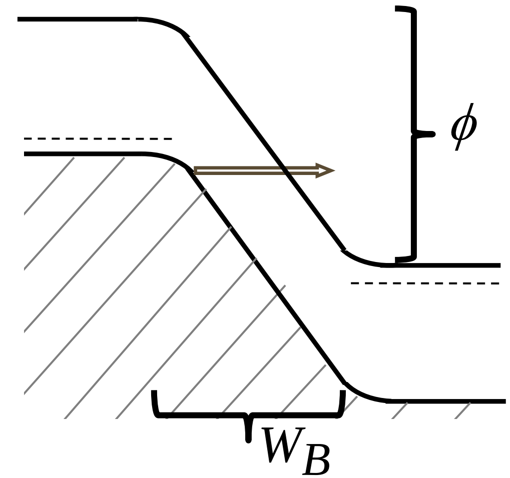
- Energy Filtering - Density of States Switch



Barrier Width Modulation Explains all Steep TFET Results and it's not Good Enough



G.Dewey, et all, *IEDM 2011* pp. 785-788, 2011



$$\text{Subthreshold Swing(SS)} \approx \frac{d\phi}{d\log(\text{T})}$$

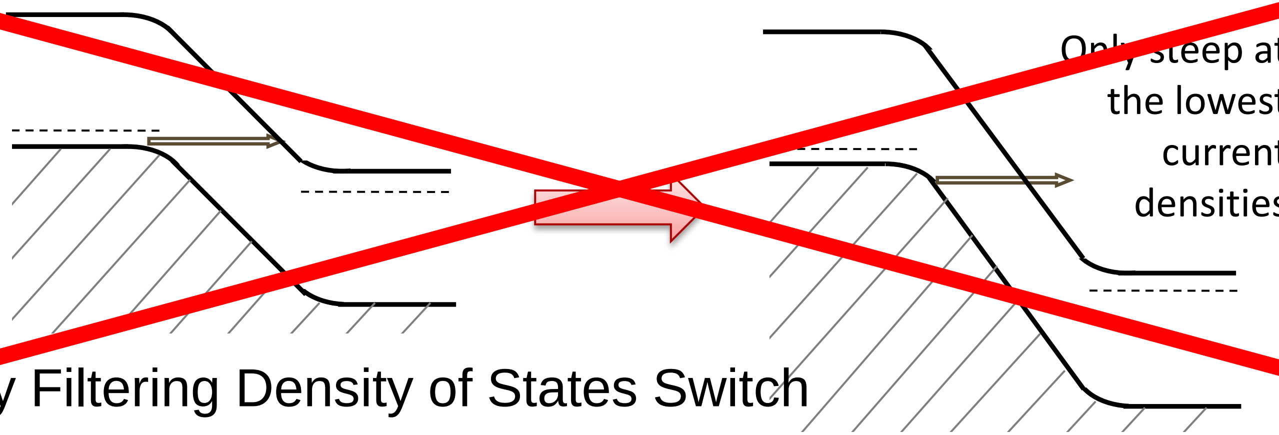
$$\text{T} = \exp\left(\frac{-\alpha}{|\vec{F}|}\right) \qquad |\vec{F}| = \frac{\phi}{W_B}$$

$$SS \approx \left|\frac{1}{\log(T)} \times \frac{F}{dF(\phi)/d\phi}\right|$$

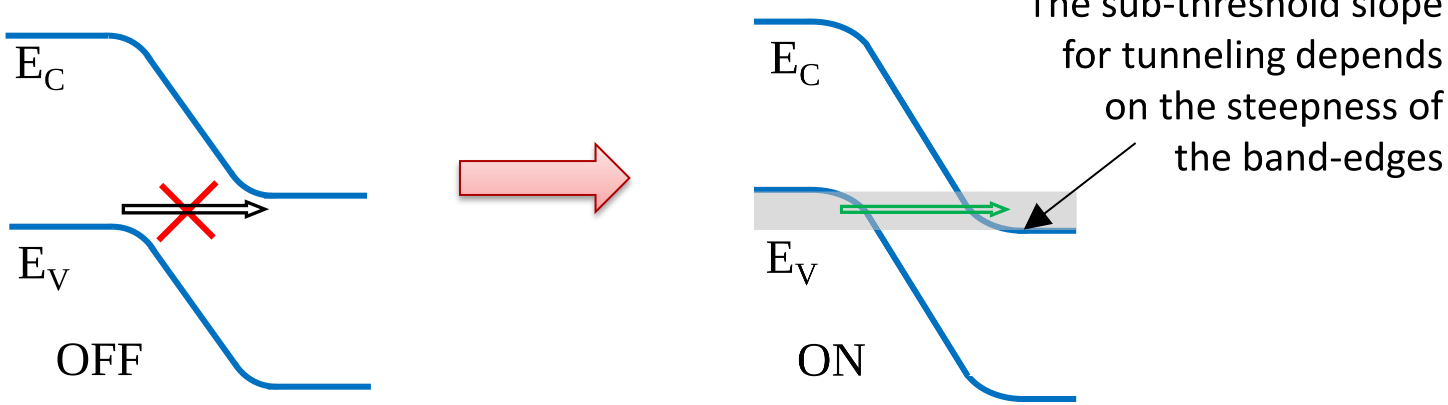
$$= \frac{\phi}{|\log(\text{T})|}$$

2 Ways to Obtain Steepness

- Modulate the Tunneling Barrier Thickness

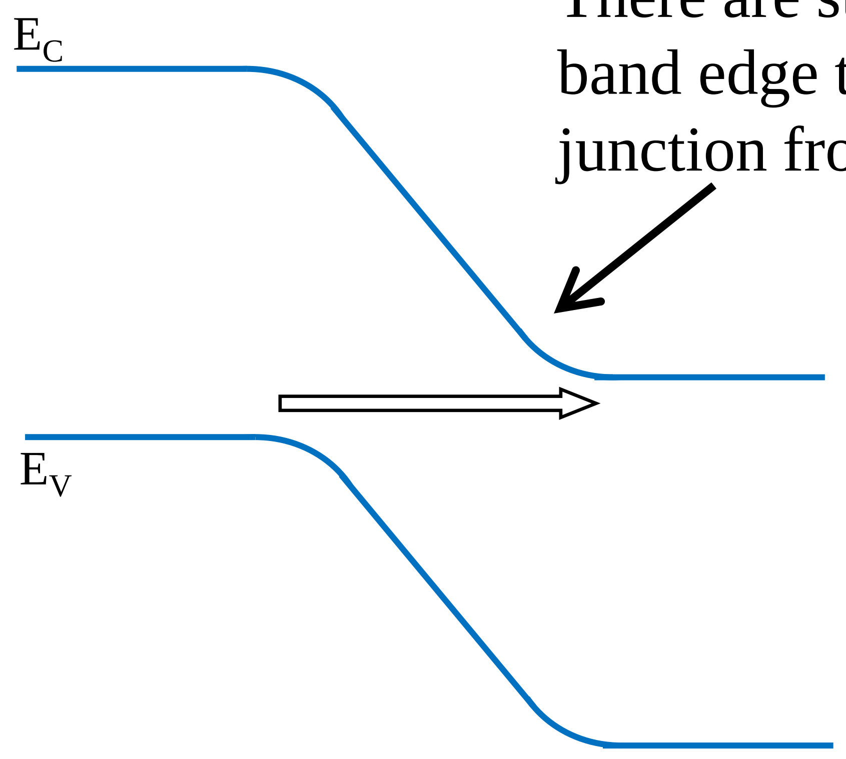


- Energy Filtering Density of States Switch

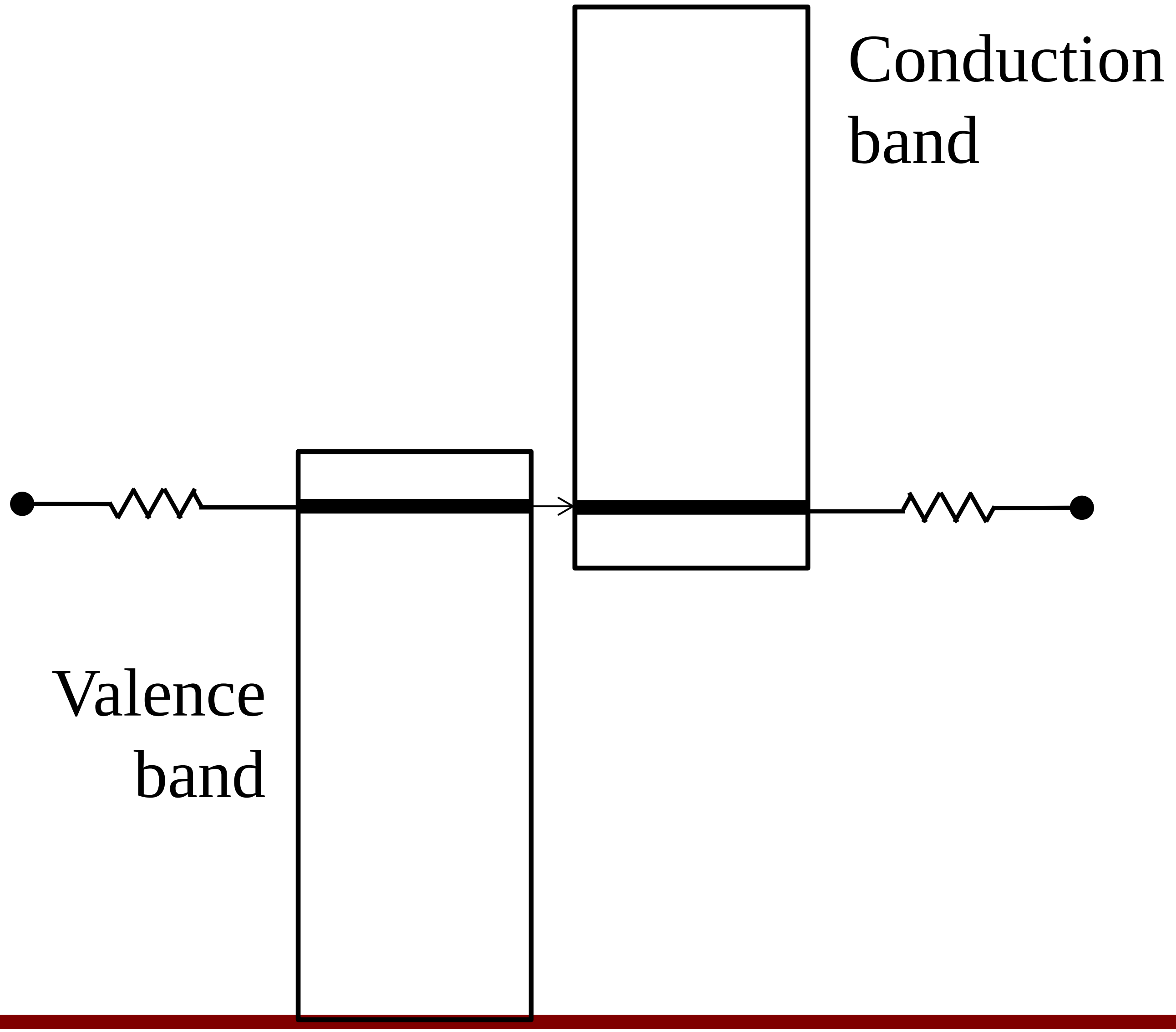


Band Tails Prevent a Steep Swing

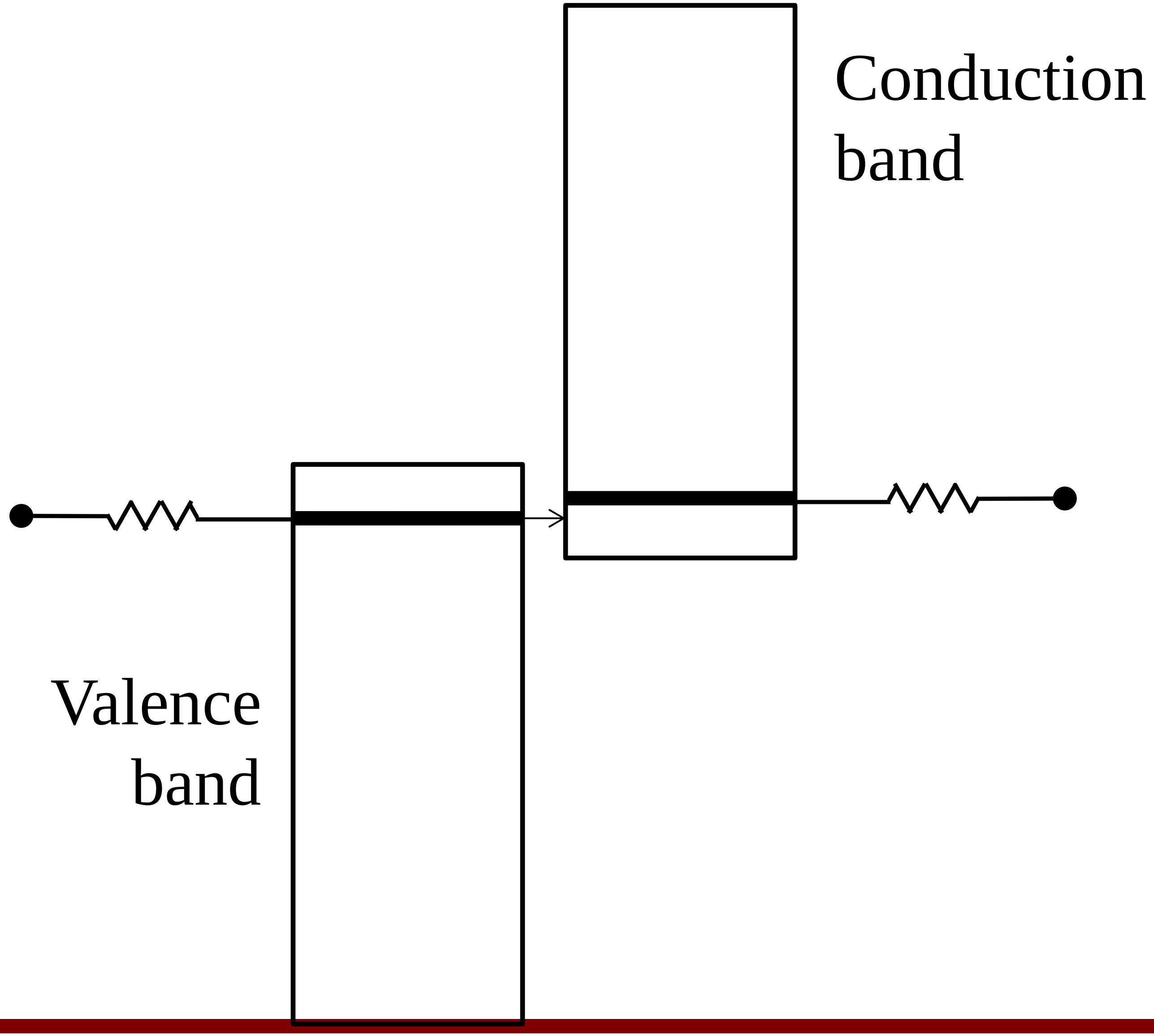
There are states below the band edge that prevent the junction from turning off



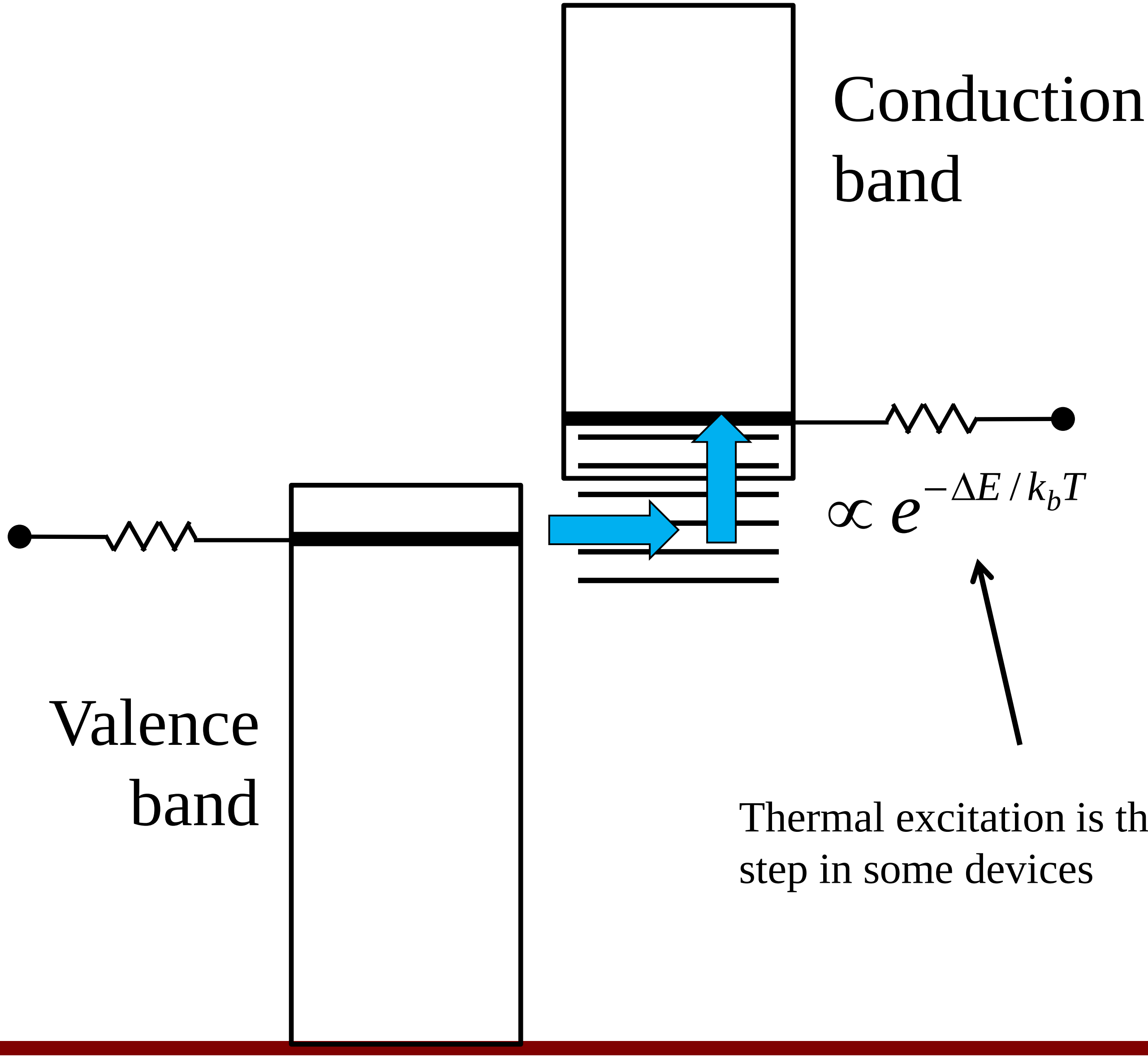
Switching Principle:



Switching Principle:



A problem arises from states where they should not be:



Thermal excitation is the rate limiting step in some devices

Interface Traps are Disastrous

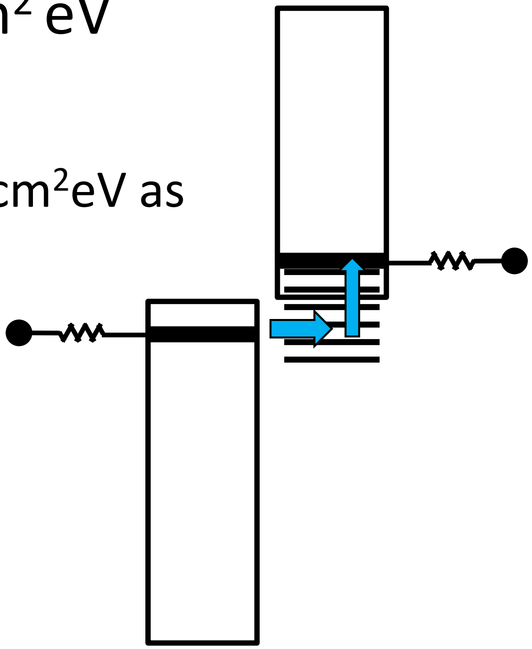
- Desired: Band-to-Band Tunneling –

  Quantum Density of States ~10^{12}/cm^2 eV

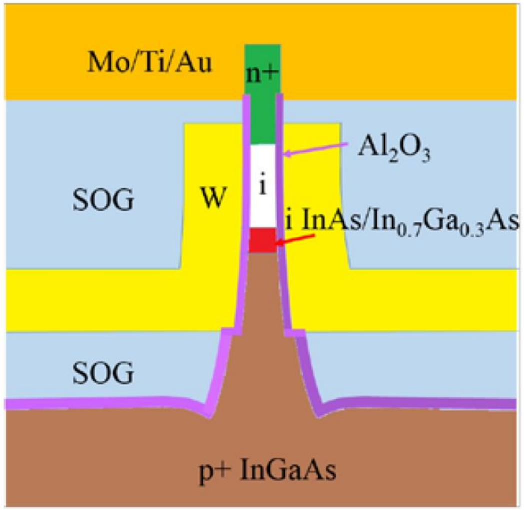
- Undesired: Tunneling into gate insulator States

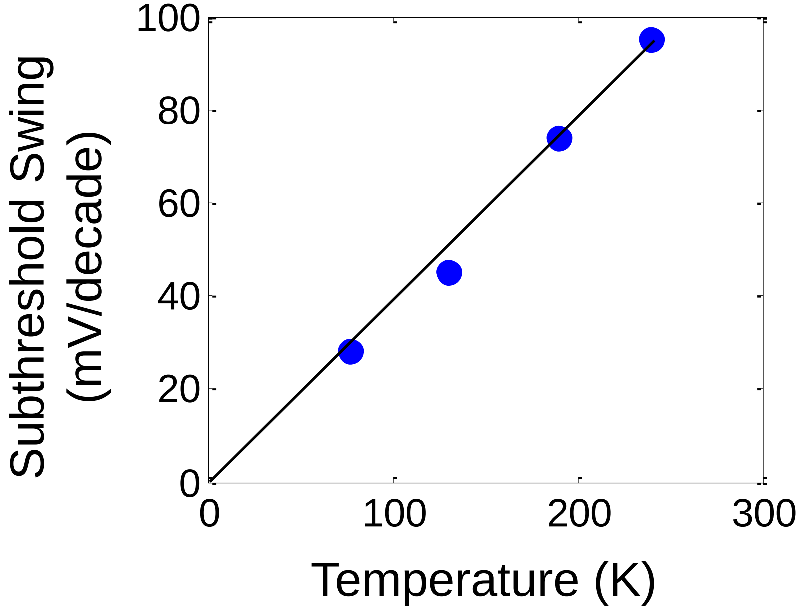
  D_{IT} ~ 10^{11}/cm^2 eV

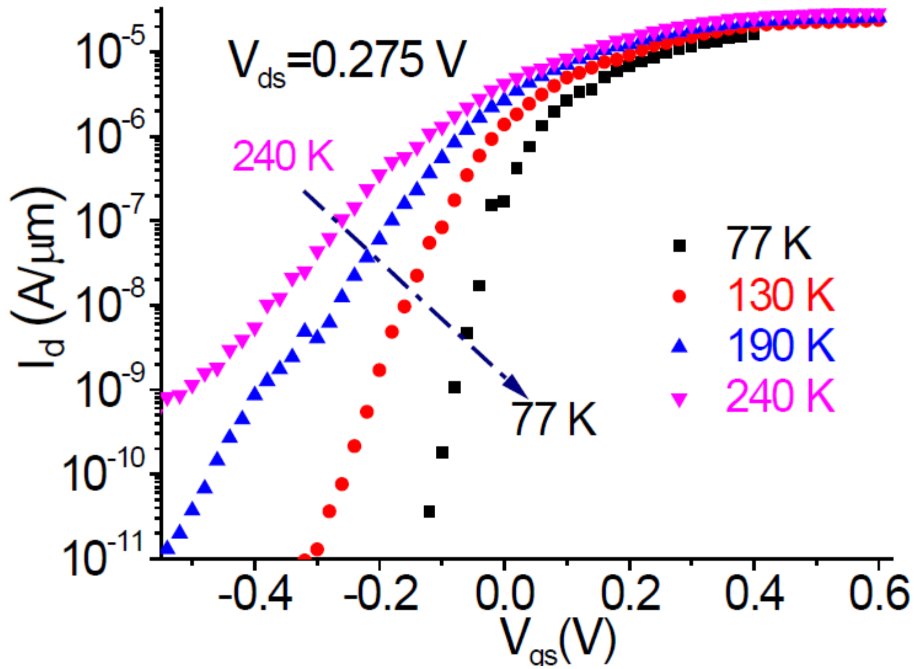
- Interface state density might have to be lowered < 10^8/cm^{2}eV as one of many pre-requisites to get a good On/Off ratio.
- This translates also into purity and reproducibility



Thermally Activated Tunneling

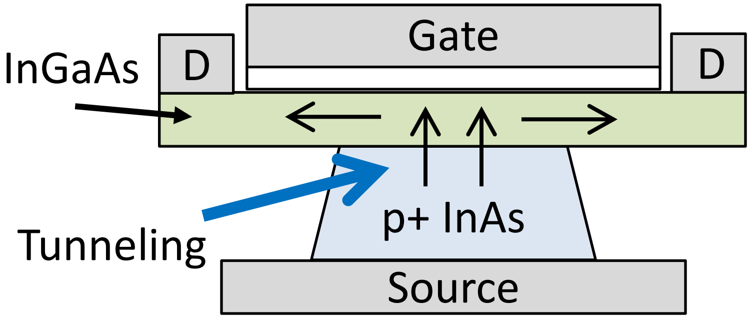


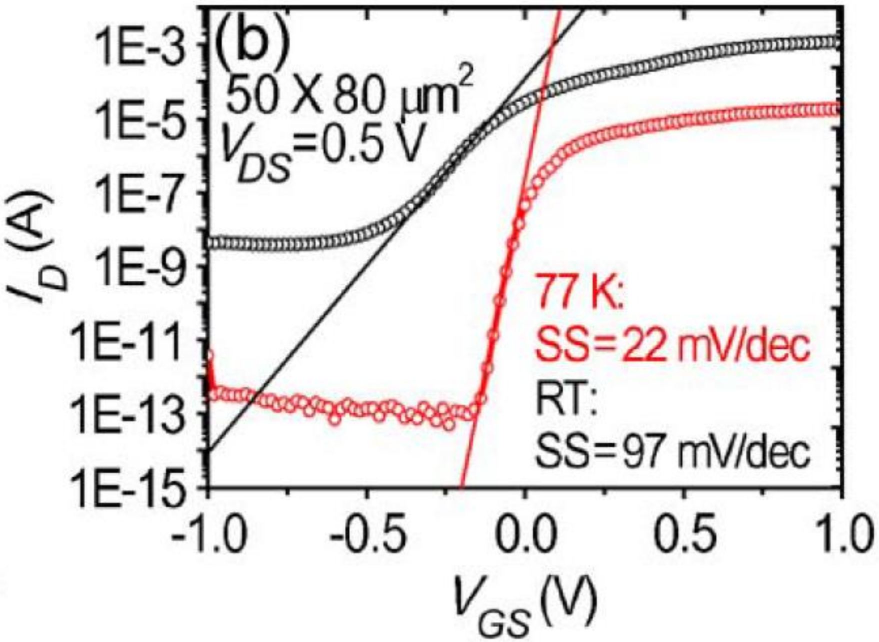


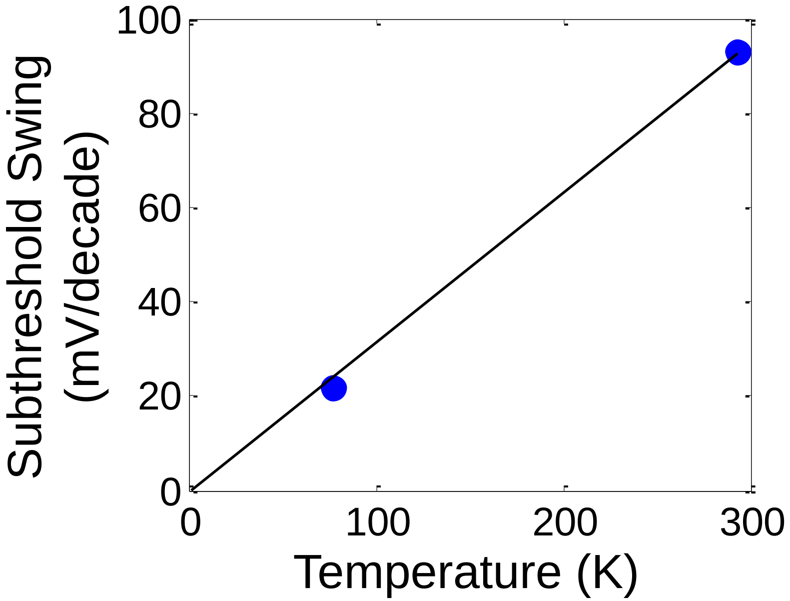


Zhao, Vardi, del Alamo, IEDM 2014

Thermally Activated Tunneling

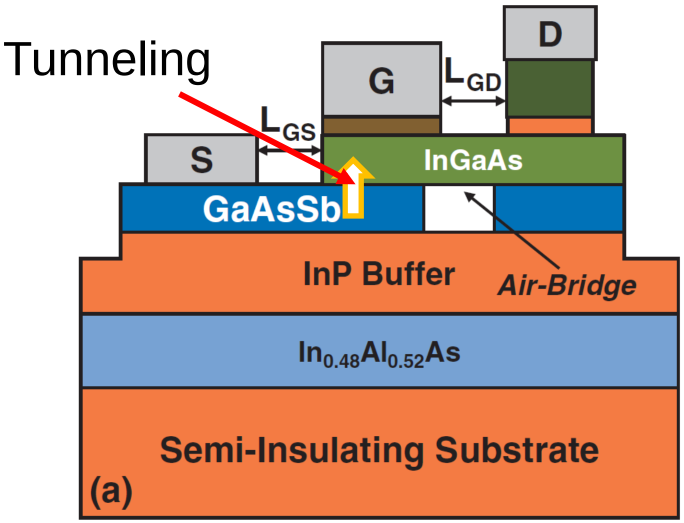


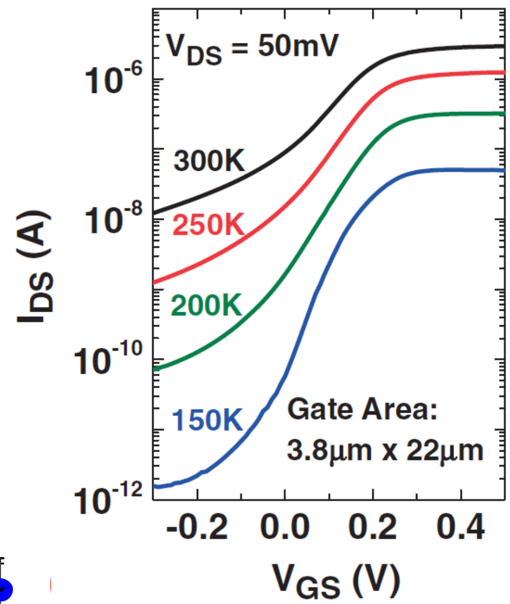


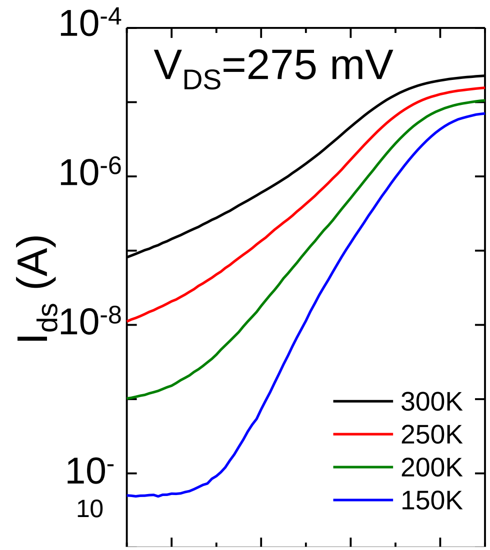


Guangle Zhou, et all, IEEE EDL 2012

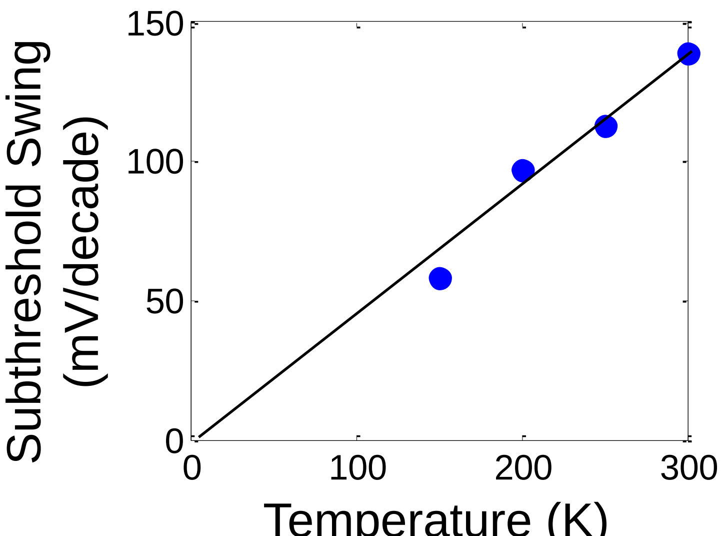
Thermally Activated Tunneling





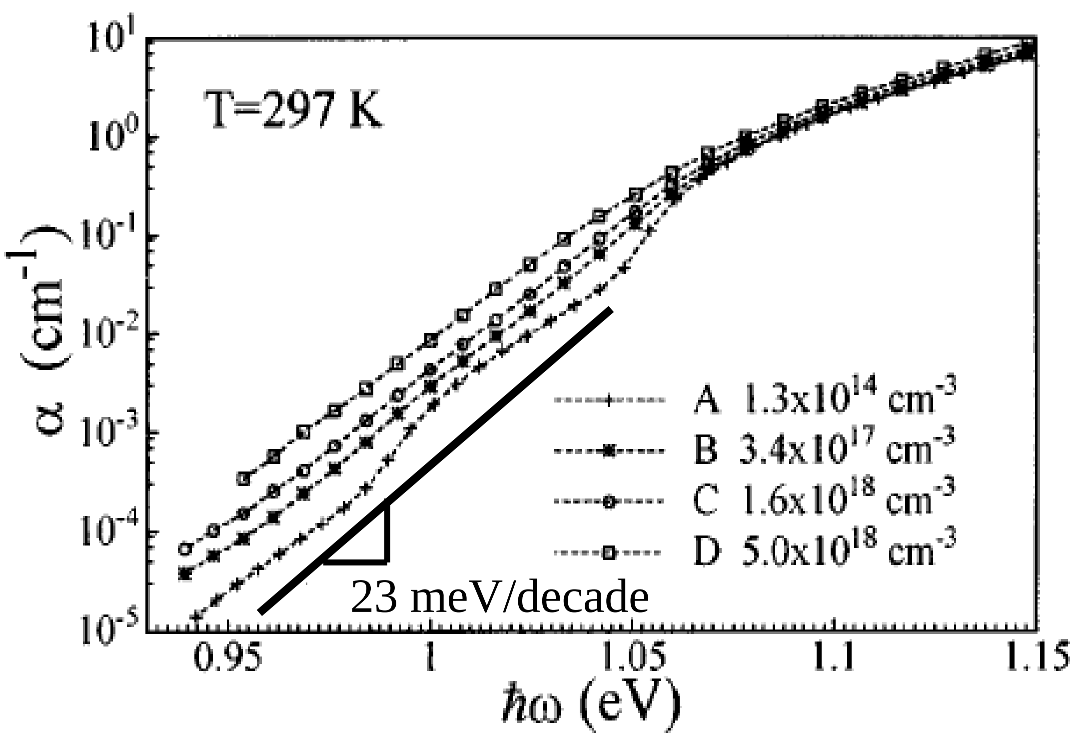


V_{gs} (V) 3.8 um x 22 um

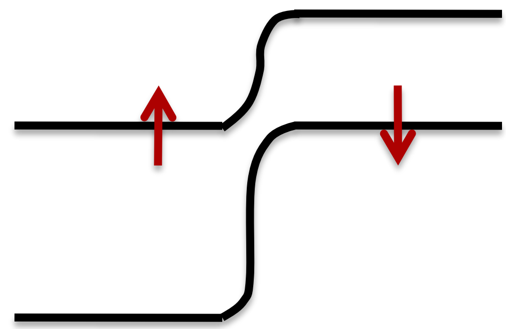


T. Yu, J. T. Teherani, D. A. Antoniadis, J. L. Hoyt, Applied Physics Express 2014

Use Optical Absorption Measurements to Measure the Band Edge Density of States



The absorption curves of Silicon at different doping levels



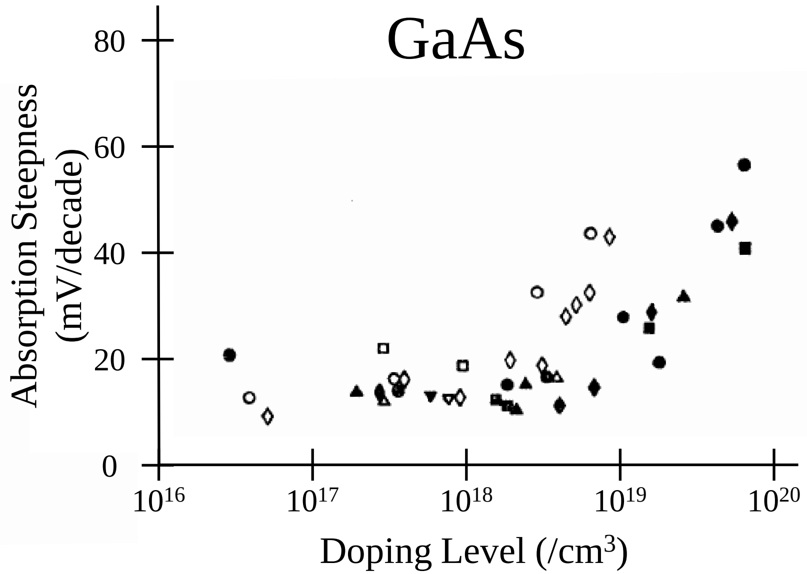
$\alpha(h\nu) \sim \exp\{(h\nu - E_g)/E_o\}$

$E_o \sim 10$meV for Silicon

~ 23 meV /decade

E. Daub and P. Wurfel, *Journal of Applied Physics,* vol. 80, pp. 5325-5331, 1996.

Optical Absorption Slope Gets Worse With Doping



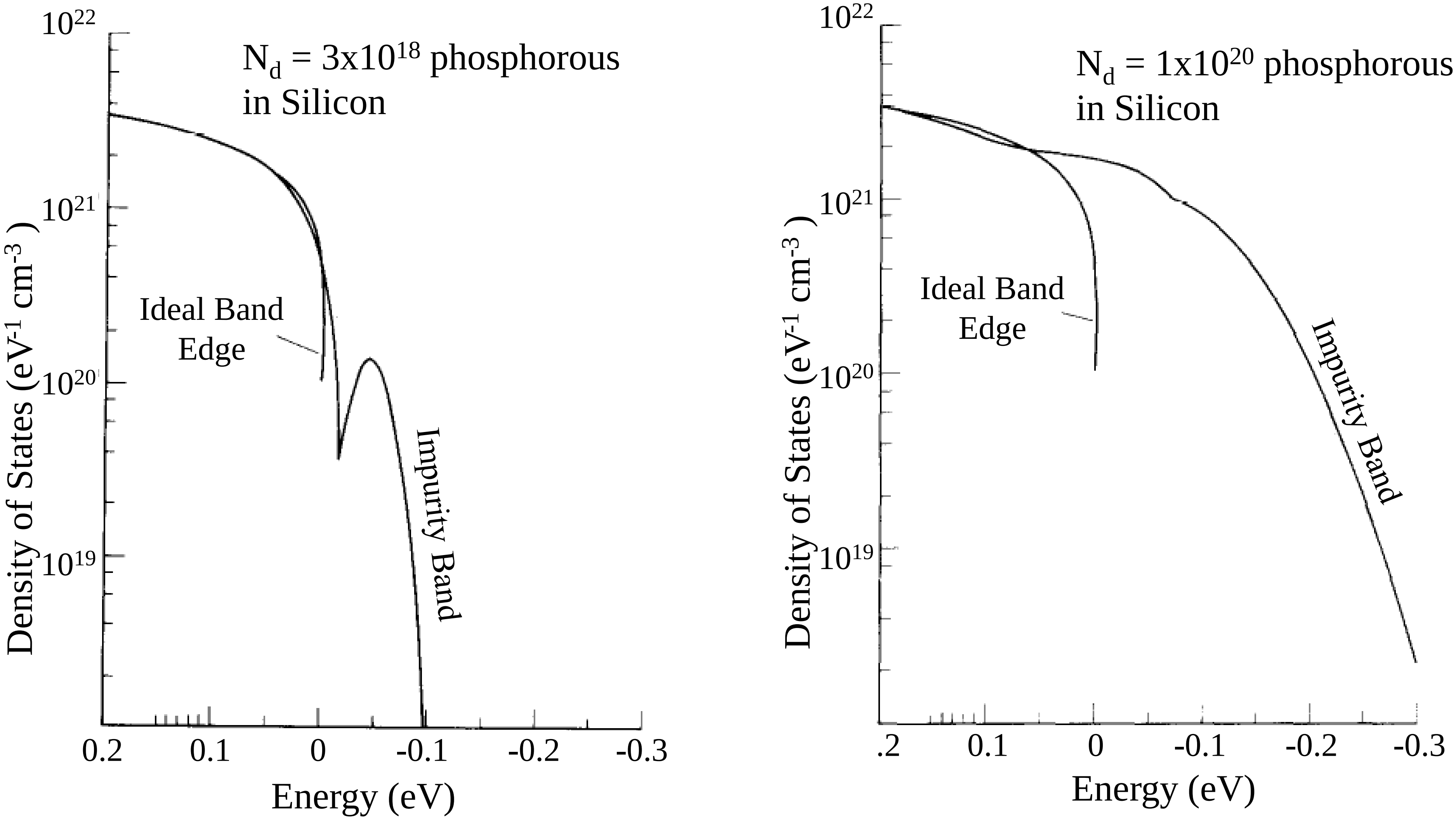
J. I. Pankove, "Absorption Edge of Impure Gallium Arsenide" *Physical Review*, vol 140 pp A2059-A2065, 1965

Undoped
~ 17 mV/decade

Heavily Doped
~ 60 mV/decade

The doping induced potential variations are screened by free carriers. The slope will be far worse in a depletion region

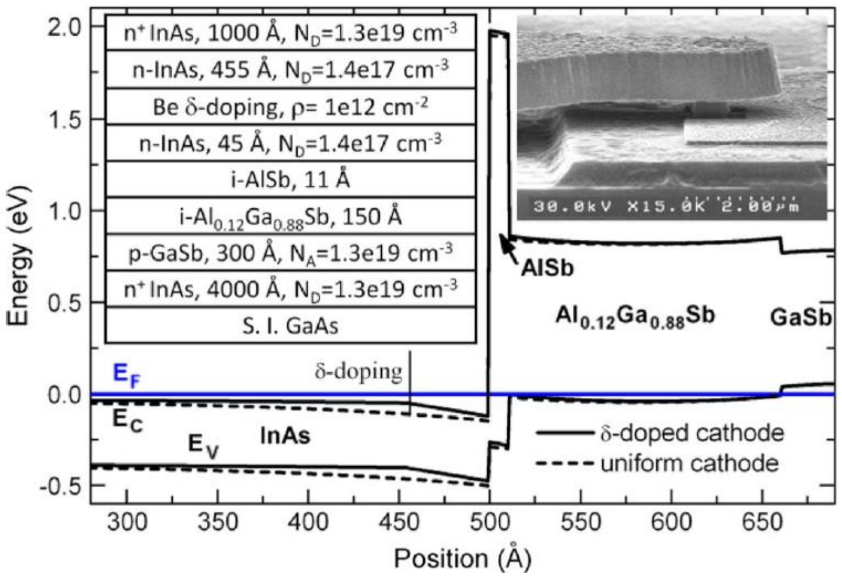
What's Going on?



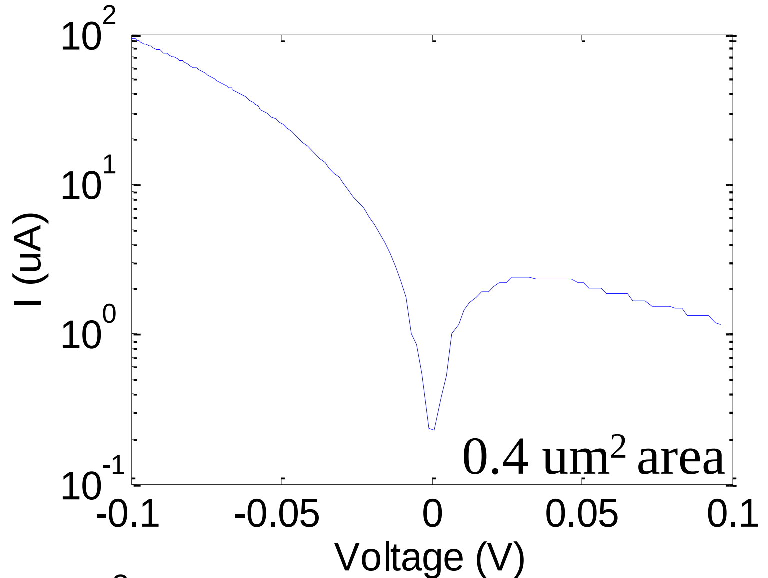
Kleppinger and Lindholm, Solid State Electronics Vol 14, pp 407-416 (1971)

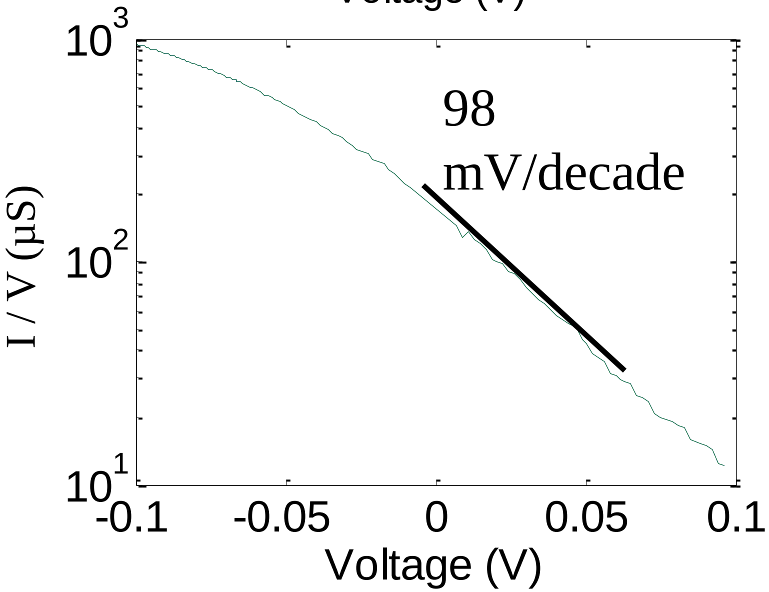
Analyze the Diode Conductance to Measure Steepness

InAs / AlGaSb Backward Diode

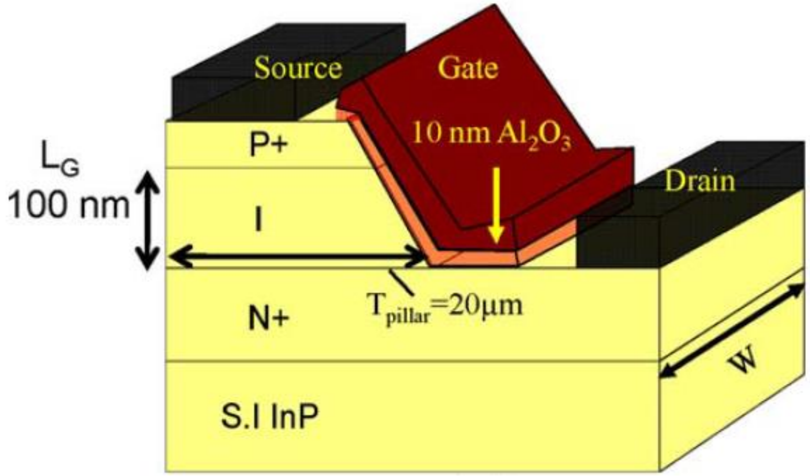


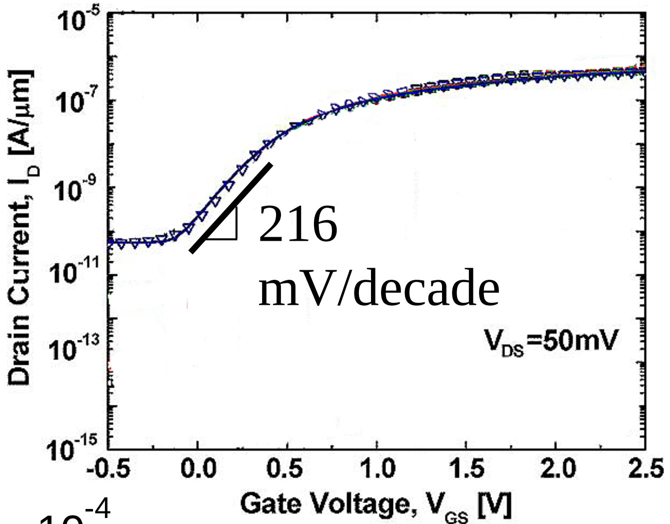
Zhang, Rajavel, Deelman, and Fay (2011)

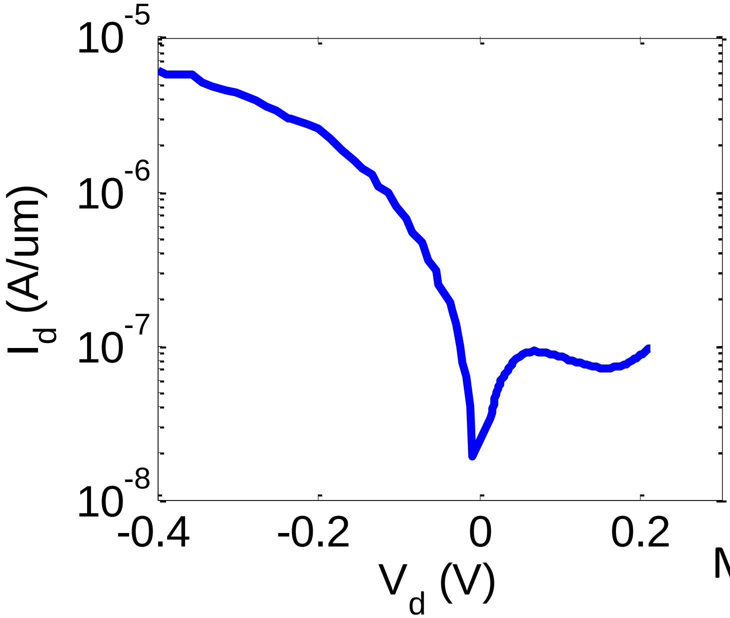




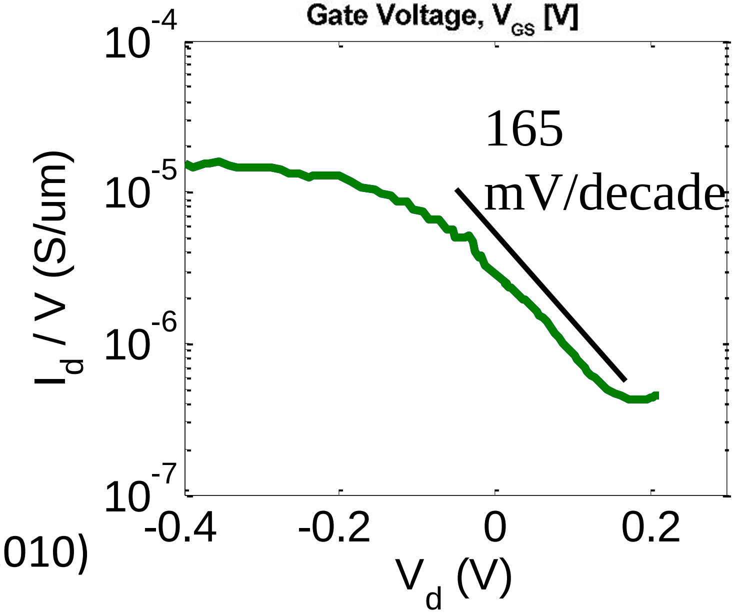
$In_{0.53}Ga_{0.47}As$ PIN Diode Characteristics Steeper than TFET!



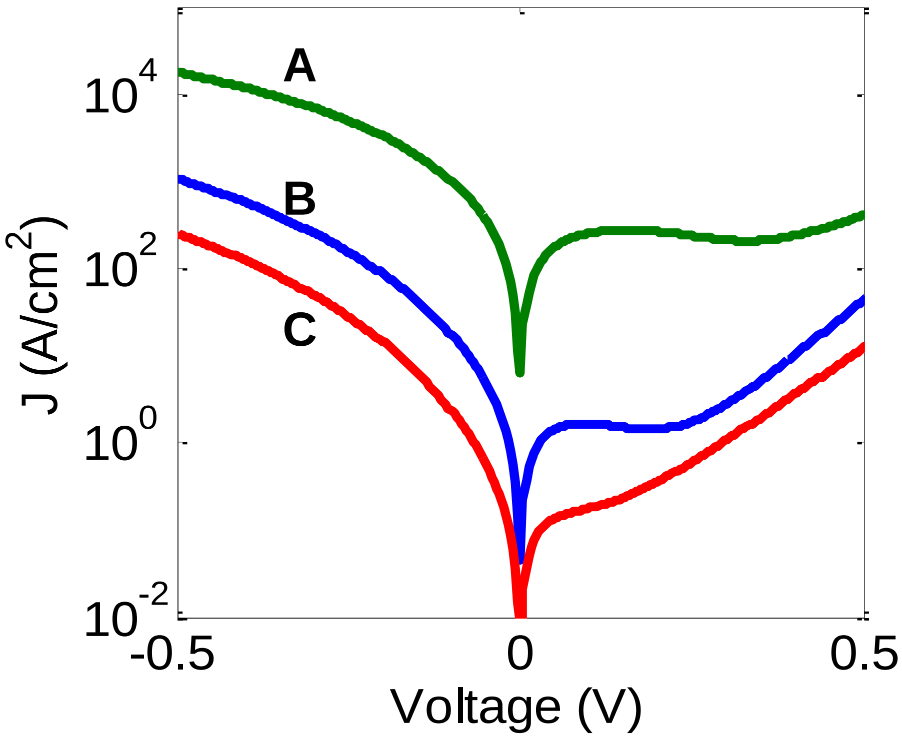


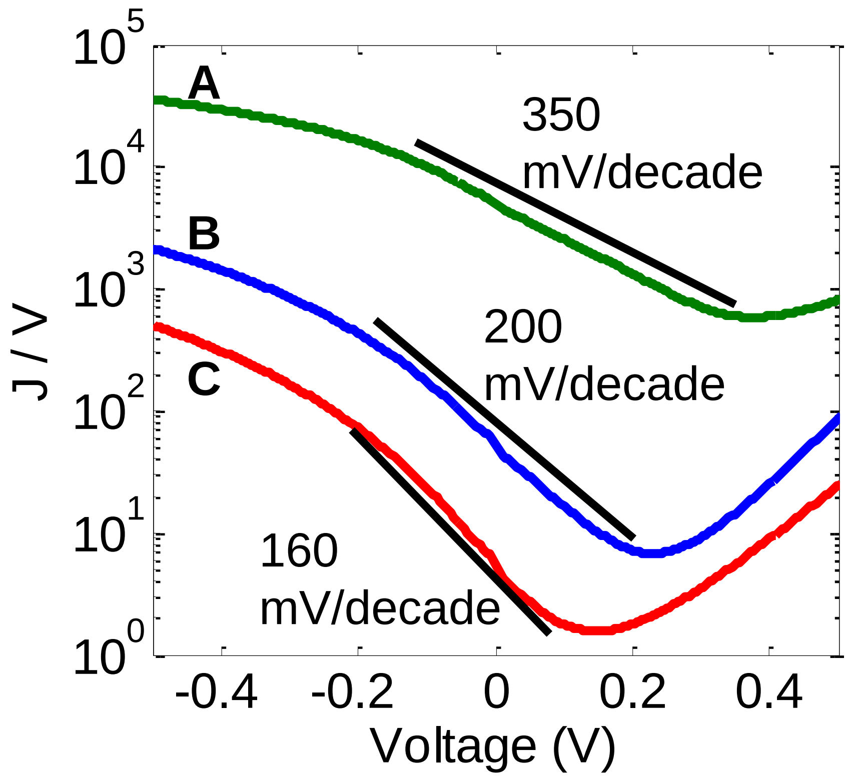


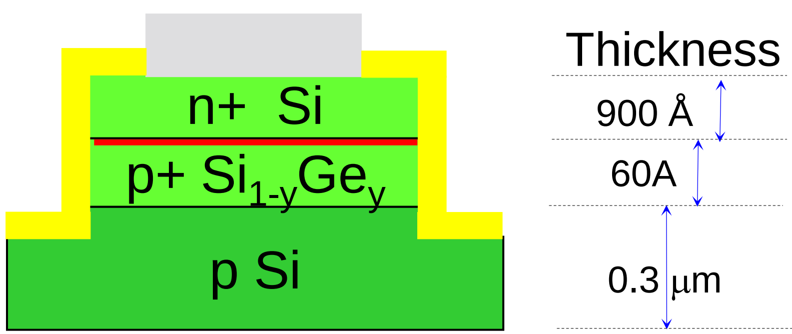
Mookerjea, (2010)



SiGe Epi Diodes Steeper at Lower Doping



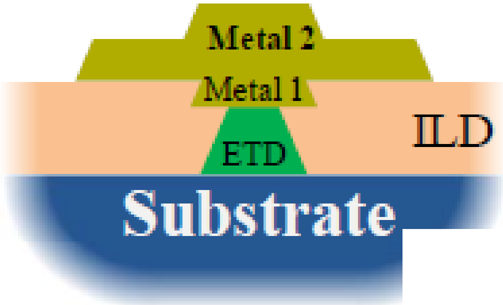




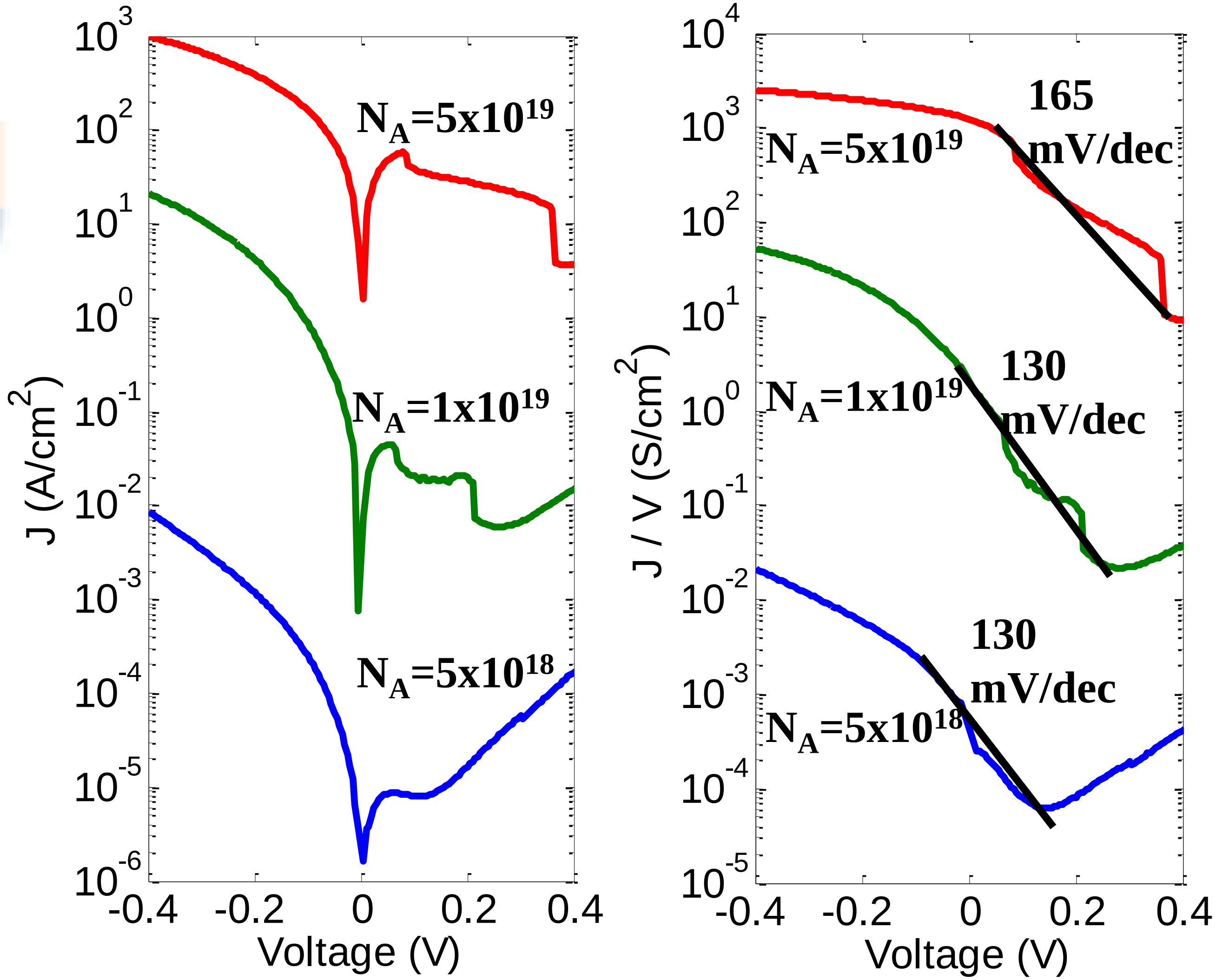
(A) 5e19/3e20/3e19 n+/p+/p
(B) 1e19/1e20/3e19 n+/p+/p
(C) 1e19/1.5e20/1e17 n+/p+/p

GaAs Homojunction Diodes

Sandia National Laboratories

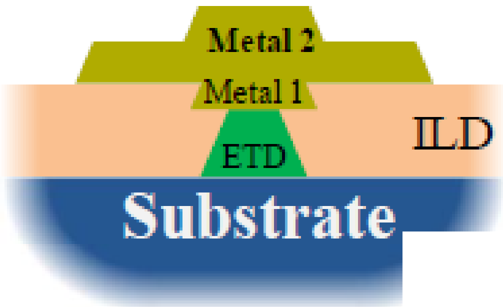


N_D=3x10^{19}

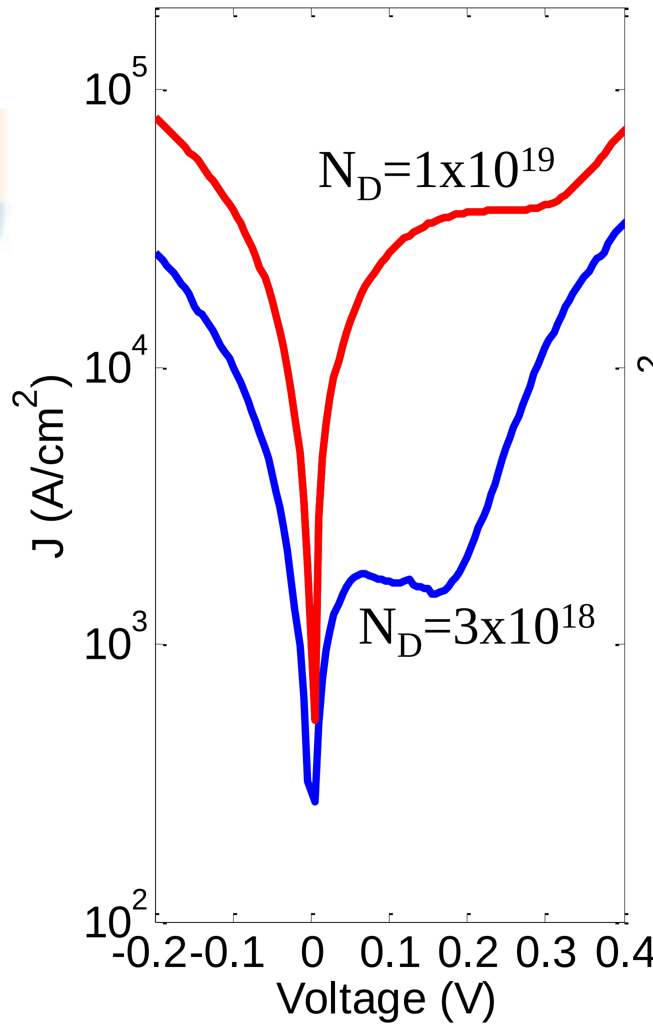


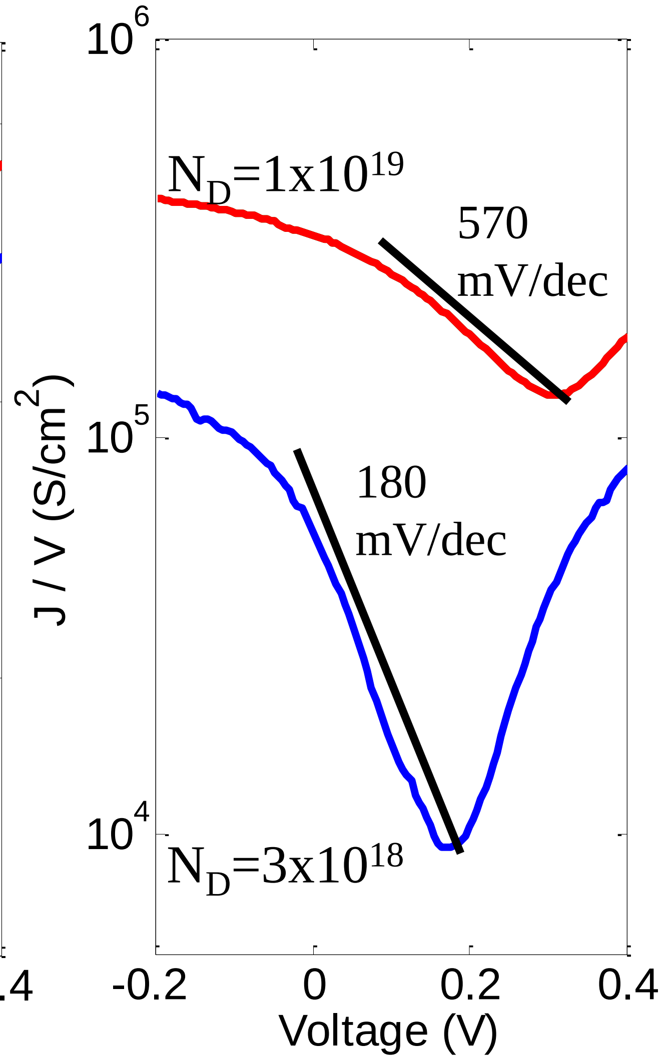
From Pawlik et all, "Benchmarking and Improving III-V Esaki Diode Performance with a Record 2.2 MA/cm2 Peak Current Density to Enhance TFET Drive Current" IEDM 2012, pp. 812-814

InAs Homojunction Diodes



N_A=1.8x10[19]

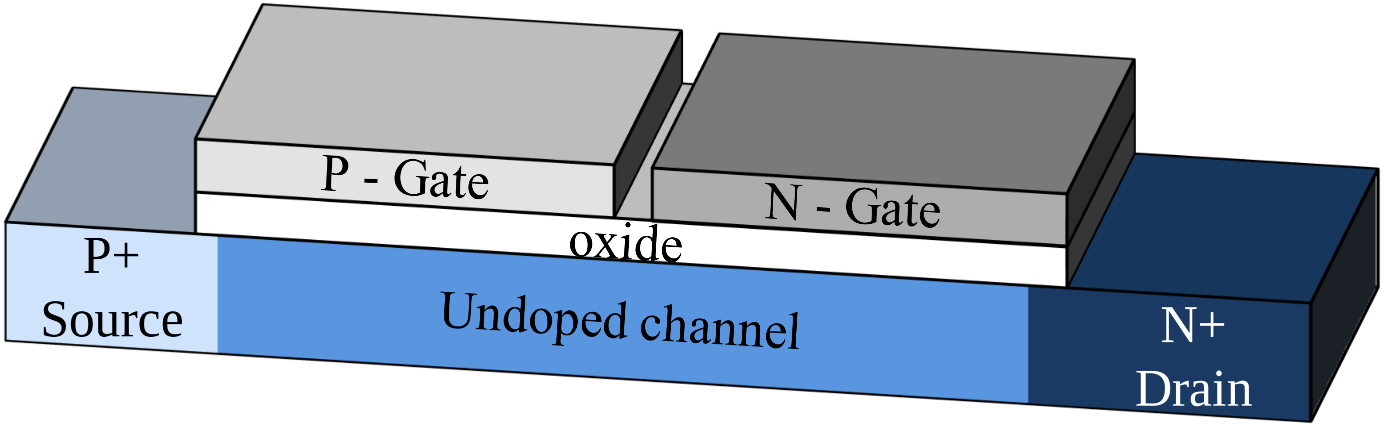


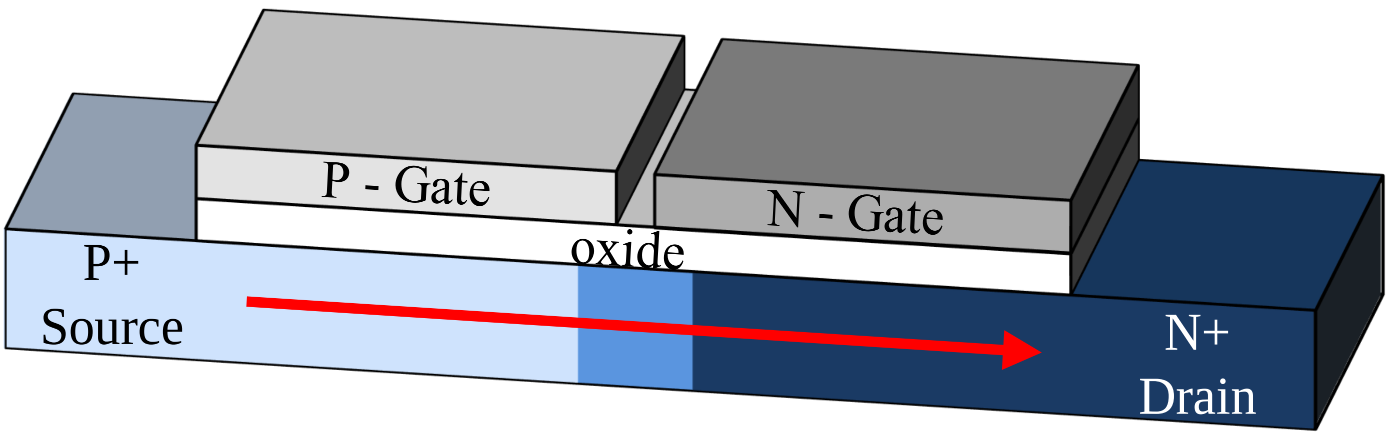


From Pawlik et all, "Benchmarking and Improving III-V Esaki Diode Performance with a Record 2.2 MA/cm2 Peak Current Density to Enhance TFET Drive Current" IEDM 2012, pp. 812-814

How to Eliminate Doping

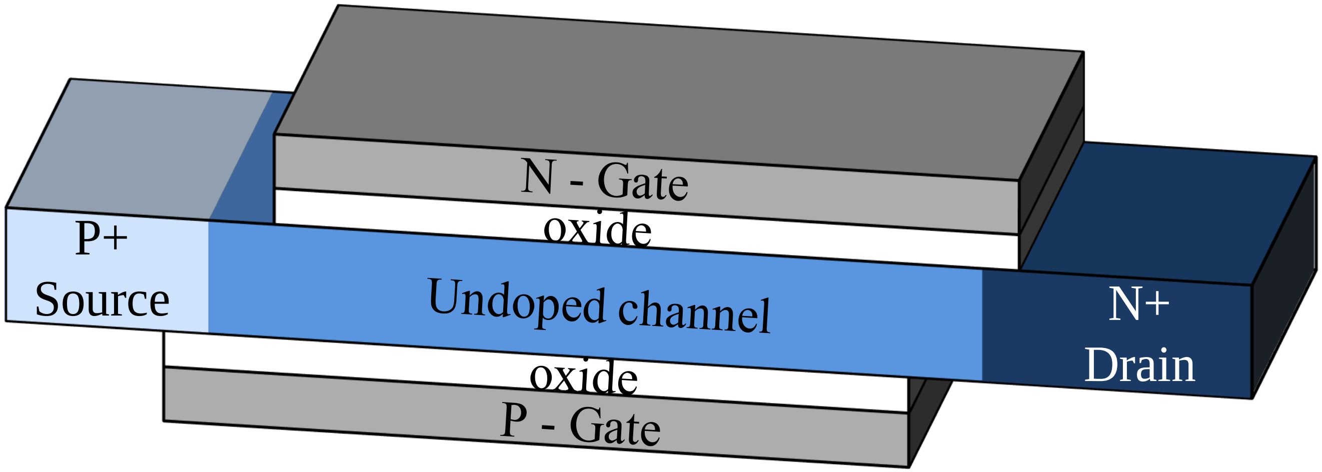
Lateral Double Gate TFET

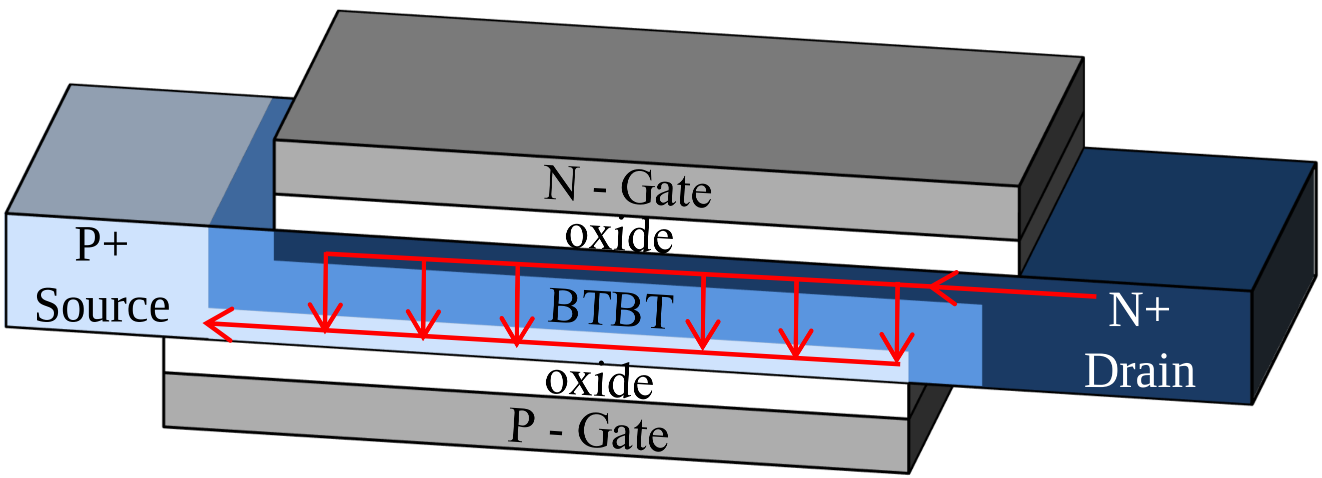




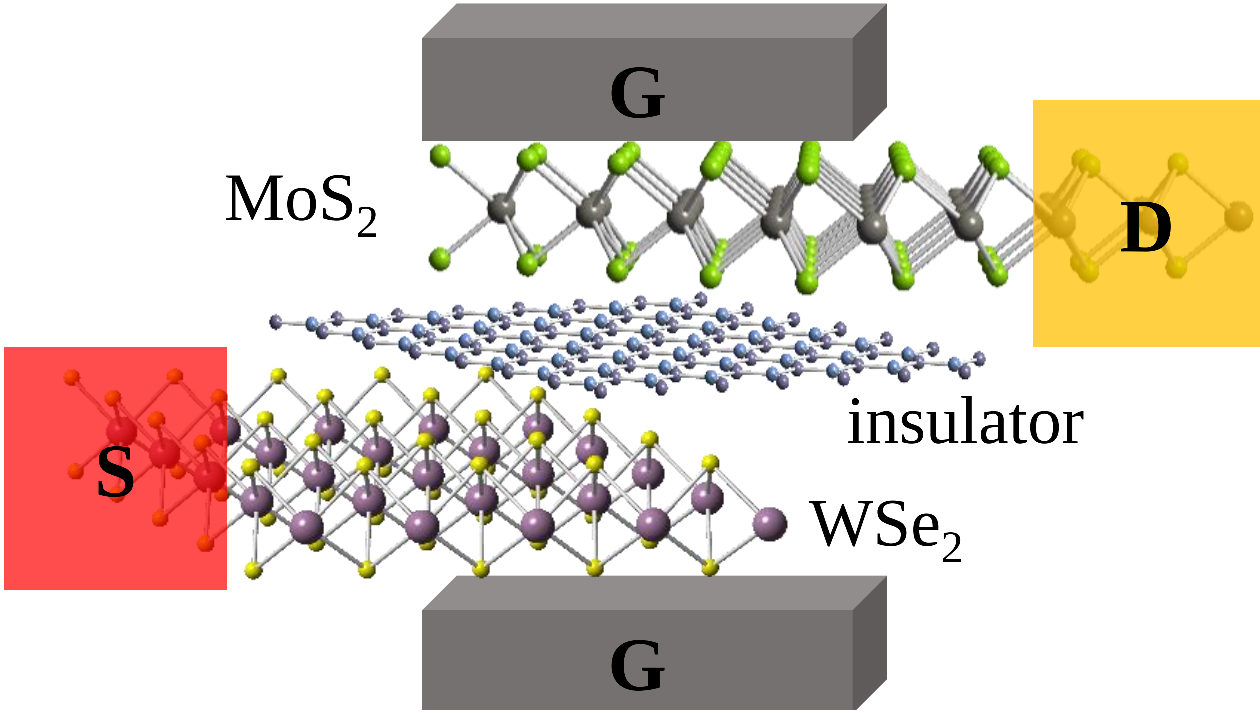
How to Eliminate Doping

Bilayer TFET



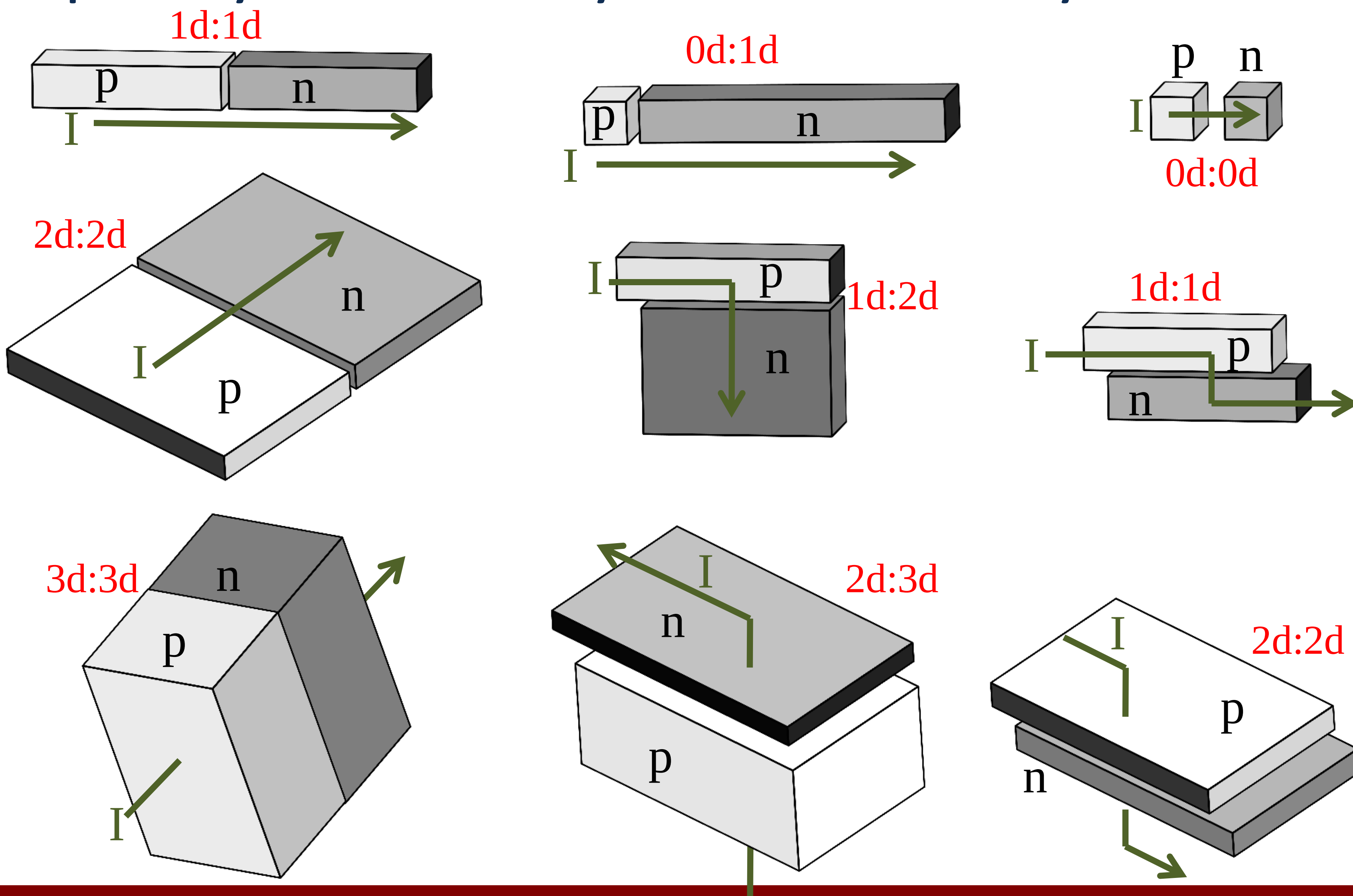


Layered chalcogenides: atomic level flatness and new opportunities



- Scalable down to a single monolayer (~ 7 Angstroms)
- Lack dangling bonds; no native oxide
- van der Waals bonding/interfaces – reduced lattice matching constraints
- Uniform thickness at the atomic level – sharp band edges

An Ideal Density of States Switch is Explicitly Affected by Dimensionality:



Fermi's Golden Rule Approach

$$I = \sum_{k_x, k_y, k_z} \frac{4q\pi}{\hbar} \left| M_{fi} \right|^2 \delta(E_i - E_f)$$

Explicitly include conservation of transverse momentum

Now include all possible states

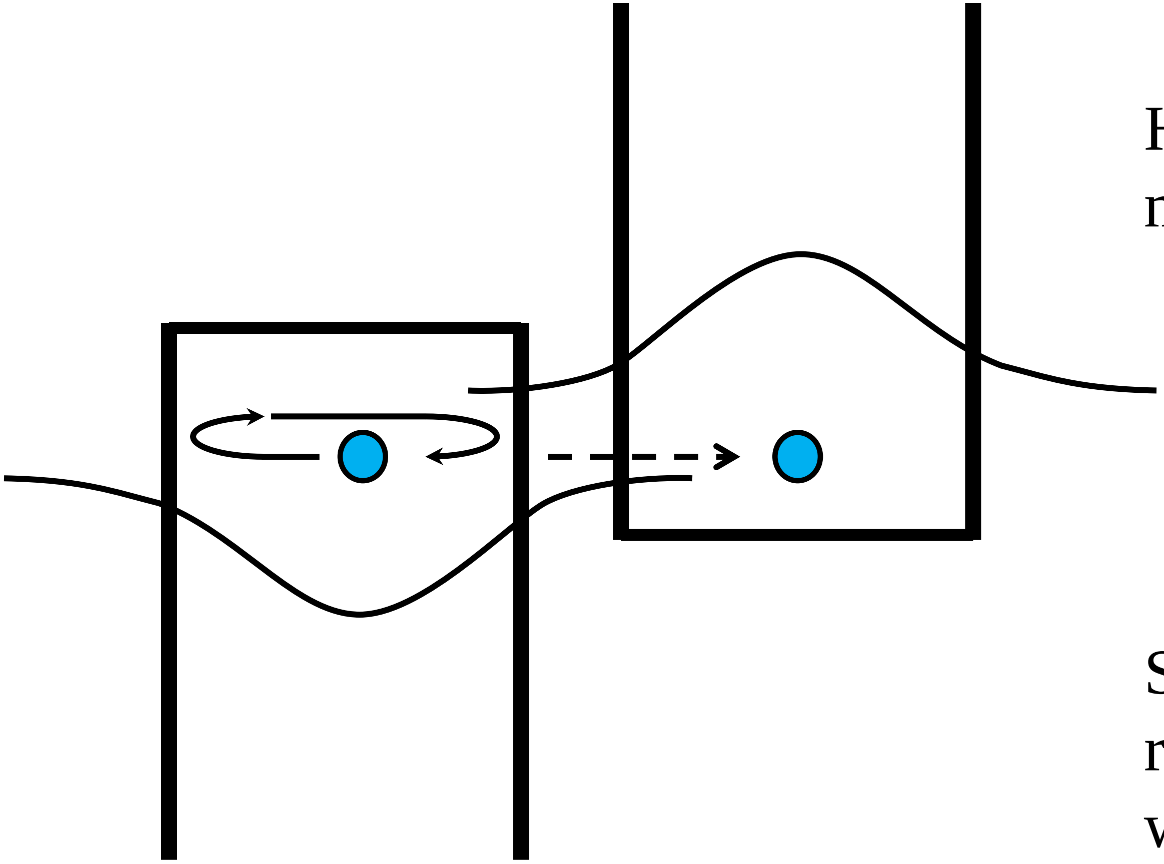
$$I = \sum_{\substack{k_{xi}, k_{yi}, k_{zi} \\ k_{xf}, k_{yf}, k_{zf}}} \frac{4q\pi}{\hbar} \left| M_{fi} \right|^2 \delta(E_i - E_f)\delta_{k_{xi}, k_{xf}} \delta_{k_{yi}, k_{yf}}$$

The number of sums is reduced for reduced dimensionality

$$\mathrm{M_{fi}} = \frac{\hbar^2}{2\mathrm{m}} \sqrt{\left(\frac{\mathrm{k_{zi} k_{zf}}}{\mathrm{L_{zi} L_{zf}}} \right)} \sqrt{\mathrm{T}}$$

References:
W. A. Harrison, "Tunneling from an independent-particle point of view," *Physical Review,* vol. 123, pp. 85-89, 1 July 1961.
C. B. Duke, *Tunneling in Solids*. New York: Academic Press, Inc, 1969.

Confinement in the Tunneling Direction Increases Conductance

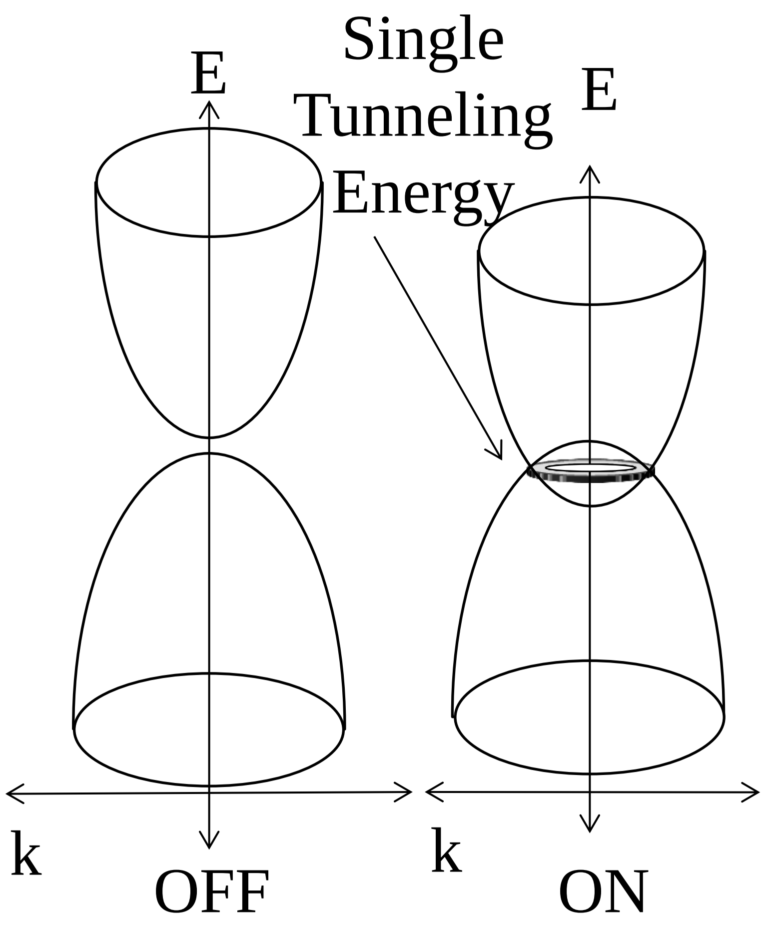


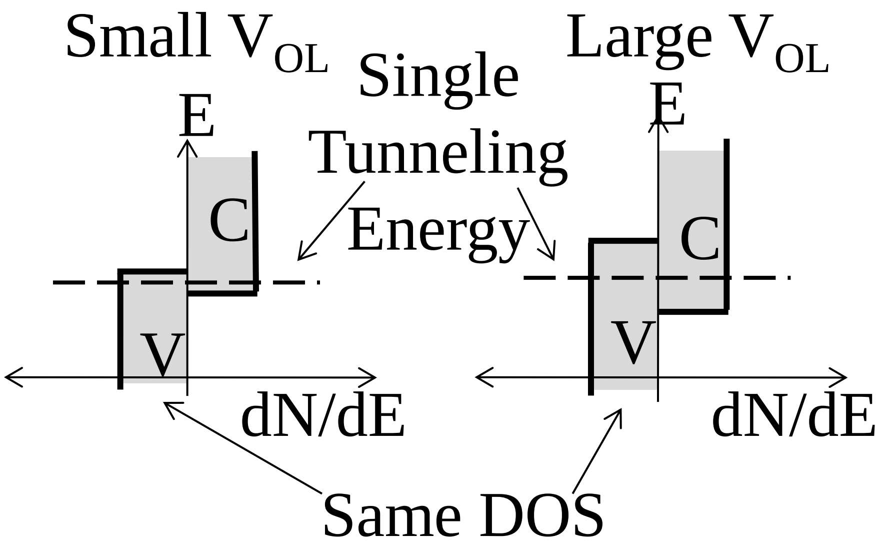
Higher energy results in more tunneling attempts

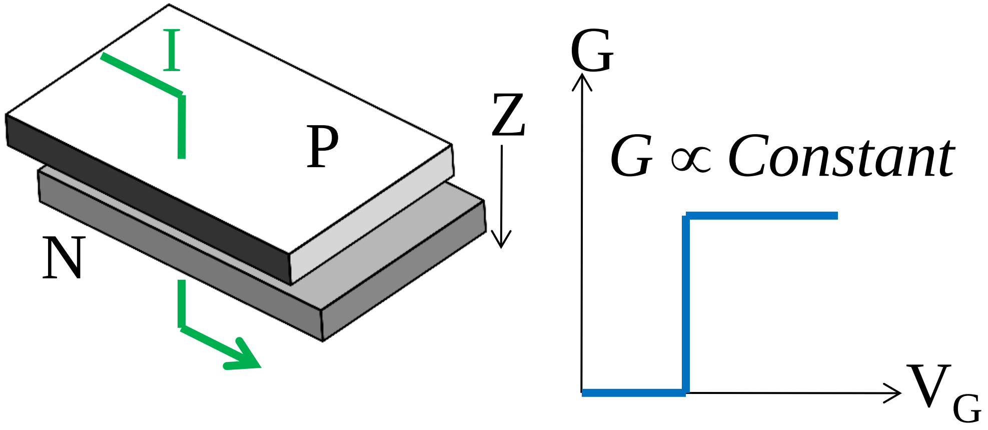
Smaller quantum well results in a larger wavefunction overlap

$$E_z = \frac{1}{2} m v_z^2$$

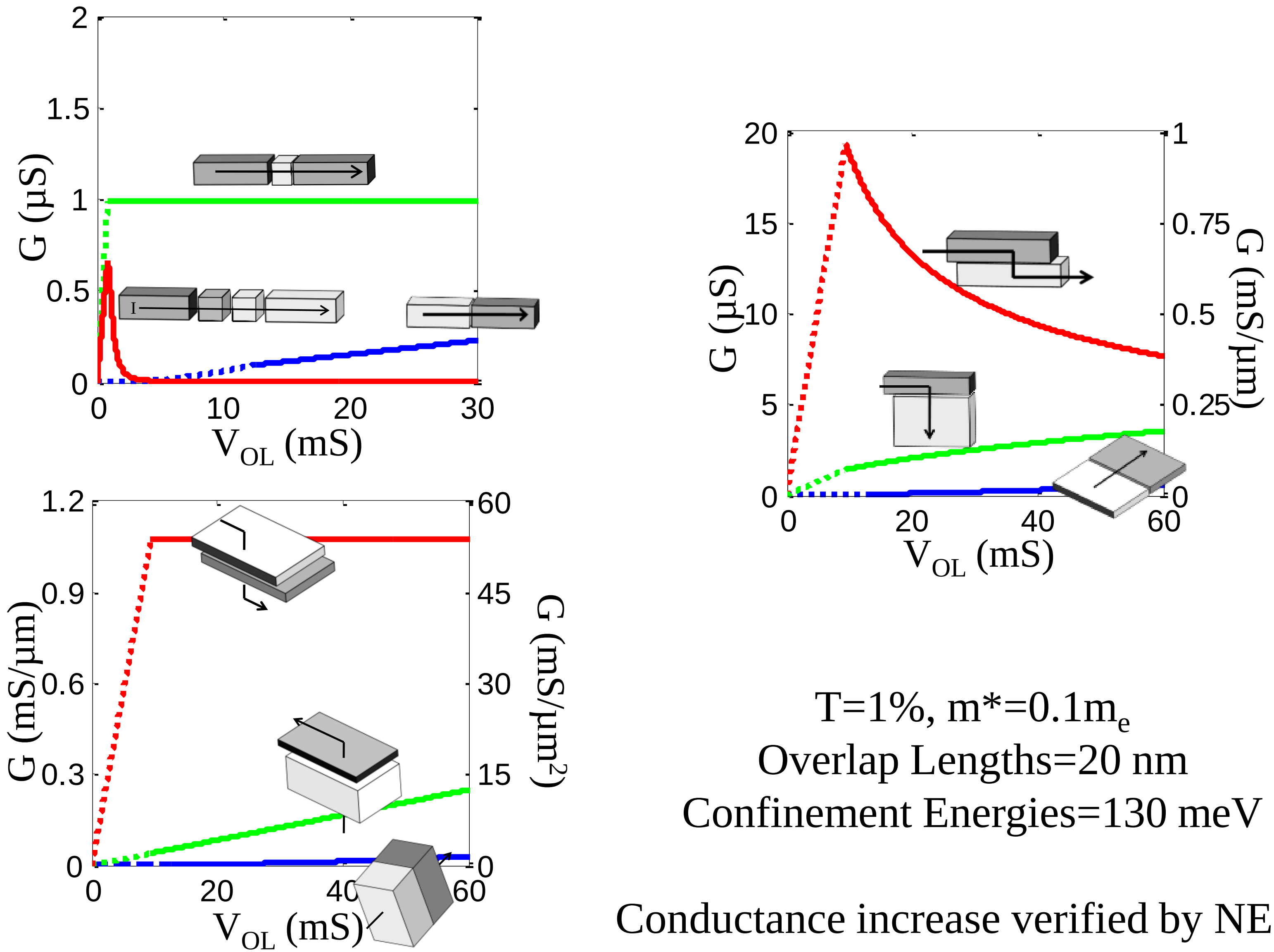
2d-2d Bilayer







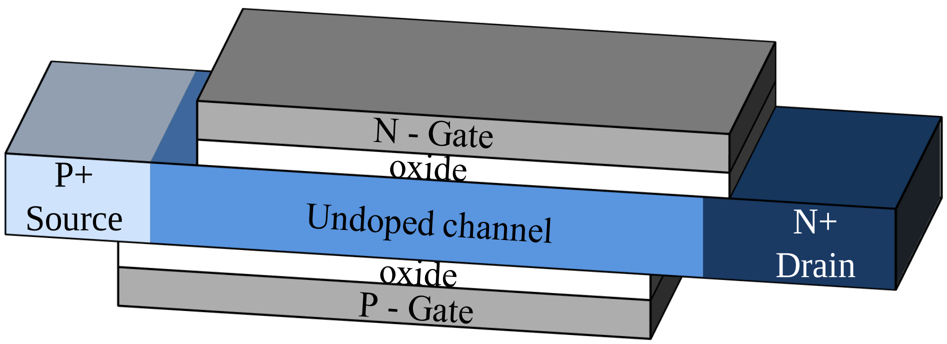
Compare the Dimensionalities

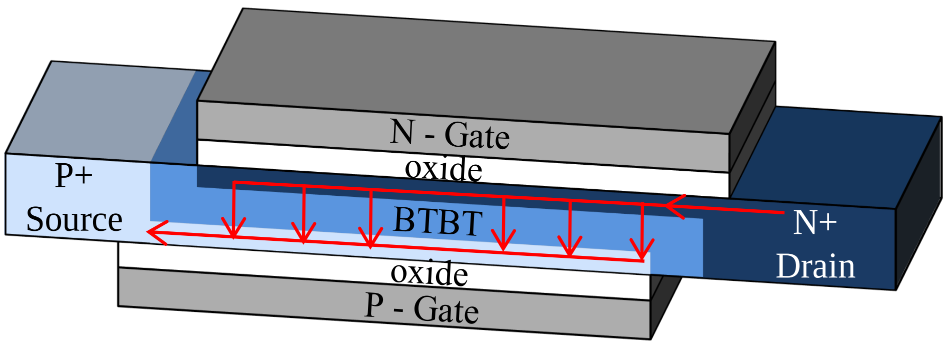


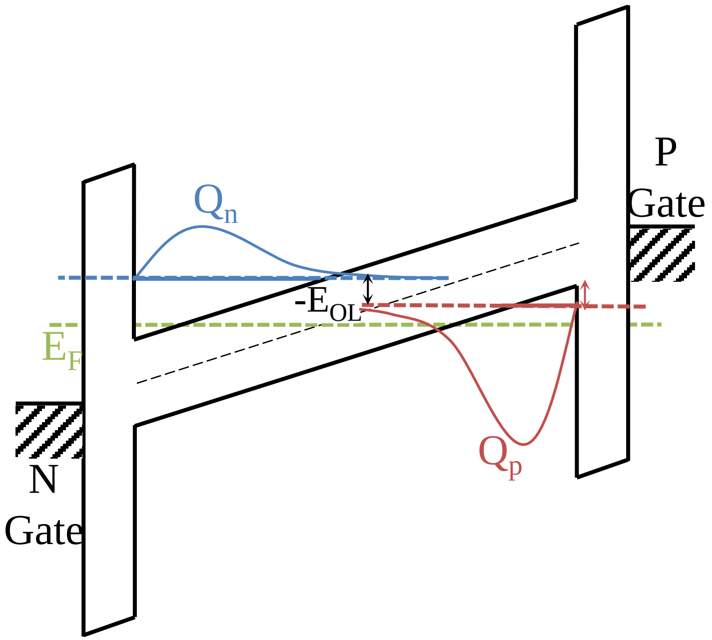
T=1%, $m^*=0.1m_e$
Overlap Lengths=20 nm
Confinement Energies=130 meV

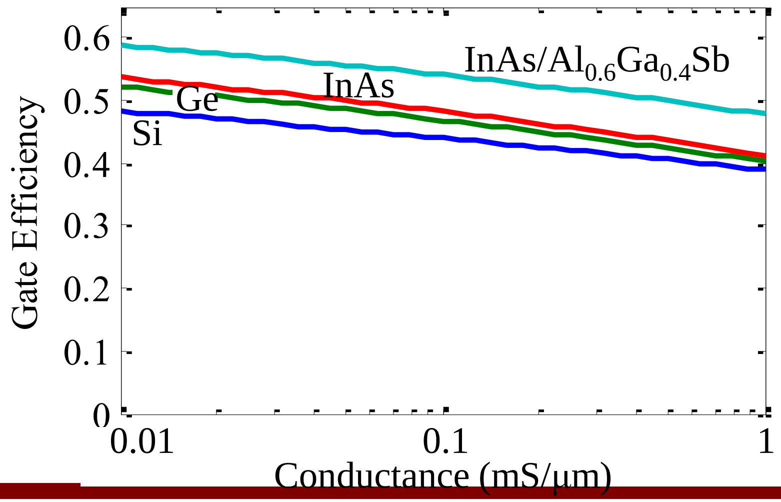
Conductance increase verified by NEGF

Putting it All Together: Bilayer TFET









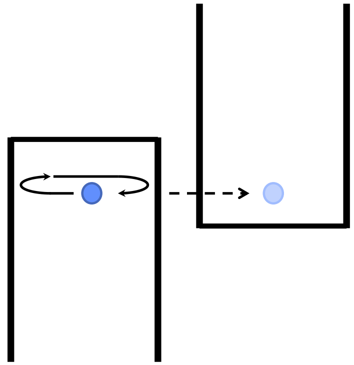
The Low Voltage TFET Demands Higher Perfection than Previously Required

- **Need a steep density of states to get a steep subthreshold swing**

- **Must drastically reduce the interface state trap density**
  - Quantum Well DOS ~10^{12}/cm^2 eV, D_{IT} ~ 10^{11}/cm^2 eV

- **No doping – use gates to electrostatically control the Fermi level**

- **Use Quantum Confinement**

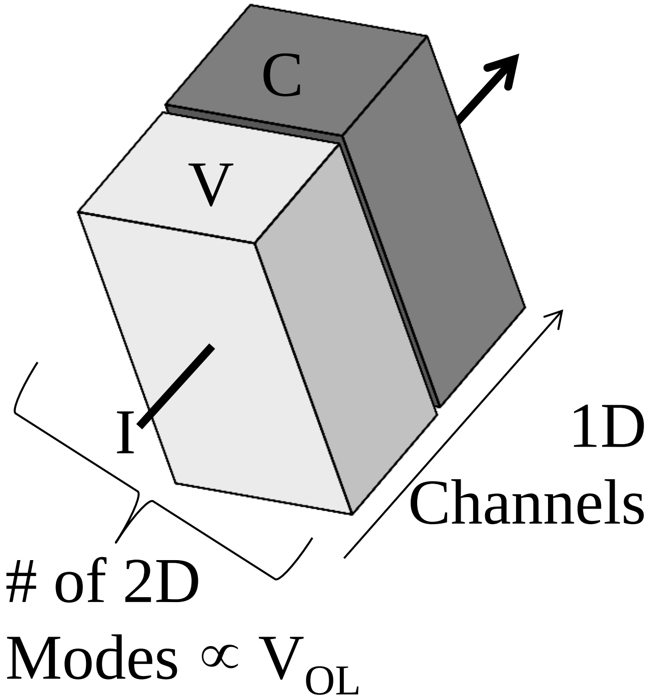


Reduce the voltage to < 100 mV

10X reduction in voltage
100X reduction in power

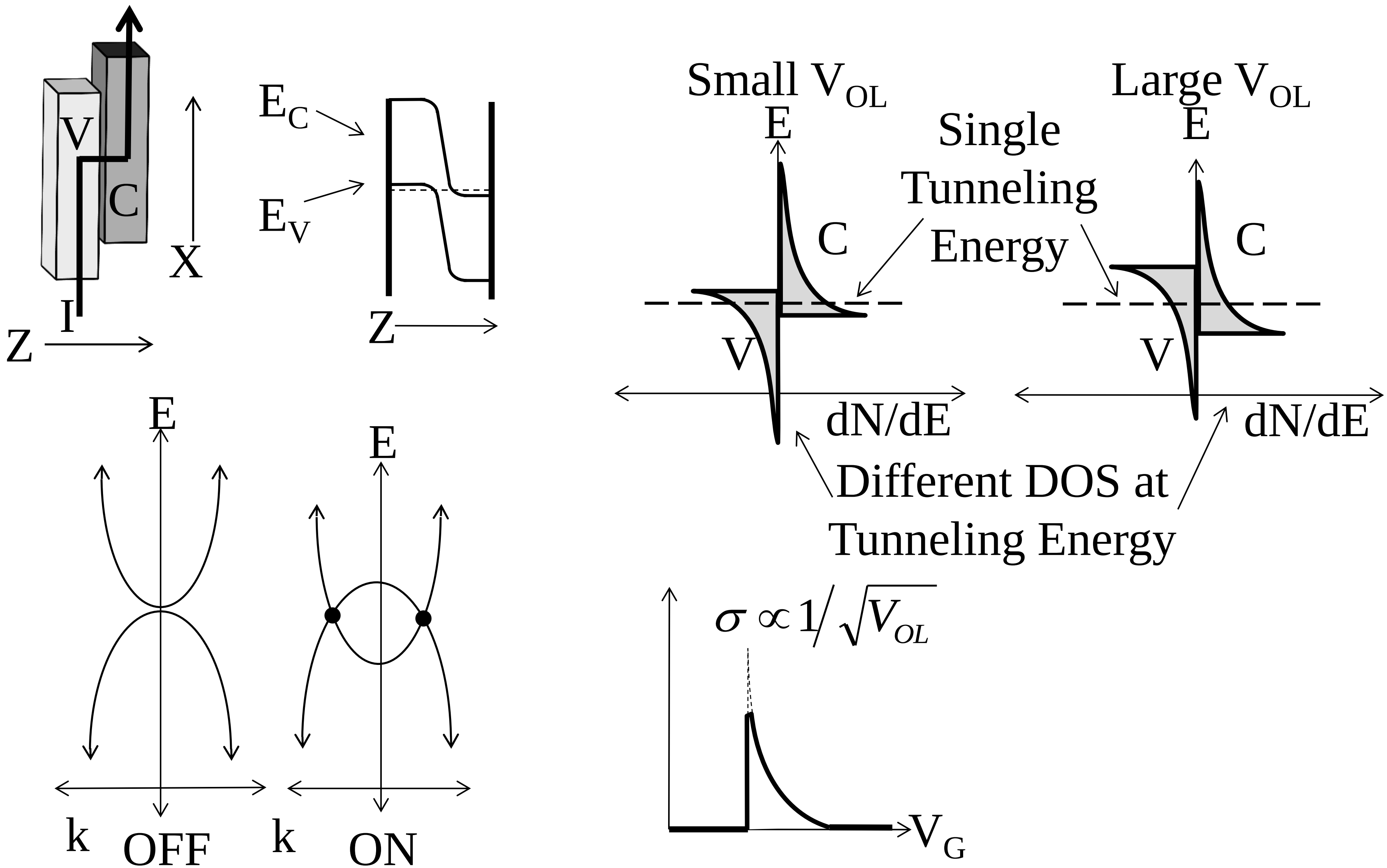
Extra Slides

3d-3d Tunneling

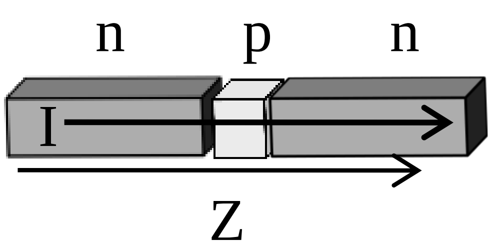


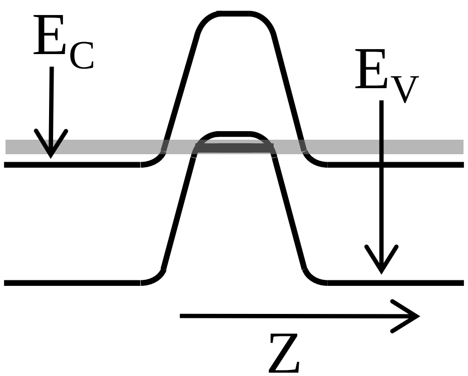
$$\partial I = N_{\perp \text{States}} \times \frac{2e}{h} \times T \times \left(f_c - f_{\text{v}}\right) \times \partial E$$

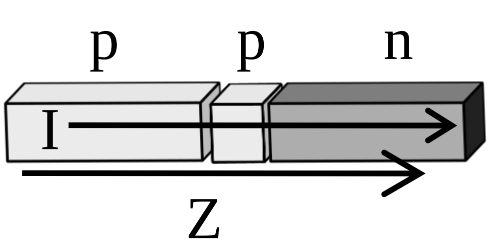
1d-1d Edge Overlap

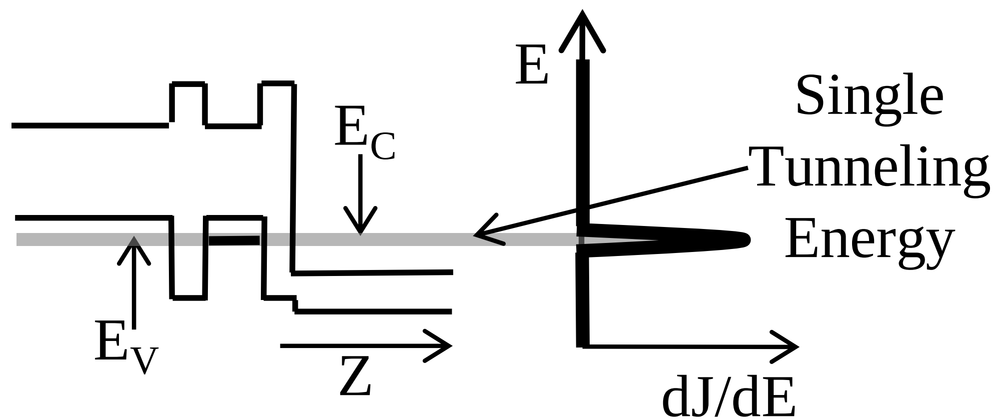


0d-1d Junction

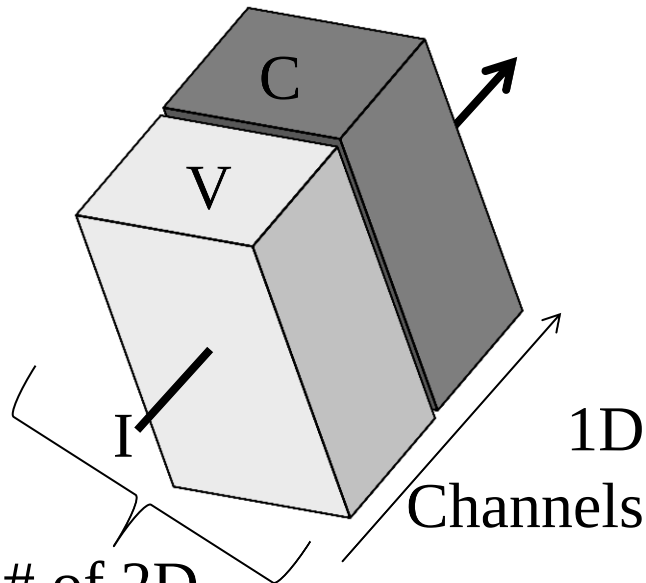




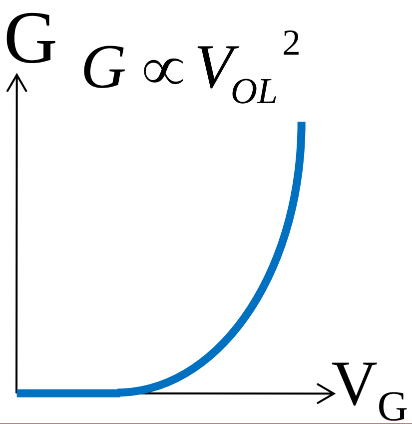


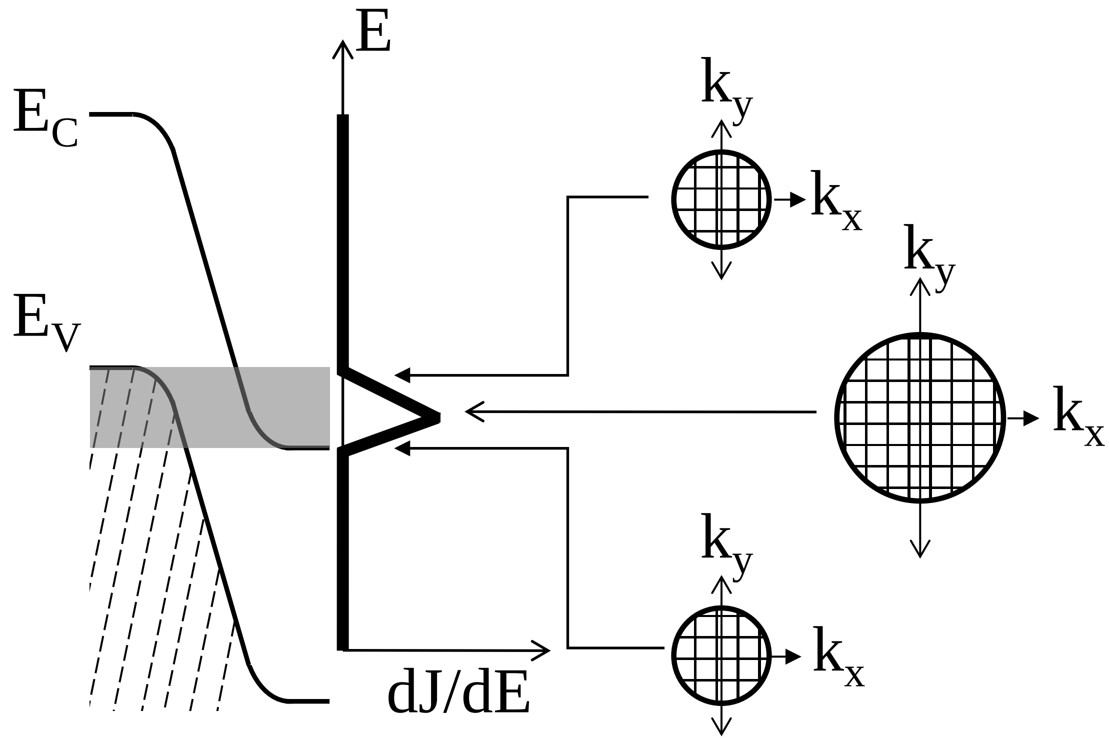


3d-3d Tunneling



# of 2D
Modes $\propto V_{OL}$

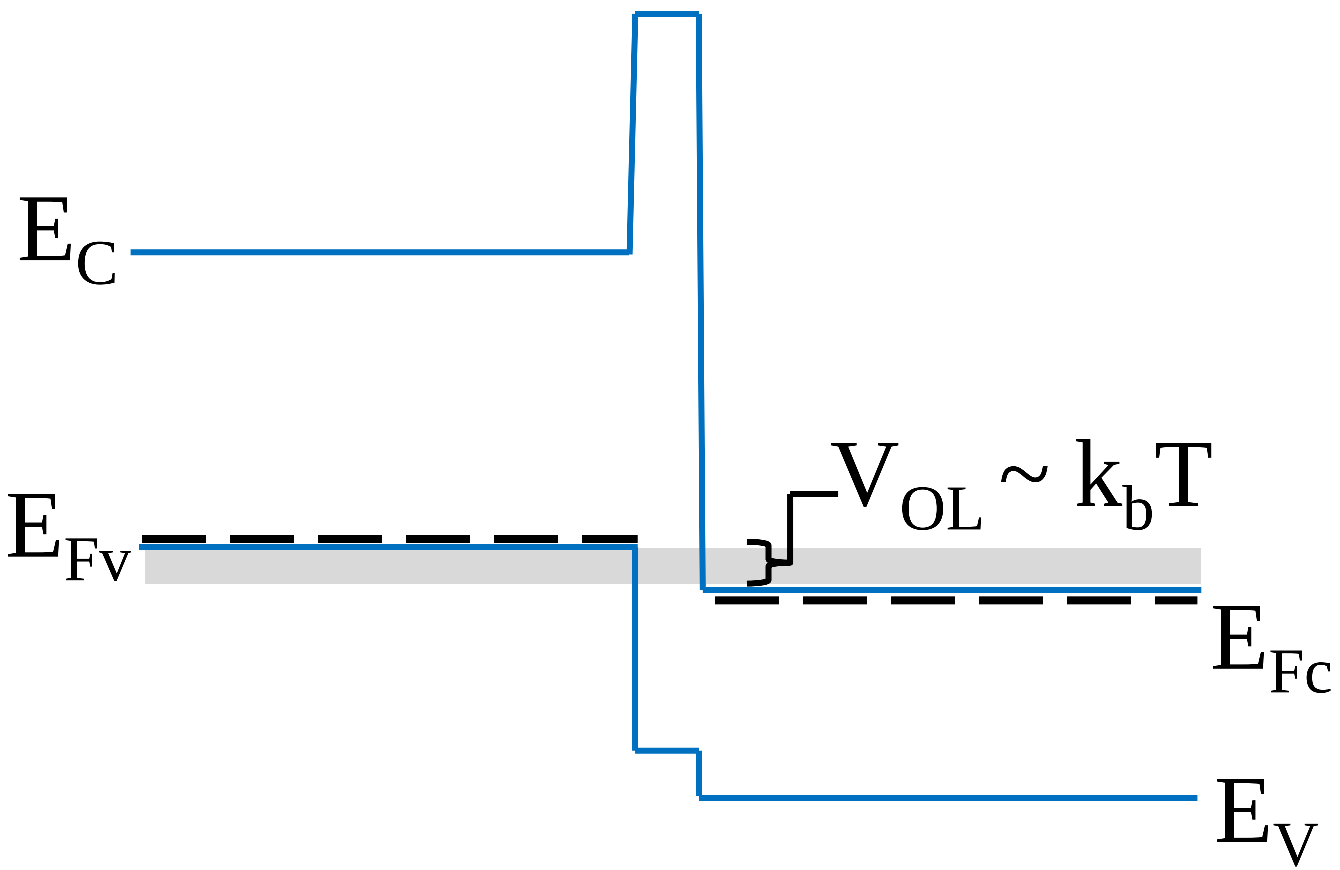




$$I_{3d-3d} \approx \left(\frac{Am^*}{4\pi\hbar^2} \times \frac{qV_{OL}}{2} \right) \times \left(\frac{2q^2}{h} V_{OL} \times T \right)$$

$$= \#\text{ of 2D Channels} \times \text{1D Conductance}$$

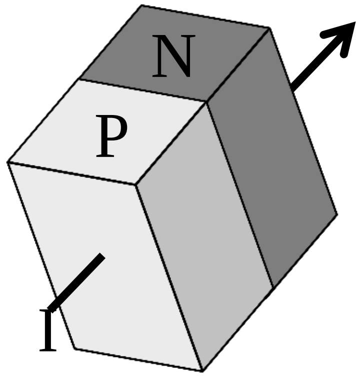
Consider an Ideal Density of States Switch

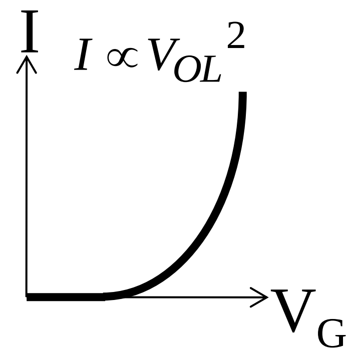


$T \approx$ constant

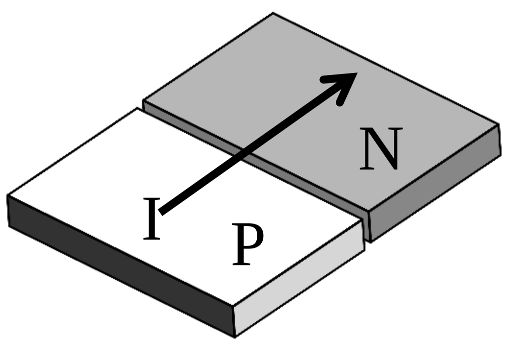
Compare the Dimensionalities

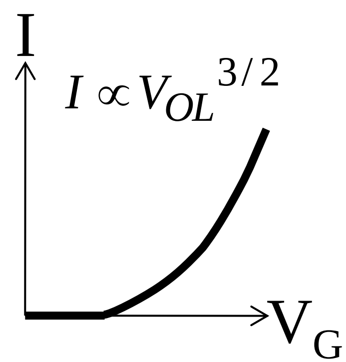
3d-3d



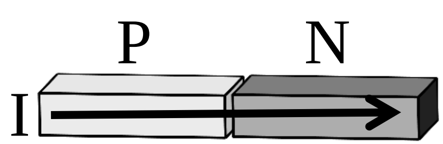


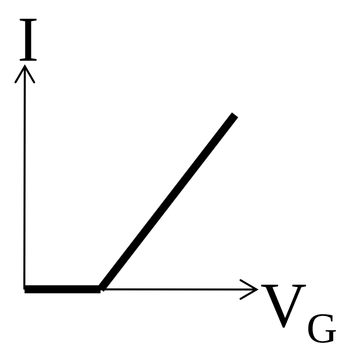
$2d\text{-}2d_{edge}$





$1d\text{-}1d_{point}$



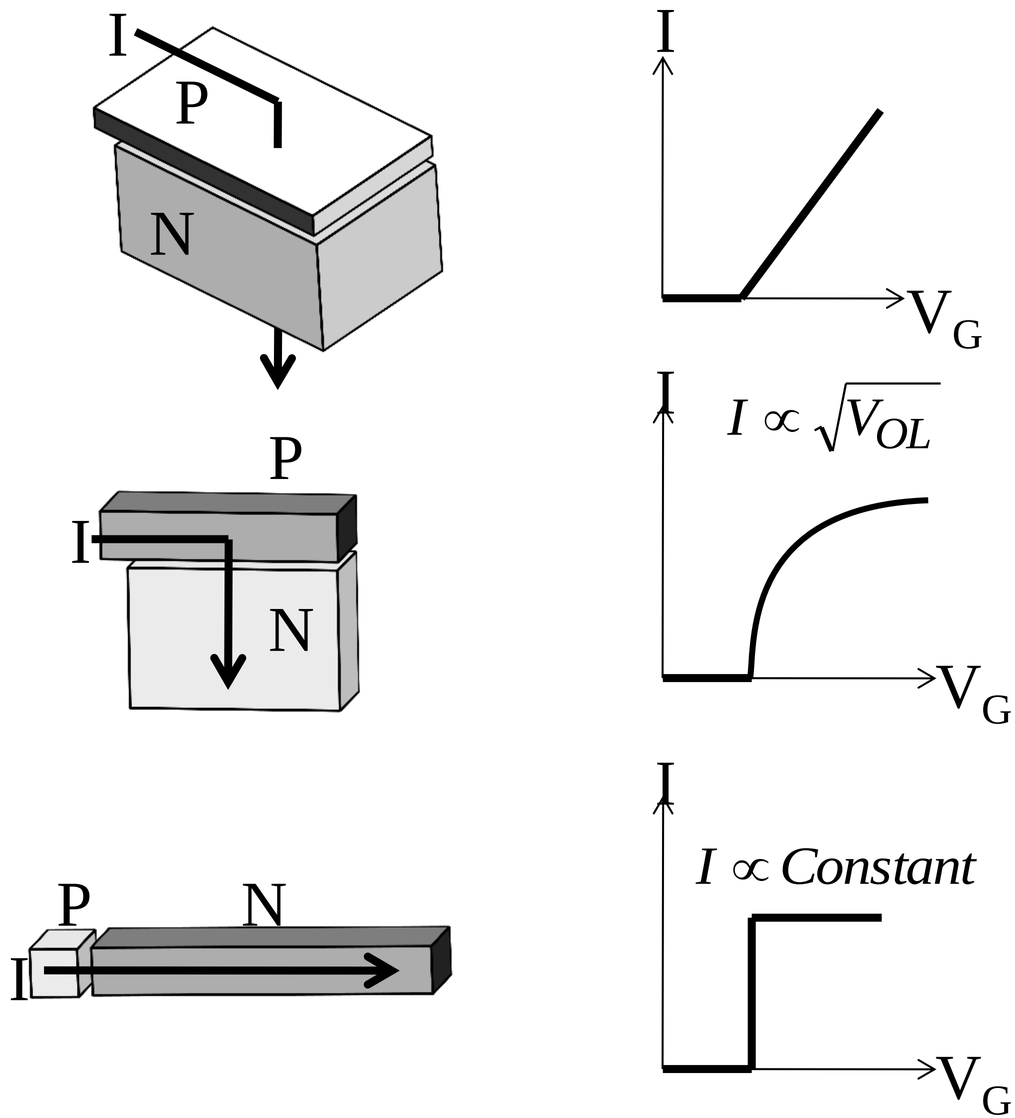


Compare the Dimensionalities

2d-3d

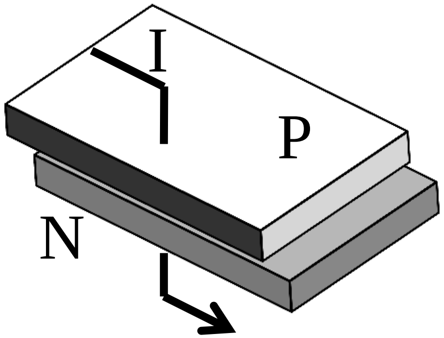
1d-2d

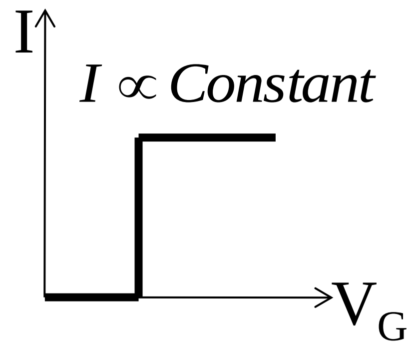
0d-1d



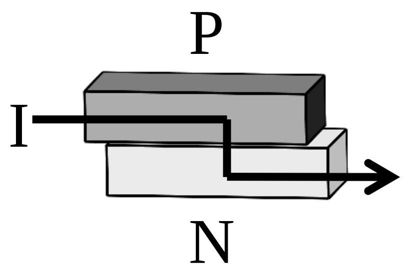
Compare the Dimensionalities

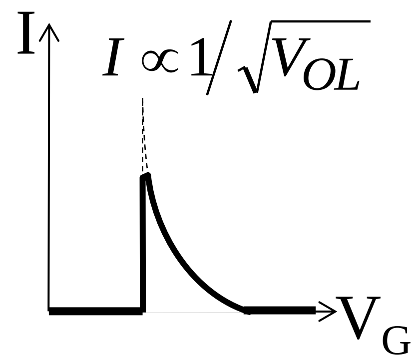
$2d\text{-}2d_{face}$



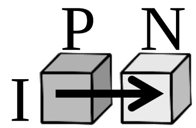


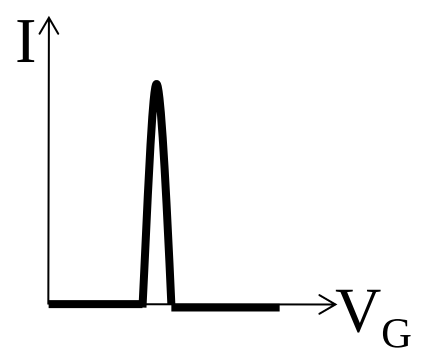
$1d\text{-}1d_{edge}$





0d-0d





Why so many Non-Steep Results?

Technological:

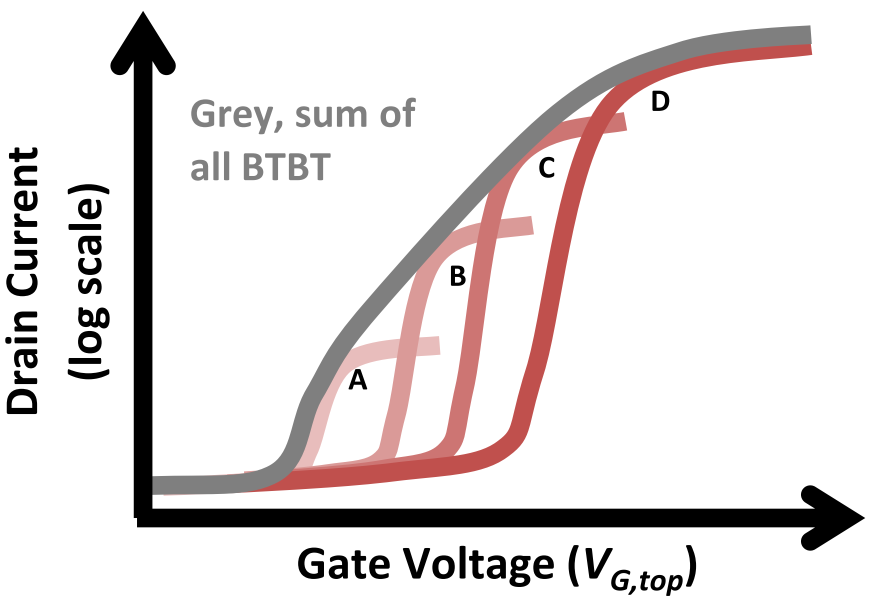
- Band-tails caused by heavy doping
- Interface traps
- Mid-gap traps
- Electrostatic design (parasitic paths)
- Spatial Inhomogeneity of semiconductor--
  - Doping & Thickness

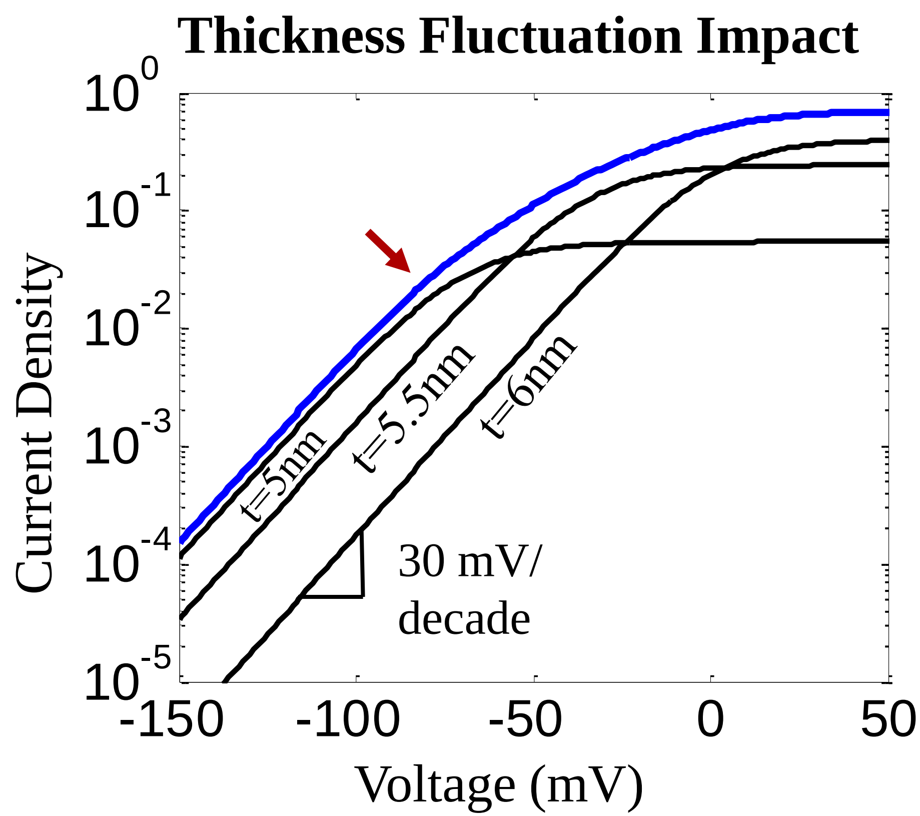
Fundamental

- Inherent level broadening (source to drain tunneling)
- Phonon effects

Eliminate Spatial Inhomogeneity

- Make the Devices Very Small.
  - The threshold may not be reproducible, but so far the field doesn't have a single steep device.





Sandia National Laboratories

Can we use $S_{Barrier}$?

$$S_{Barrier} \approx \left| \frac{\phi_S}{\log(T)} \right|$$

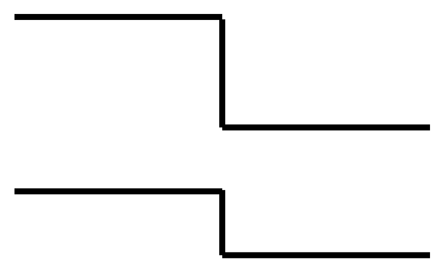
Consider T~ 1%

Log(T) = -2

For $S_{Barrier}$ = 60 mV/decade, need φ_S of 120 meV

Is this reasonable?

$\log(I_{ON}/I_{OFF})$= 120 meV / S_{DOS}



For 5 orders of magnitude on/off need $S_{DOS} < 24$ mV/decade

Use steep S_{DOS} for steep subthreshold swing

Find $S_{Barrier}$

$$S_{Barrier} \approx \frac{d\phi_s}{d\log(T)}$$

$$T(\vec{F}) = \exp\left(\frac{-\pi(m_{tunnel}^{*})^{1/2} E_g^{3/2}}{2\sqrt{2}\hbar q\,|\vec{F}\,|}\right) = \exp\left(\frac{-\alpha}{|\vec{F}\,|}\right)$$

$$S_{Barrier} \approx \left(\log(e) \times \alpha \times \frac{1}{\left|\vec{F}\right|^2} \times \frac{d\vec{F}(\phi_s)}{d\phi_s}\right)^{-1}$$

$$\text{use } \left|\vec{F}\right| = -\frac{\log(e)\times\alpha}{\log(T)}$$

$$S_{Barrier} \approx \left|\frac{1}{\log(T)} \times \frac{F}{d\vec{F}(\phi_s)/d\phi_s}\right|$$

Lateral/point TFET

$$\left|\vec{F}\right| = \frac{\phi_s}{l_{screening}}$$

$$\frac{\left|\vec{F}\right|}{dF/d\phi_s} = \phi_s$$

Bilayer TFET

$$\left|\vec{F}\right| = \frac{\phi_s}{t_{body}}$$

$$\frac{\left|\vec{F}\right|}{dF/d\phi_s} = \phi_s$$

$$\boxed{S_{Barrier} \approx \left|\frac{\phi_s}{\log(T)}\right|}$$

Find $S_{Barrier}$

Vertical TFET

$$\left|\vec{F}\right| = \frac{\phi_S}{W_{depletion}} = \frac{\phi_S}{\sqrt{\varepsilon_S \phi_S / 2qN_d}}$$

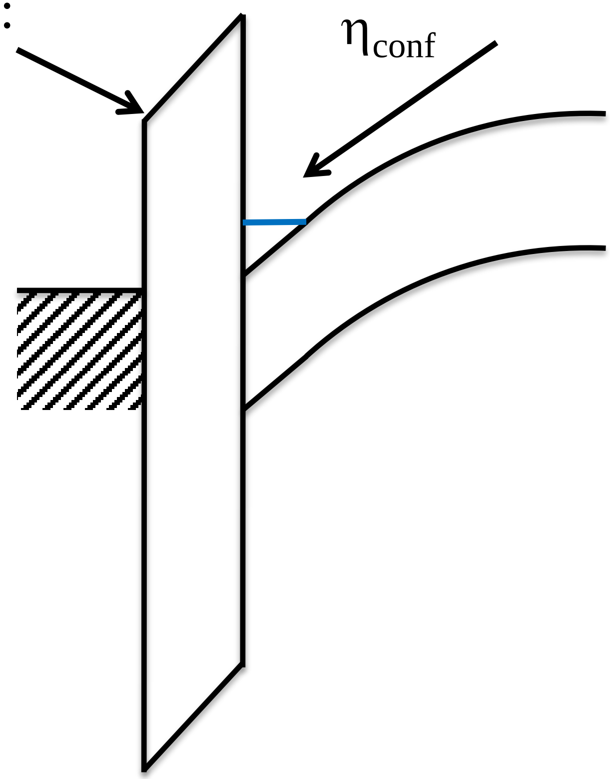
$$\frac{d\vec{F}}{\phi_S} = \frac{1}{2}\sqrt{\frac{2qN_d}{\varepsilon_S}}\phi_S^{-1/2} = \frac{1}{2\phi_S}\vec{F}$$

$$\boxed{S_{Barrier} \approx \left|\frac{2 \times \phi_s}{\log(T)}\right|}$$

Need to Maximize Gate Efficiency

Voltage lost on
the gate oxide:
η_{el}

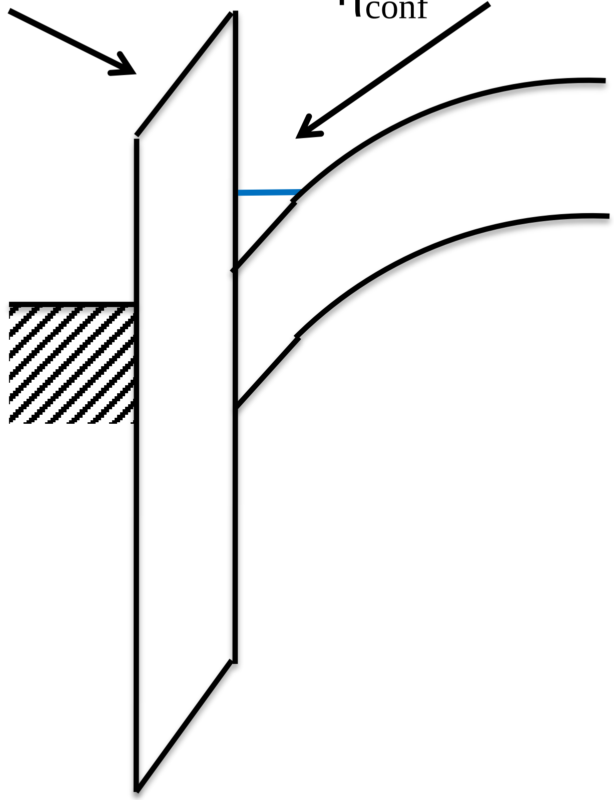
Triangular barrier gets
steeper, which increases
the confinement energy:
η_{conf}



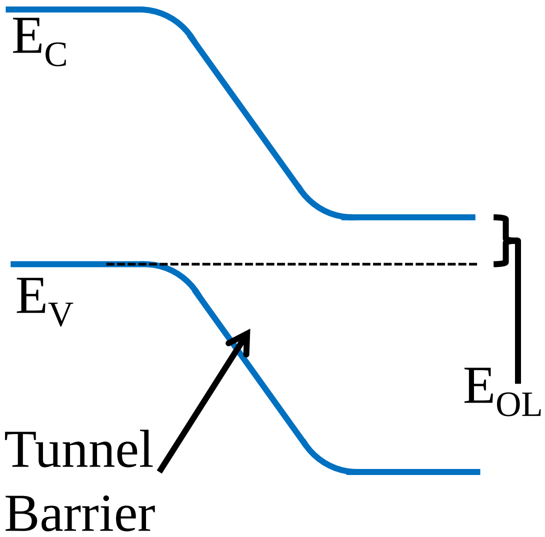
Need to Maximize Gate Efficiency

Voltage lost on the gate oxide: η_{el}

Triangular barrier gets steeper, which increases the confinement energy: η_{conf}



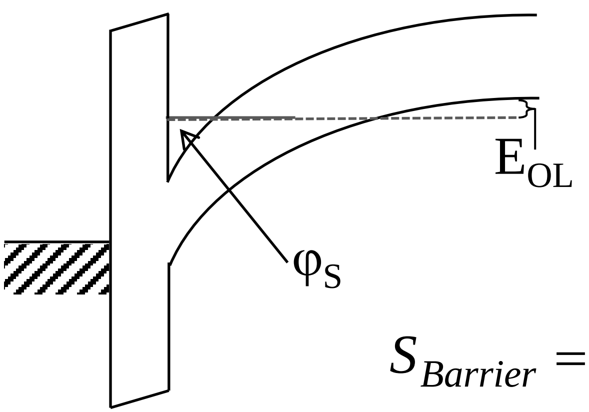
Four Factors Determine The Subthreshold Swing



$$I \propto DOS \times \text{Tunneling Probability}$$

$$SS = \left(\frac{d\log(I)}{dV_G} \right)^{-1}$$

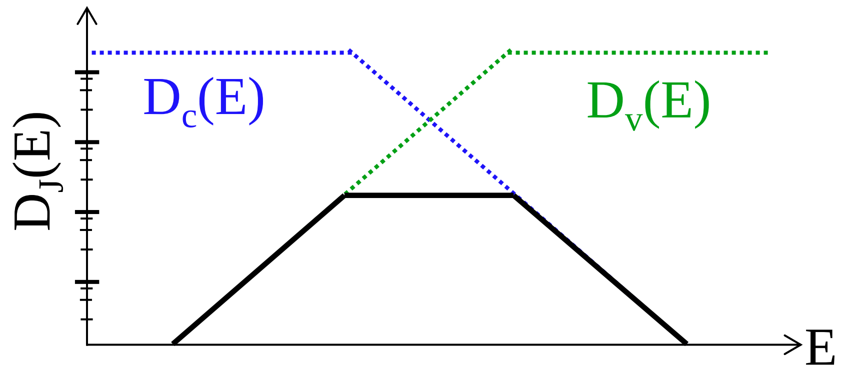
$$= \frac{1}{\eta_{el}} \left(\frac{\eta_{conf}}{S_{DOS}} + \frac{1}{S_{Barrier}} \right)^{-1}$$



$$S_{Barrier} = \frac{d\log(T)}{d\phi_s} \quad S_{DOS} = \frac{d\log(DOS)}{dE_{OL}} \quad \eta_{conf} = \frac{dE_{OL}}{d\phi_s} \quad \eta_{el} = \frac{d\phi_s}{dV_G}$$

Modeling the Tunneling Current

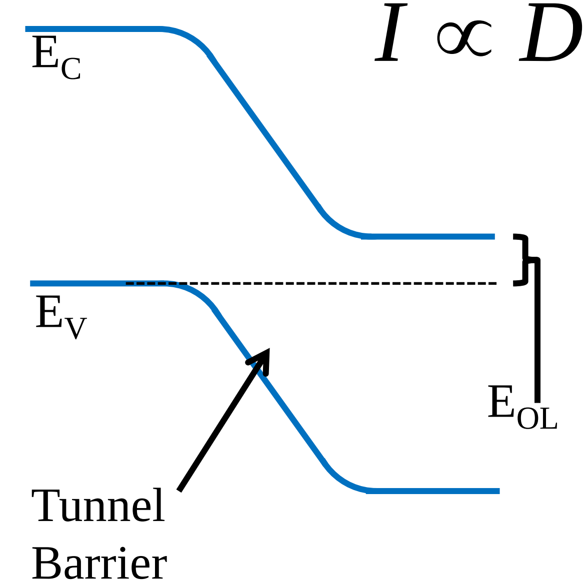
$$I \propto \int (f_C - f_V) \times T \times D_J(E) \times \partial E$$



$$I \propto e^{-|E_{OL}|/qV_0} \times \int_{E_V'}^{E_C'} (f_C - f_V) \times T \times D_0 \times \partial E$$

$$I \propto DOS \times \text{Tunneling Current}$$

Four Factors Determine The Subthreshold Swing

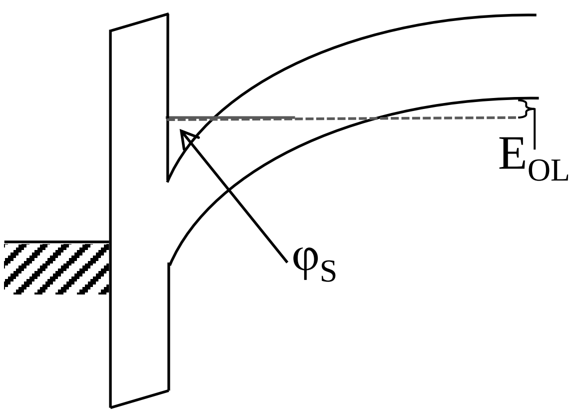


$$I \propto DOS \times \text{Tunneling Probability}$$

$$SS = \left(\frac{d\log(I)}{dV_G} \right)^{-1} = \left(\frac{d\log(DOS)}{dV_G} + \frac{d\log(T)}{dV_G} \right)^{-1}$$

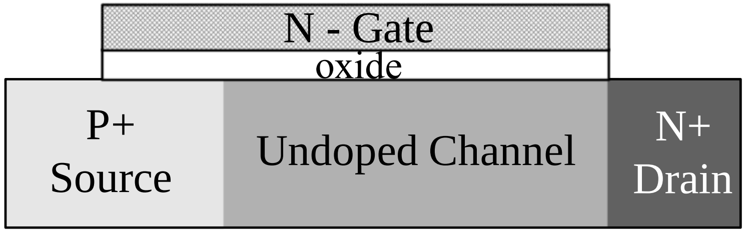
$$= \left(\frac{d\phi_s}{dV_G}\frac{dE_{OL}}{d\phi_s}\frac{d\log(DOS)}{dE_{OL}} + \frac{d\phi_s}{dV_G}\frac{d\log(T)}{d\phi_s} \right)^{-1}$$

$$= \left(\frac{\eta_{el}\eta_{conf}}{S_{DOS}} + \frac{\eta_{el}}{S_{Barrier}} \right)^{-1}$$

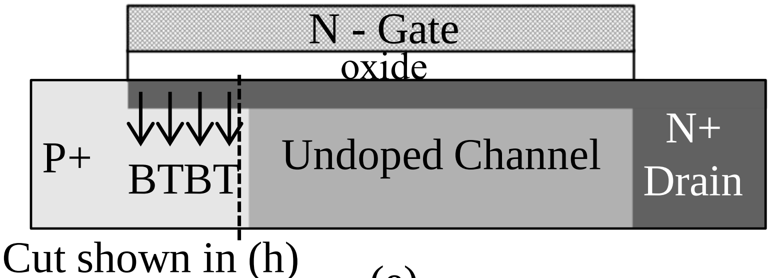


$$\frac{1}{\eta_{el}}\left(\frac{\eta_{conf}}{S_{DOS}} + \frac{1}{S_{Barrier}} \right)^{-1}$$

Vertical TFET



(b)

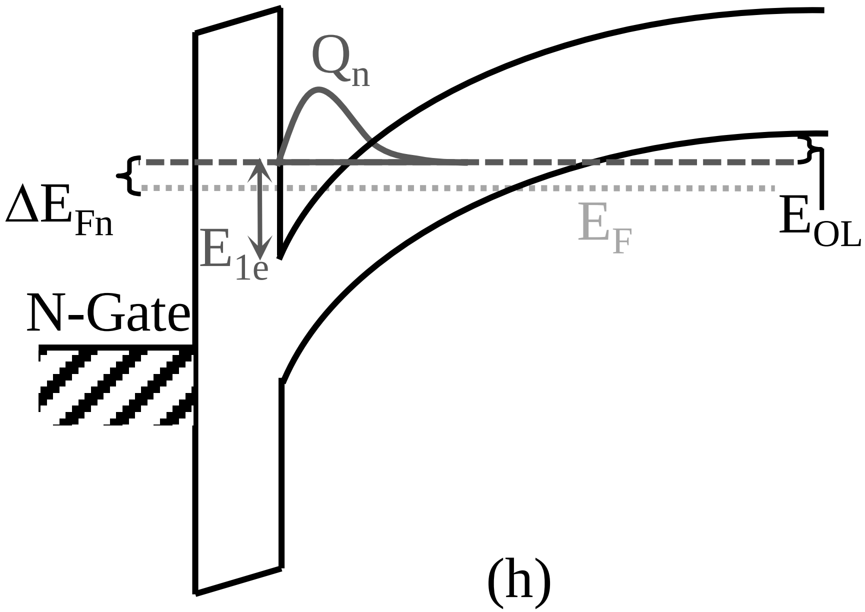


(e)

$$\eta_{conf} \approx \frac{1}{3}\left(\frac{9\pi}{8}\right)^{2/3} \times \left(\frac{N_d \hbar^2}{m^*_{e,z}\varepsilon_s}\right)^{1/3} \times \phi_s^{-2/3}$$

$\sim 80 - 90\%$

η_{el} is standard planar MOSFET gate efficiency

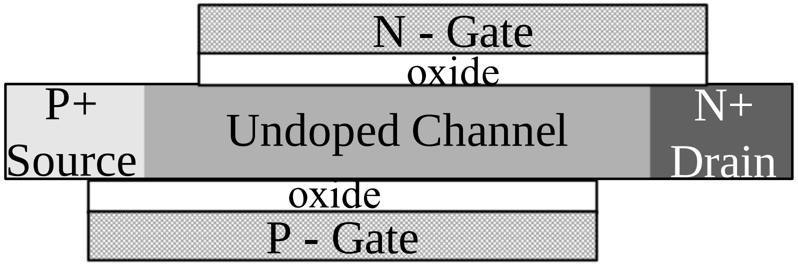


(h)

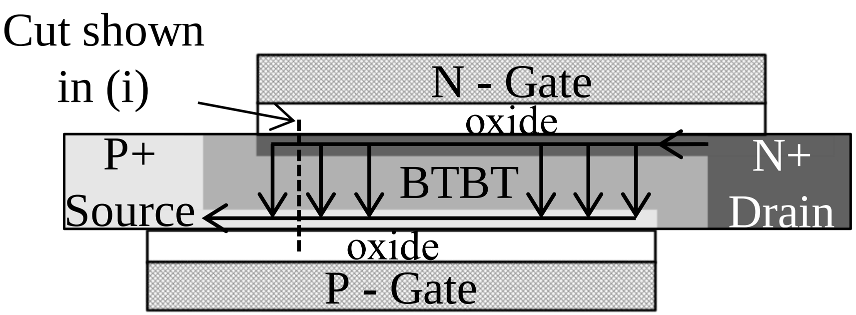
Higher I_{ON}

Always requires doping to get band bending -> poor S_{DOS}

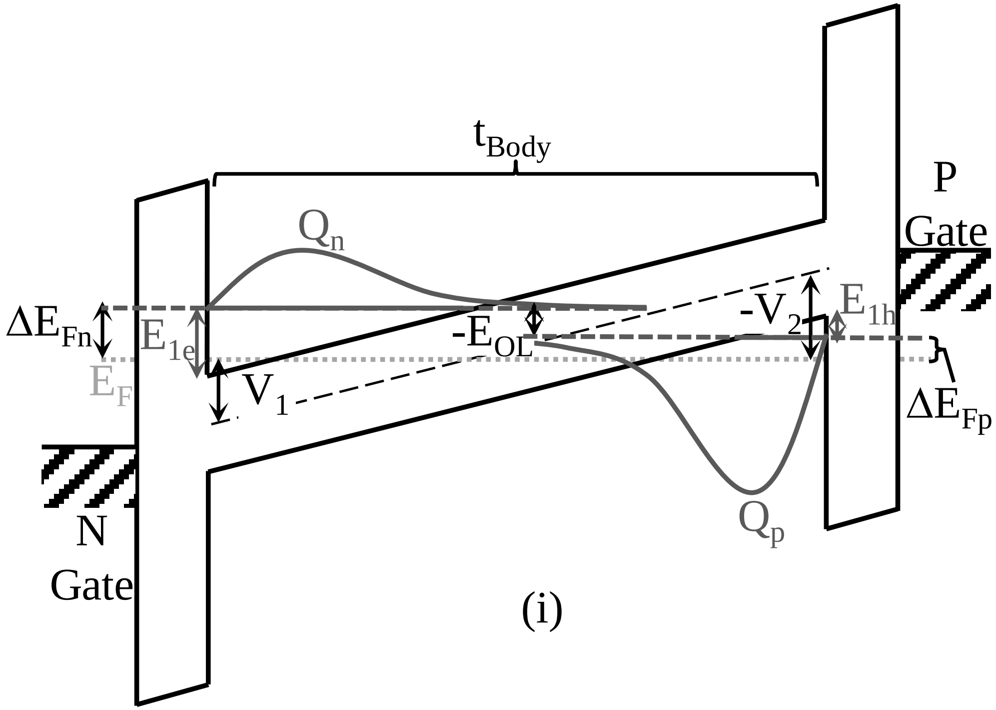
Bilayer TFET



(c)



(f)



(i)

Two gate oxides and thin body

$\rightarrow \eta_{el} \sim 60\text{-}70\%$

Confined Electron and Hole Levels

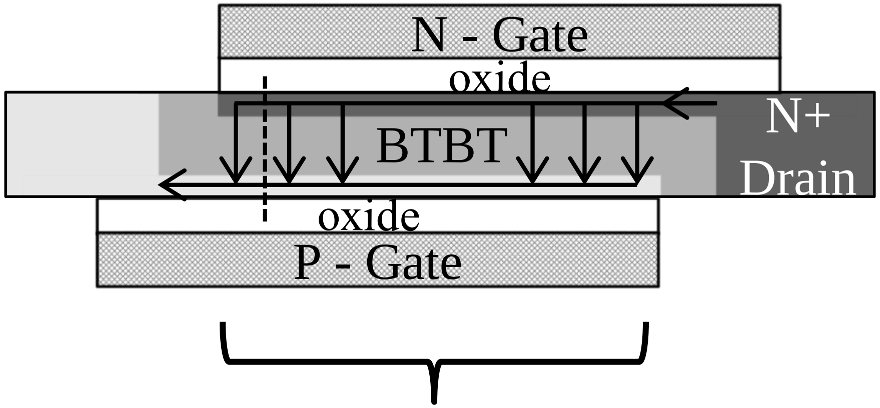
$\rightarrow \eta_{conf} \sim 60\text{-}70\%$

$\eta_{conf} \times \eta_{el} \sim 40\text{-}50\%$

Highest I_{ON}

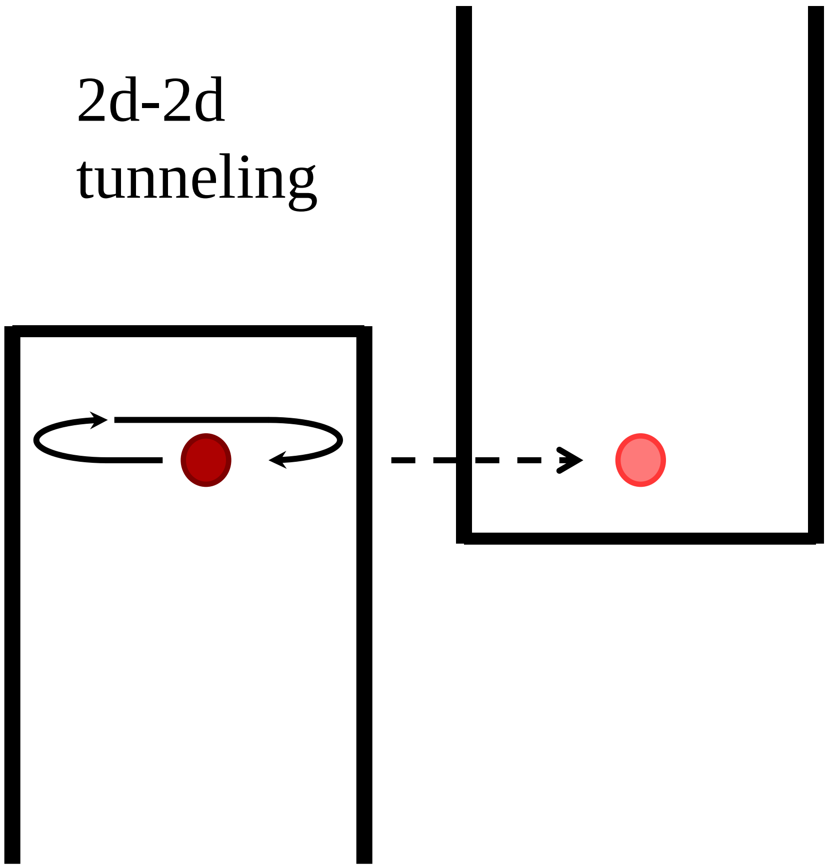
Lowest Overdrive Voltage

High Bilayer Conductance



Large Tunneling Area

2d-2d
tunneling



$$E_z = \frac{1}{2} m \mathrm{v}_z^2$$

What is Happening in a Diode at Small Bias?

$$I \propto \int (f_C - f_V) \times T \times D_J(E) \times \partial E$$

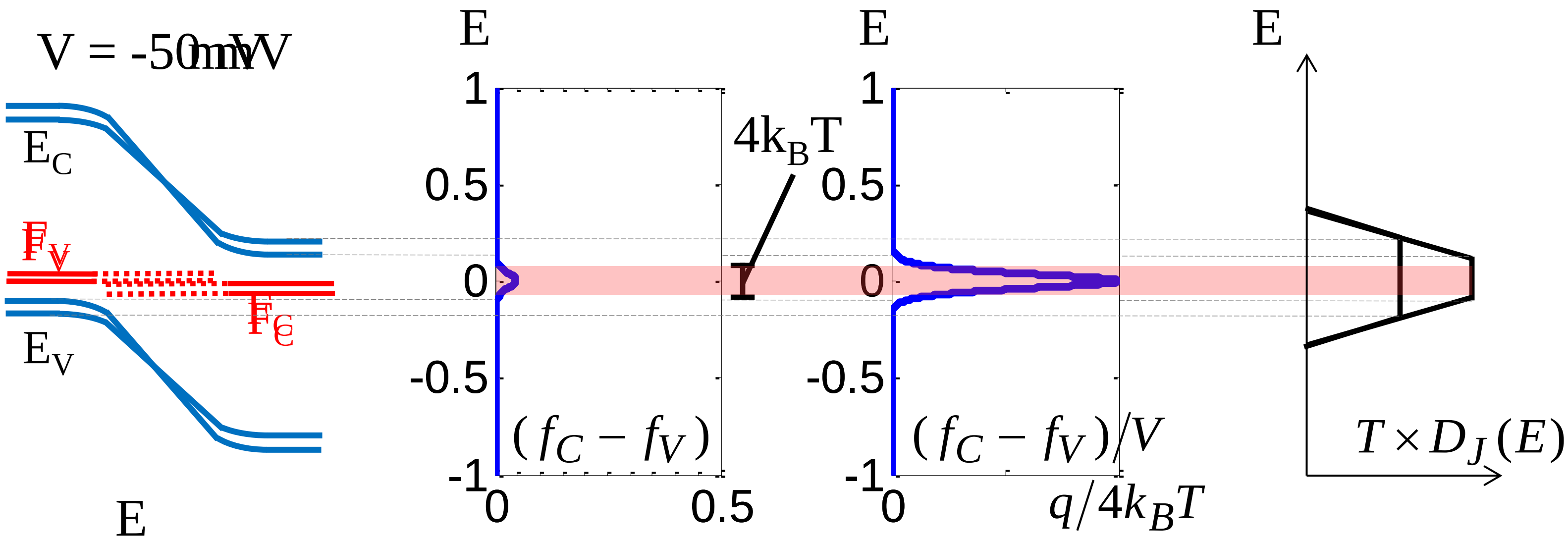
Fermi Functions   Tunneling probability   Joint Density of States

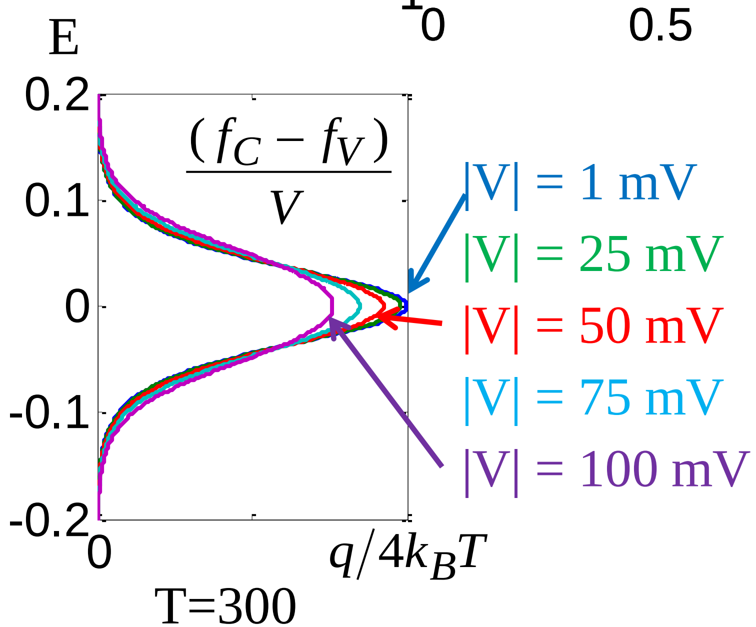
Consider Small Bias

$$I \propto \int (f_C - f_V) \times \partial E \times \frac{\int (f_C - f_V) \times T \times D(E) \times \partial E}{\int (f_C - f_V) \times \partial E}$$

$$= \qquad qV \qquad \times \qquad \left\langle T \times D(E) \right\rangle \Big|_{-2k_{BT}}^{2k_B T}$$

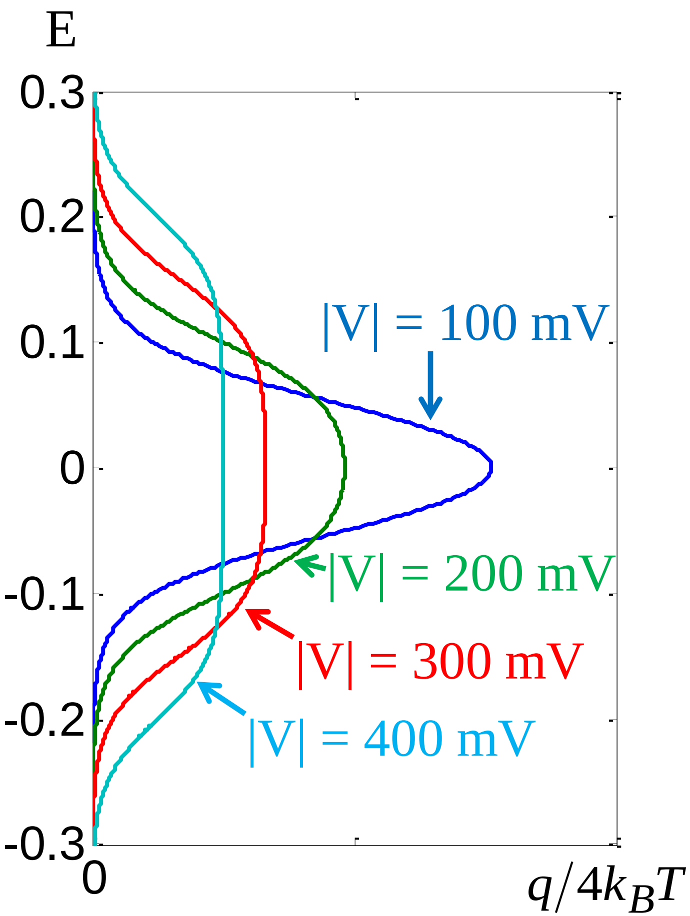
What is Happening in a Diode at Small Bias?





$$I \propto \quad qV \quad \times \quad \langle T \times D_J(E) \rangle \Big|_{-2k_BT}^{2k_BT}$$

What is Happening in a Diode at Large Bias > $4k_BT$?



$$(f_C - f_V)/V$$

$$I \propto \int (f_C - f_V)\partial E \times \frac{\int (f_C - f_V) \times T \times D(E) \times \partial E}{\int (f_C - f_V)\partial E}$$

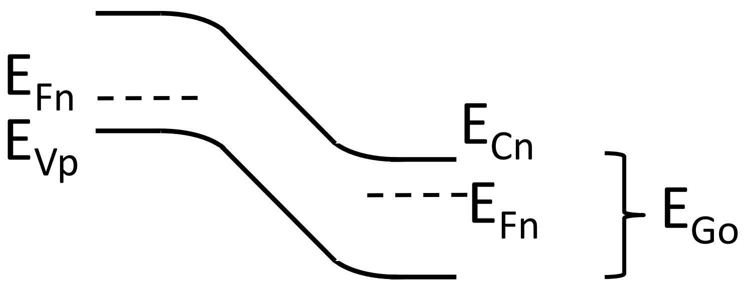
$$= \quad qV \quad \times \quad \langle T \times D(E) \rangle \Big|_{-V/2}^{V/2}$$

The Band Tails Can be Modeled

$$J = J_0 \int \partial E \times T \times (f_C - f_V) \times D_n(E) \times D_p(E)$$

$$D_p(E) = \begin{cases} 1, & E < E_{Vp} \\ e^{-(E-E_{Vp})/qV_O}, & E > E_{Vp} \end{cases}$$

$$D_n(E) = \begin{cases} 1, & E > E_{Cn} \\ e^{+(E-E_{Cn})/qV_O}, & E \le E_{Cn} \end{cases}$$



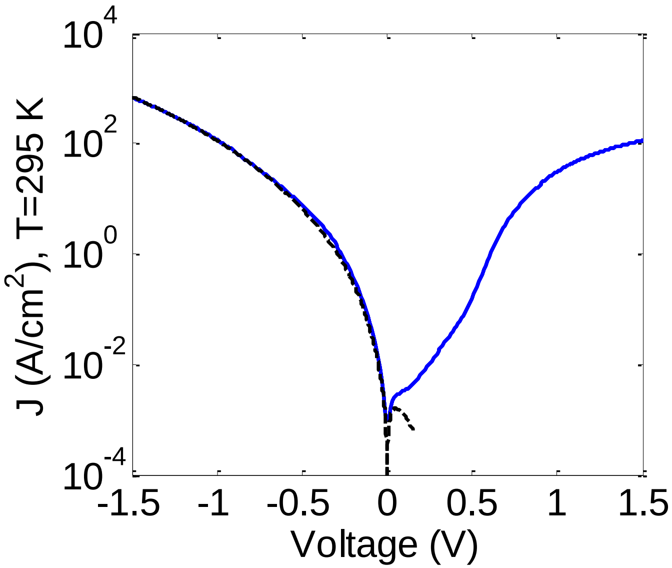
$$f_c = \frac{1}{1 + e^{(E-E_{fn})/k_b T}}$$

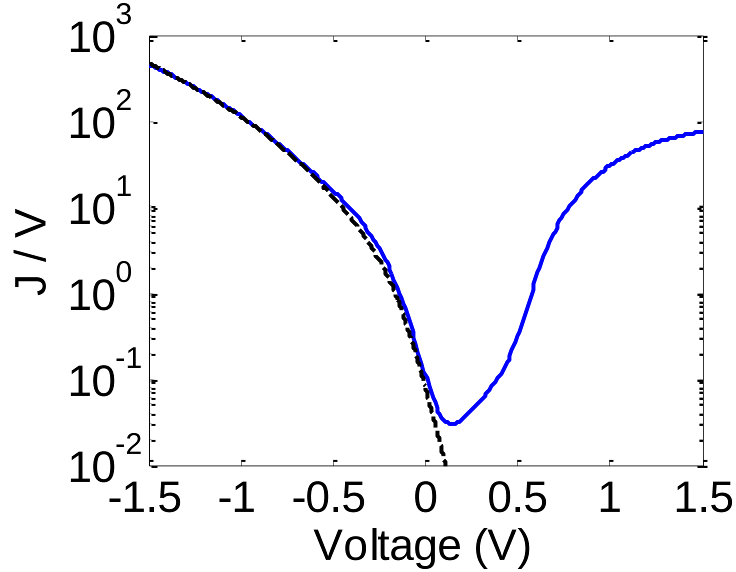
$$f_v = \frac{1}{1 + e^{(E-E_{fp})/k_b T}}$$

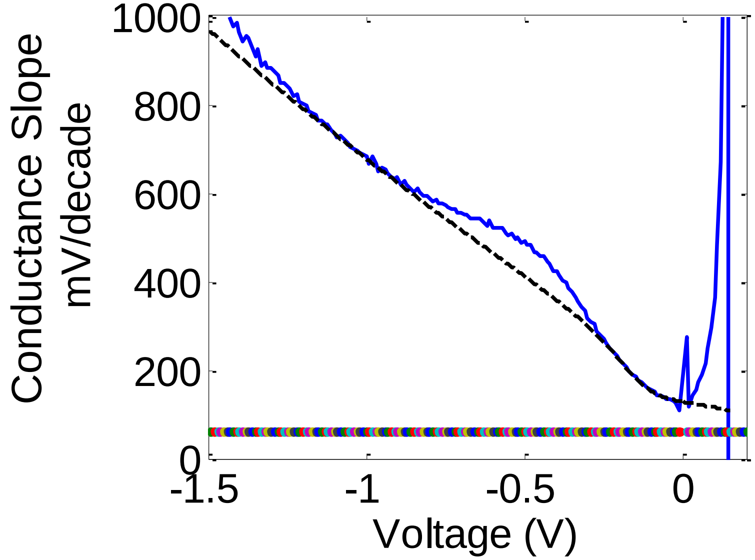
$$T(V_{SD}) = e^{\frac{-\alpha}{(V_{bi}-V_{SD})^{1/2}}}$$

V_{bi} =0.91 V
E_{go} =1.12 eV
V_o =0.126 V
J_0 =3.84e7
α =0.843

I-V Fits Band Tail Model Well







Band Edge Tunneling Current

$$j_t \propto \int \partial E * T * \underbrace{(f_C - f_V)} * D_{BandEdge}(E)$$

Band Edge Density of States

Fixed by source-drain bias in a transistor and is a CONSTANT with gate voltage

Varies with voltage in a diode

At small bias:

$$(f_C - f_V) \approx \left(\frac{1}{2} - \frac{E - F_C}{4K_B T}\right) - \left(\frac{1}{2} - \frac{E - F_V}{4K_B T}\right) = \frac{F_C - F_V}{4k_b T} = \frac{qV}{4k_b T}$$

At larger biases it becomes energy dependent, but

$$\int (f_C - f_V) dE = qV_{SD}$$

Simply dividing the diode current by voltage will approximately give the transistor response!

Polycrystalline Silicon is Very Bad!

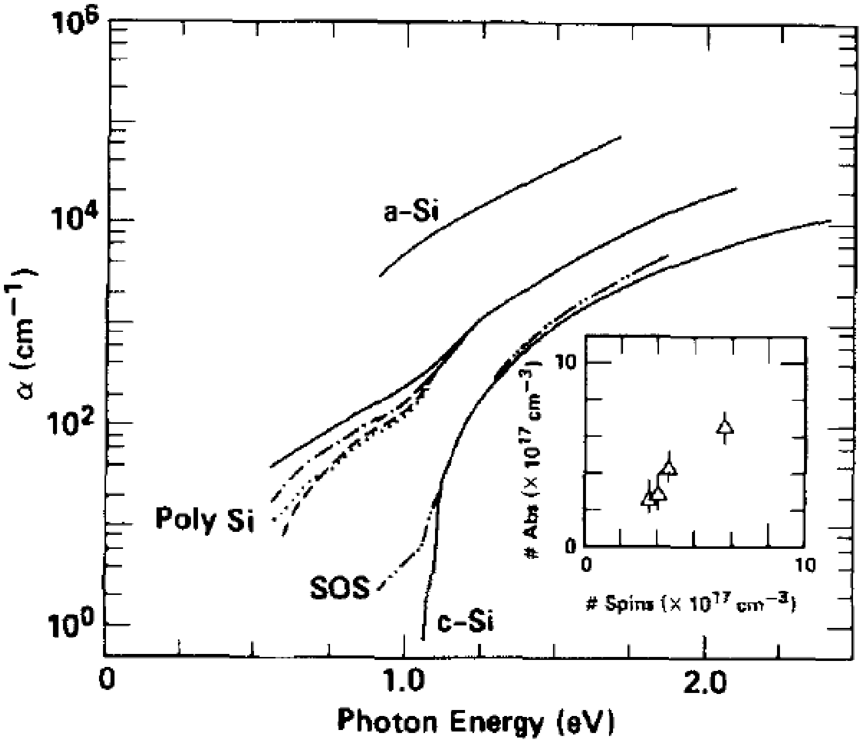


FIG. 1. Absorption vs photon energy for different intervals of atomic hydrogenation exposure. Evaporated amorphous silicon (*a*-Si) from Ref. 16. Fine grained polysilicon, unhydrogenated (solid), 60 min (dot-dash), 120 min (dash), 30 min (dotted), silicon-on-sapphire (SOS). Bulk crystallline silicon (*c*-Si) from Ref. 17. Inset shows the integrated density of optically absorbing defects with a cross section of 1.2×10^{-16} cm^{-2} (Ref. 8) vs the dangling bond spin density.

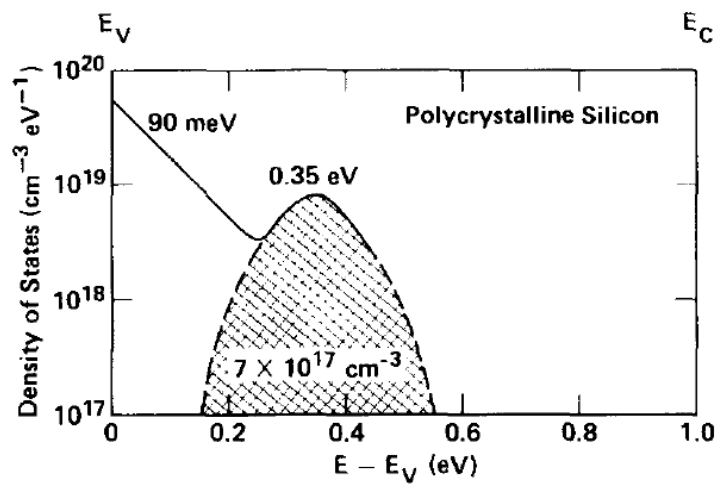
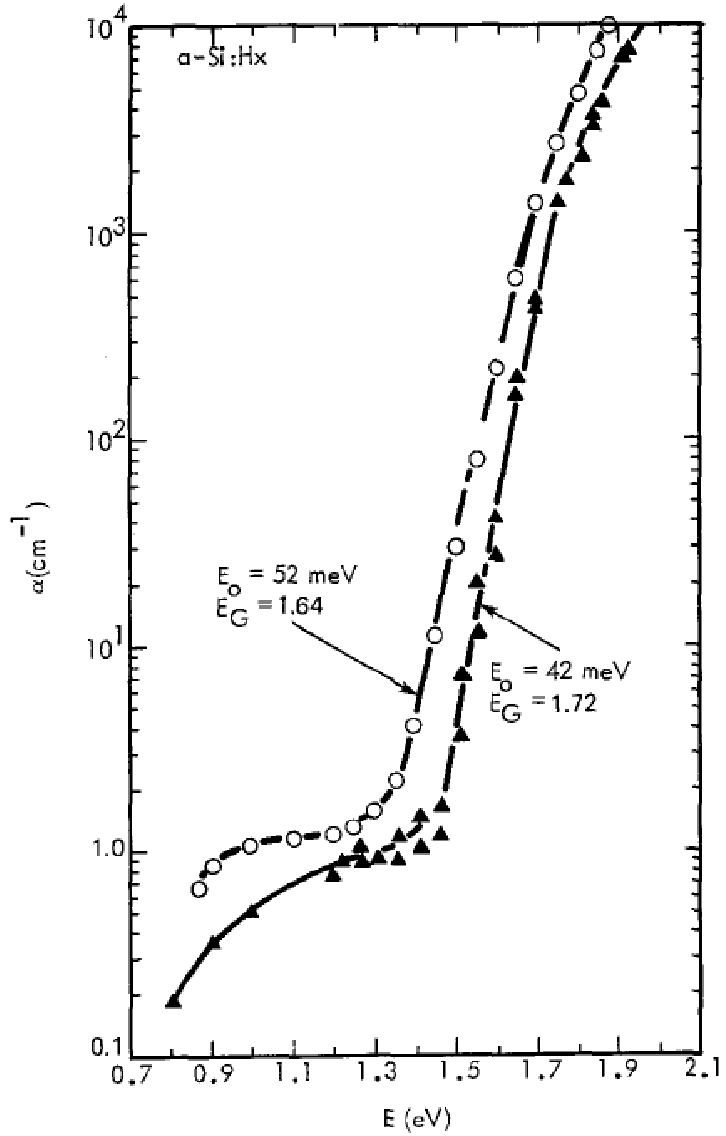


FIG. 3. Features of the grain boundary density of states derived from optical absorption and ESR measurements.

Jackson, Johnson and Biegelsen, "Density of Gap States of Silicon Grain boundaries Determined by Optical Absorption," 1982

Amorphous Silicon is Very Bad!

Sandia National Laboratories



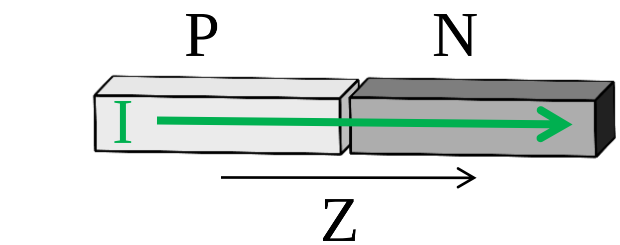
$$\alpha = \alpha_0 \exp[E - E_F/E_0(T, X)]$$

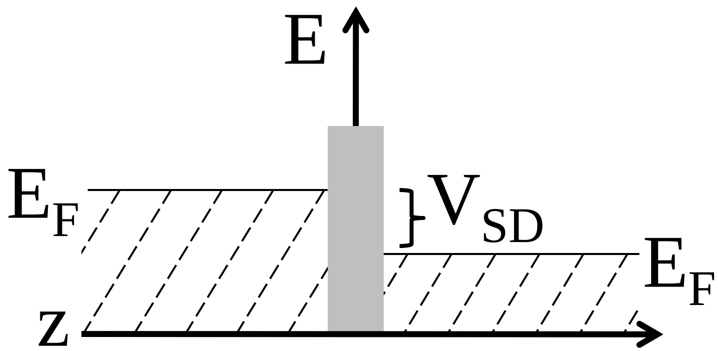
Fig. 1. Absorption edge of two films of amorphous silicon hydride (a-Si:H). The film with the higher Tauc gap was grown at a substrate temperature of 250°C compared with 200°C for the lower gap film. It has a hydrogen content of 14 at.% compared with 9 at.% for the lower gap film (adapted from ref. [2]).

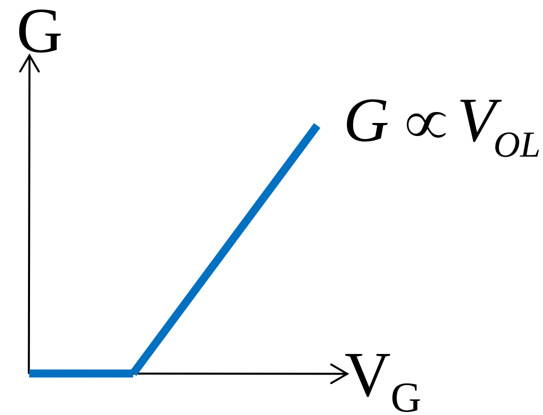
Cody, "Urbach Edge of crystalline and amorphous silicon: a personal review" (1992)

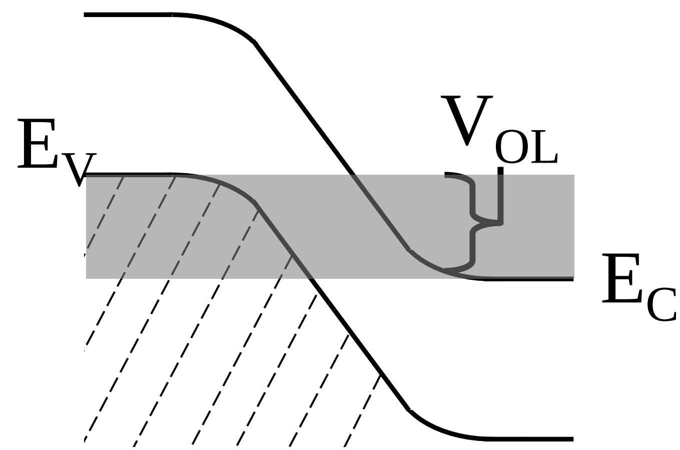
Sandia
National
Laboratories

1d-1d Point Overlap









$$I_{1d-1d,\text{Point}} = \frac{2e^2}{h} \times V_{OL} \times T$$

Consider a Very Small V_{SD}

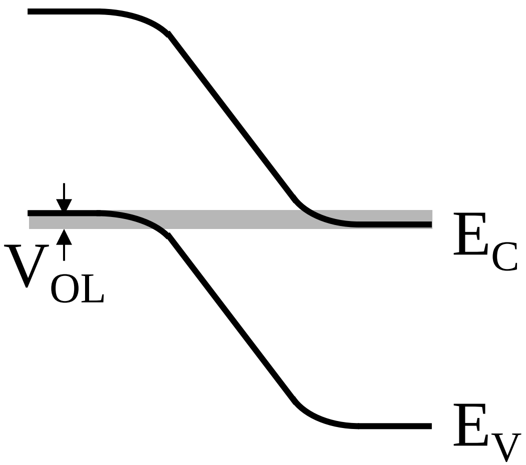
- We are interested in thee case where all voltages < kT
- All states are roughly half occupied,

  and current flows both ways according

  to the difference in occupation probability:

$$f_c = \frac{1}{e^{(E-E_{Fc})/kT} + 1}$$

$$f_c - f_v \approx \frac{(E_{Fc} - E_{Fv})}{4kT} \approx \frac{qV_{SD}}{4kT}$$

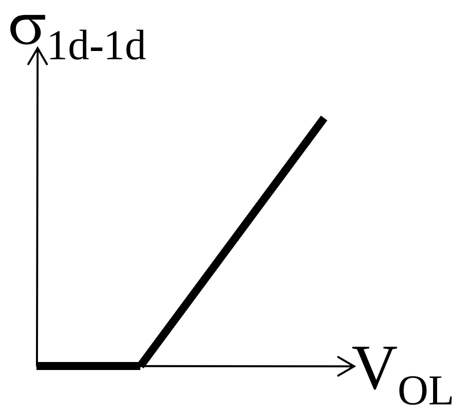


- Take the cold current and multiply by $qV_{SD}/4kT$

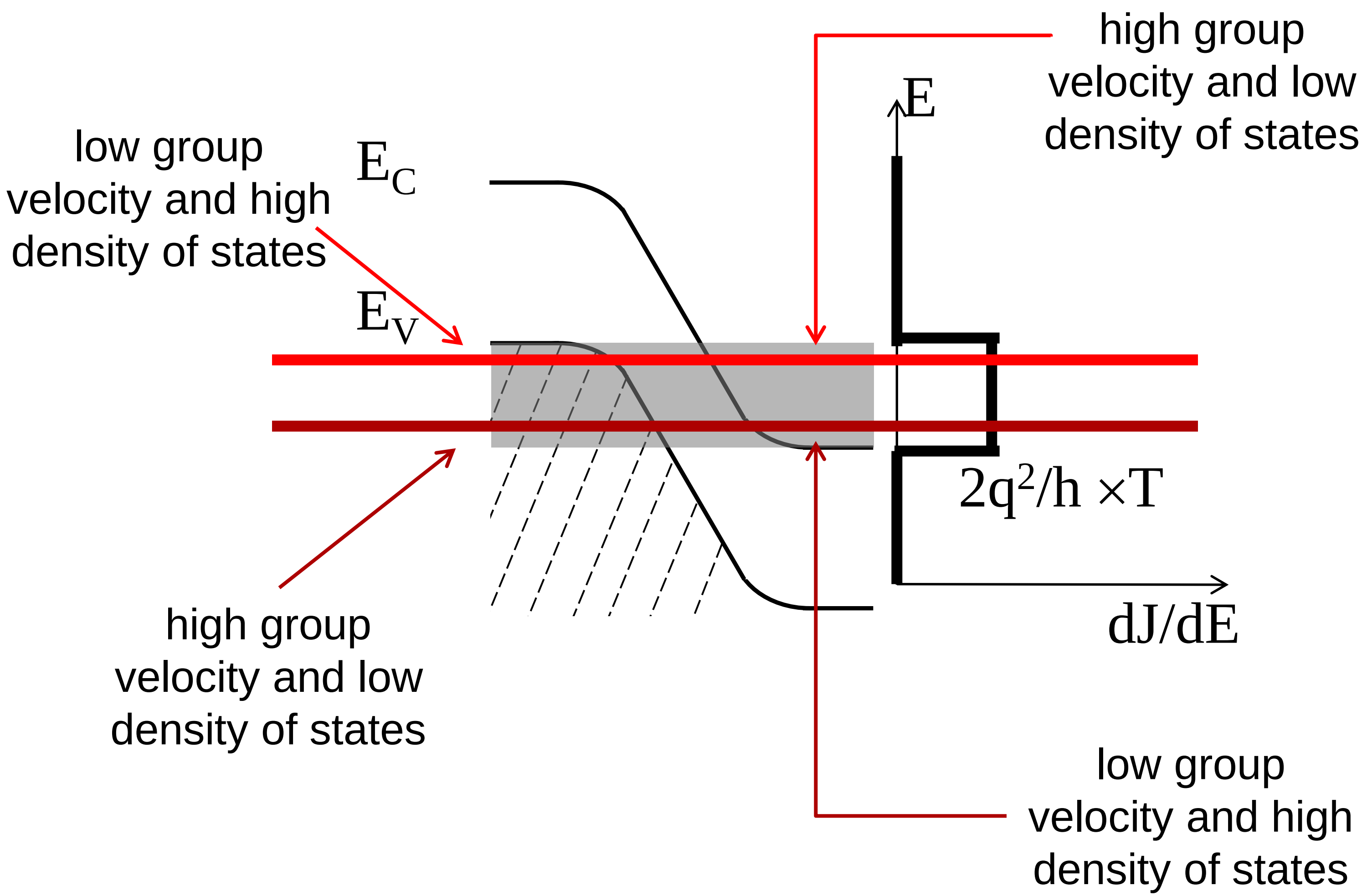
$$I_{1d-1d,Point} \times \frac{qV_{SD}}{kT} = \frac{2q^2}{h} \times V_{OL} \times \frac{qV_{SD}}{4kT}$$

- Therefore conductance of the diode is:

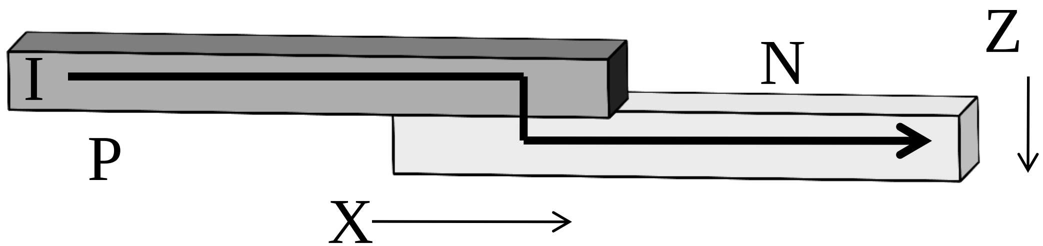
$$\sigma_{1d-1d,Point} = \frac{2q^2}{h} \times V_{OL} \times \frac{q}{4kT}$$



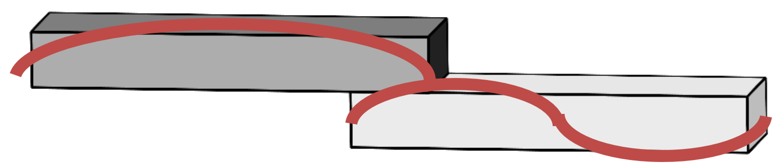
Why is it Still a Quantum of Conductance?



Turn on Broadening

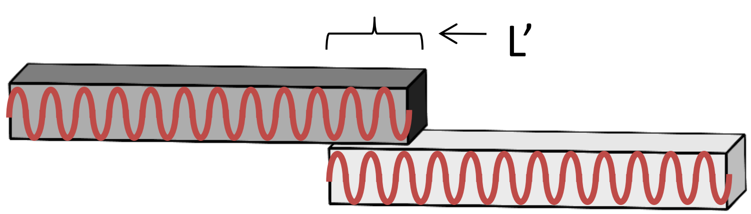


Transverse Momentum is NOT Conserved at Low k

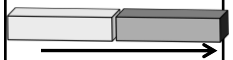
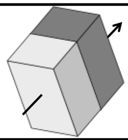
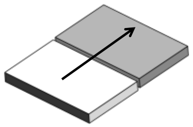
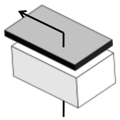
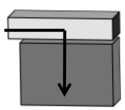
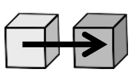
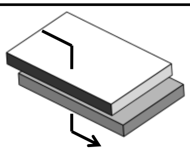
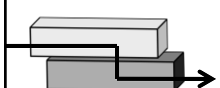


k1≠k2
overlap integral is
NOT zero

Transverse Momentum is Conserved at High k



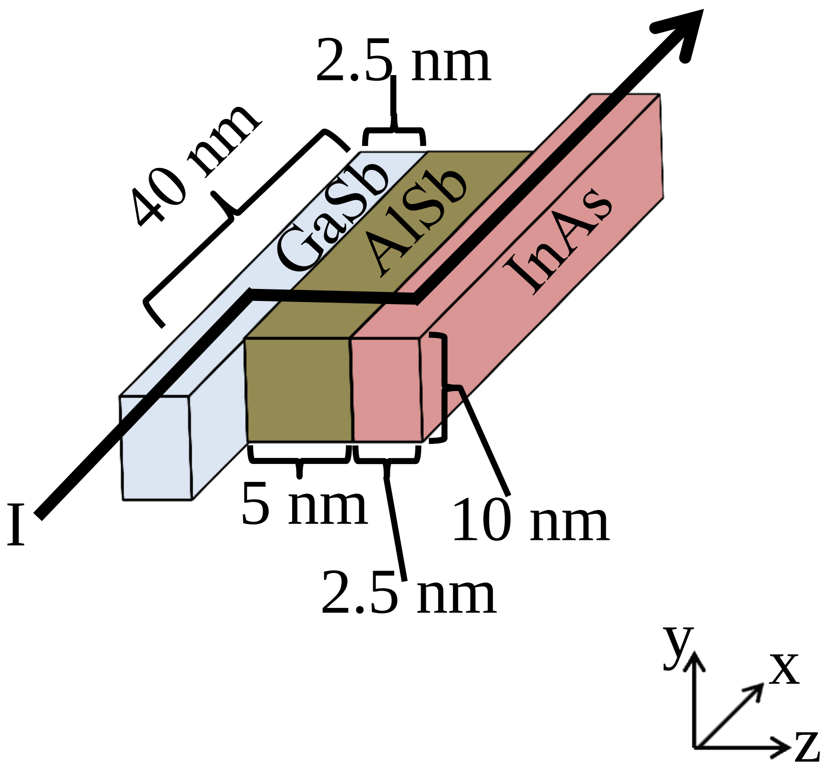
Transverse momentum conserved once λ ~ L’

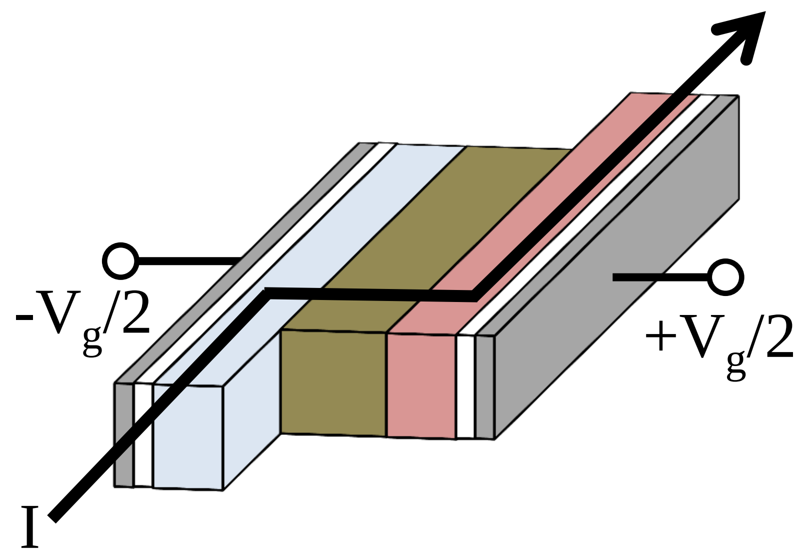
Case	Picture	Current	Conductance, G	Maximum G for pert. theory to be valid	Maximum G for end contacts $\gamma=(2/\pi)E_X$
1d-1d		$\frac{2q^2}{h}\times V_{OL}\times\mathcal{T}_{device}$	$\frac{2q^2}{h}\times V_{OL}\times\mathcal{T}_{device}\times\frac{q}{4k_bT}$	N/A	N/A
3d-3d		$\frac{Am^*}{4\pi\hbar^2}\times\frac{qV_{OL}}{2}\times\frac{2q^2}{h}V_{OL}\times\mathcal{T}_{device}$	$\frac{Am^*}{4\pi\hbar^2}\times\frac{qV_{OL}}{2}\times\frac{2q^2}{h}V_{OL}\times\mathcal{T}_{device}\times\frac{q}{4k_bT}$	N/A	N/A
2d-2d$_{edge}$		$\frac{2L_X\sqrt{qm^*V_{OL}}}{3\pi\hbar}\times\frac{2q^2}{h}\times V_{OL}\times\mathcal{T}_{device}$	$\frac{2L_X\sqrt{qm^*V_{OL}}}{3\pi\hbar}\times\frac{2q^2}{h}\times V_{OL}\times\mathcal{T}_{device}\times\frac{q}{4k_bT}$	N/A	N/A
0d-1d		$\frac{2q}{h}\times E_Z\times\mathcal{T}_{device}$	$\frac{2q}{h}\times E_Z\times\mathcal{T}_{device}\times\frac{q}{4k_bT}$	N/A	N/A
2d-3d		$\frac{Am}{2\pi\hbar^2}\times\frac{qV_{OL}}{2}\times\frac{4q}{h}\times E_Z\times\mathcal{T}_{device}$	$\frac{Am}{2\pi\hbar^2}\times\frac{qV_{OL}}{2}\times\frac{4q}{h}\times E_Z\times\mathcal{T}_{device}\times\frac{q}{4k_bT}$	N/A	N/A
1d-2d		$\frac{L_X}{\pi\hbar}\times\sqrt{qm^*V_{OL}}\times\frac{4q}{h}\times E_Z\times\mathcal{T}_{device}$	$\frac{L_X}{\pi\hbar}\times\sqrt{qm^*V_{OL}}\times\frac{4q}{h}\times E_Z\times\mathcal{T}_{device}\times\frac{q}{4k_bT}$	N/A	N/A
0d-0d		$\frac{4q}{\hbar}E_{Z,i}\times\frac{\mathcal{T}_{device}}{\mathcal{T}_{contact}}$	$\frac{4q}{\hbar}E_{Z,i}\times\frac{\mathcal{T}_{device}}{\mathcal{T}_{contact}}\times\frac{q}{4k_bT}$	$\frac{2q^2}{h}\times\pi^2\times\frac{\gamma}{k_bT}$	$\frac{2q^2}{h}\times\pi^2\times\frac{\gamma}{k_bT}$
2d-2d$_{face}$		$\frac{qmA}{\pi^2\hbar^3}\times E_{Z,i}\times E_{Z,f}\times\mathcal{T}_{device}$	$\frac{qmA}{\pi^2\hbar^3}\times E_{Z,i}\times E_{Z,f}\times\mathcal{T}_{device}\times\frac{q}{4k_bT}$	$\frac{2q^2}{h}\times\frac{\pi^3}{2}\times\gamma^2\times\frac{1}{4k_bT}\times\frac{2mA}{\hbar^2\pi^2}$	$\frac{2q^2}{h}\times\frac{\pi^2}{4}\times\frac{W}{L_X}\times\frac{\gamma}{k_bT}$
1d-1d$_{edge}$		$2\frac{qL_X}{\pi^2\hbar^2}E_{Z,i}\times E_{Z,f}\times\sqrt{\frac{m}{qV_{OL}}}\times\mathcal{T}_{device}$	$2\frac{qL_X}{\pi^2\hbar^2}E_{Z,i}\times E_{Z,f}\times\sqrt{\frac{m}{qV_{OL}}}\times\mathcal{T}_{device}\times\frac{q}{4k_bT}$	$\frac{2q^2}{h}\times\sqrt{2}\pi^2\times\gamma^{3/2}\times\frac{1}{4k_bT}\times\sqrt{\frac{2mL_X^2}{\pi^2\hbar^2}}$	$\frac{2q^2}{h}\times\frac{2\pi^{3/2}}{4}\times\frac{\gamma}{k_bT}$

Sandia National Laboratories

Use NEGF to Model a 1d-1d Edge Overlapped Junction

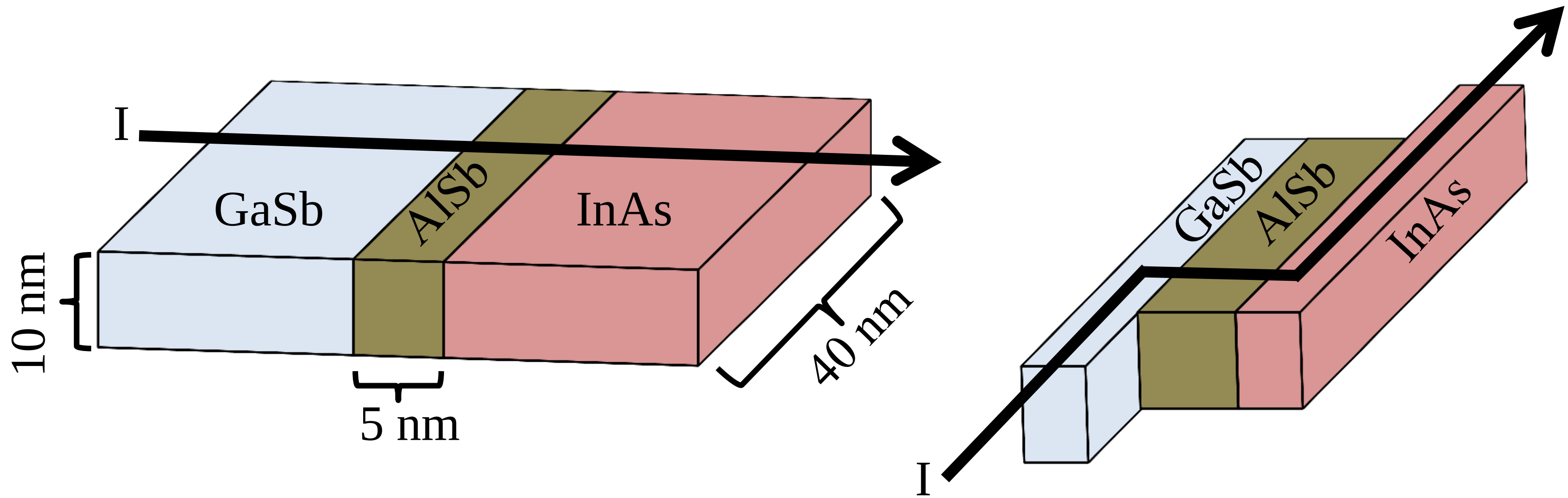
- Define a 1d-1d$_{edge}$ Geometry
  - Let contacts extend to infinity

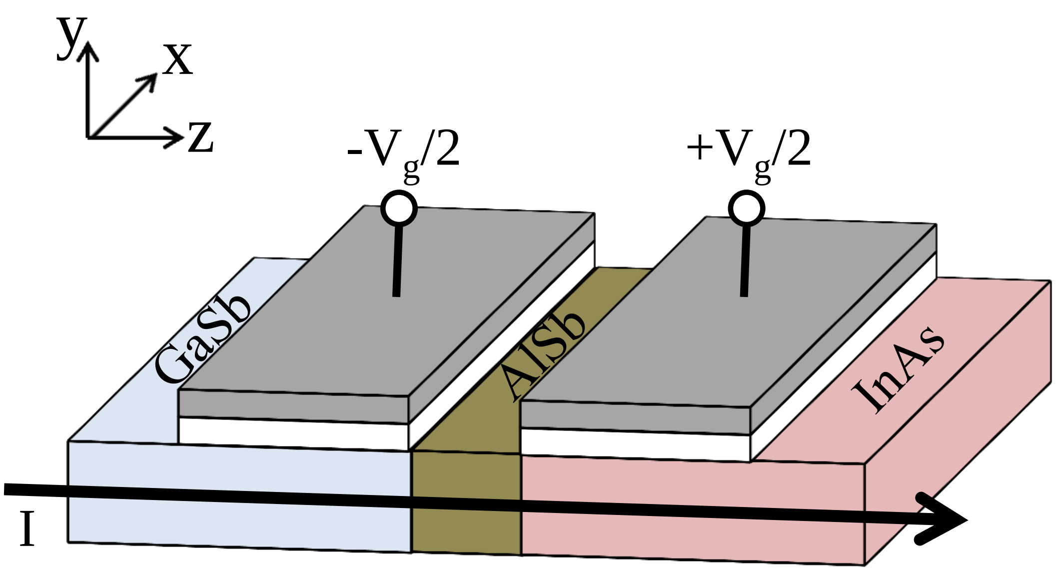


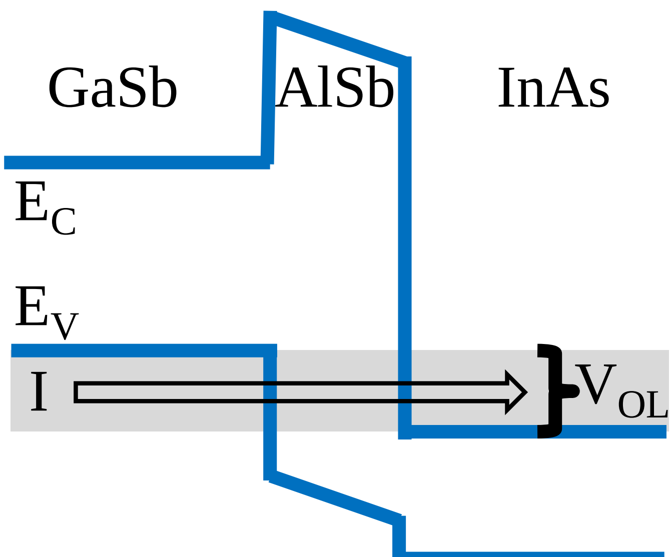


Use an 8 band k.p based basis for the NEGF Modeling

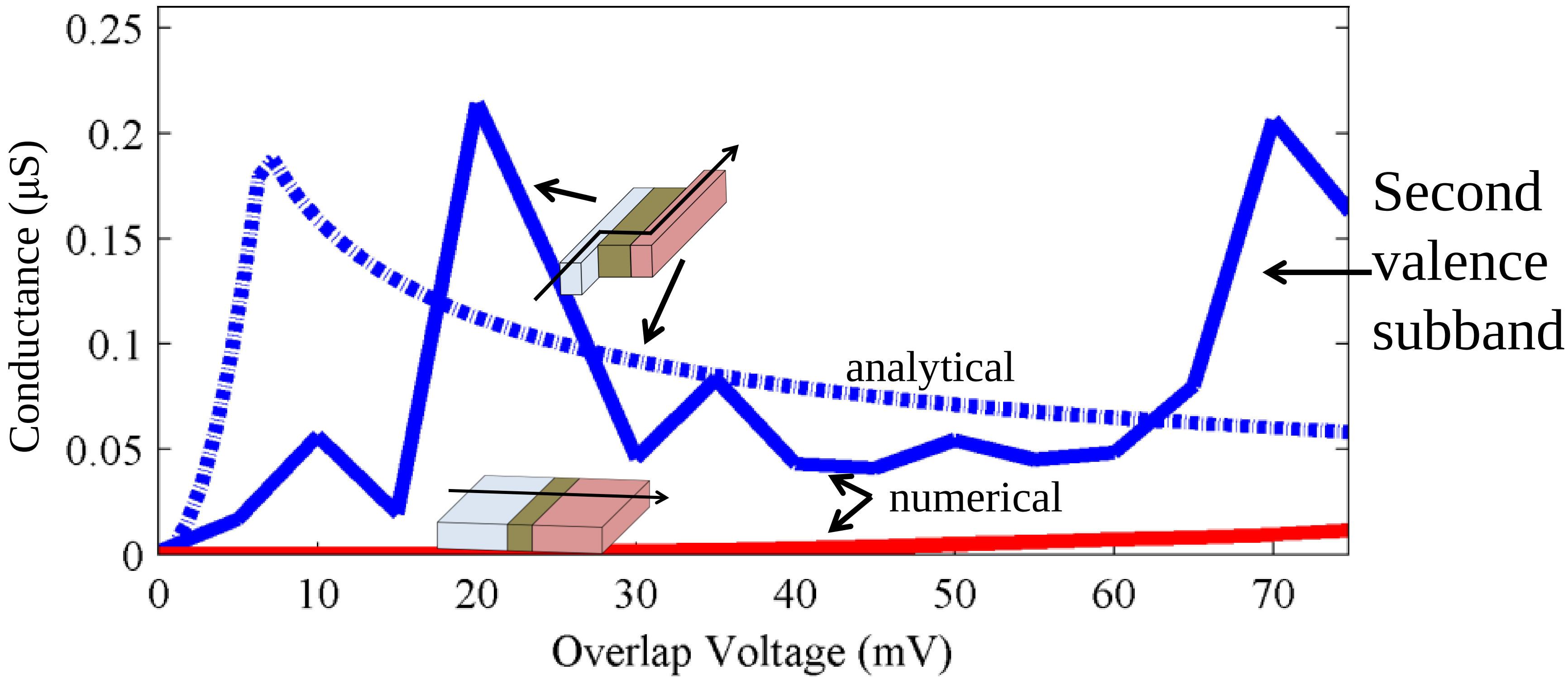
Compare to an Unconfined 2d-2d$_{edge}$ Structure





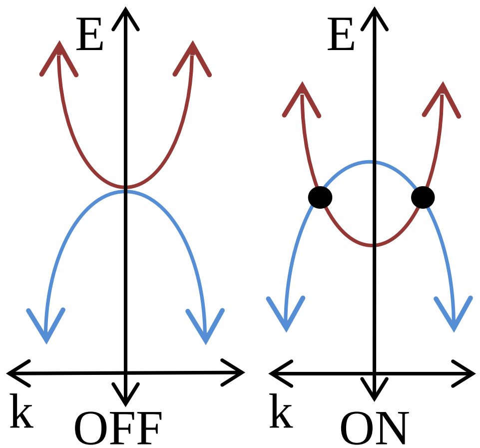


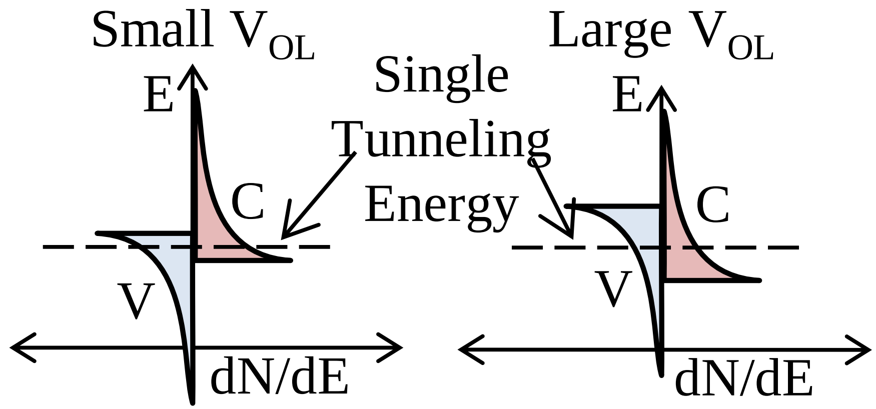
Compare the Structures

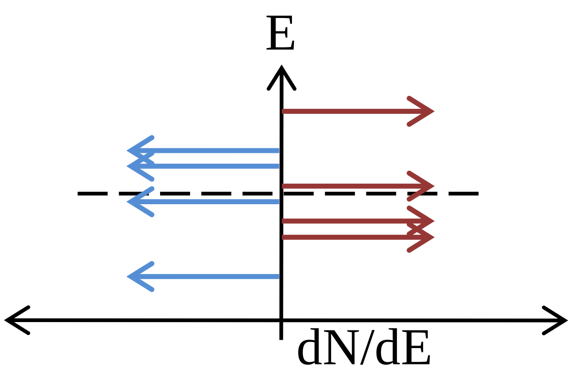


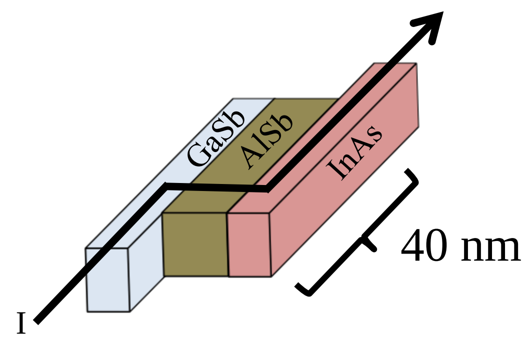
$G_{1d\text{-}1d,\ edge}$ is 10 times larger than $G_{2d\text{-}2d,\ edge}$!

What is the Difference Between the Analytic Model and Simulation?



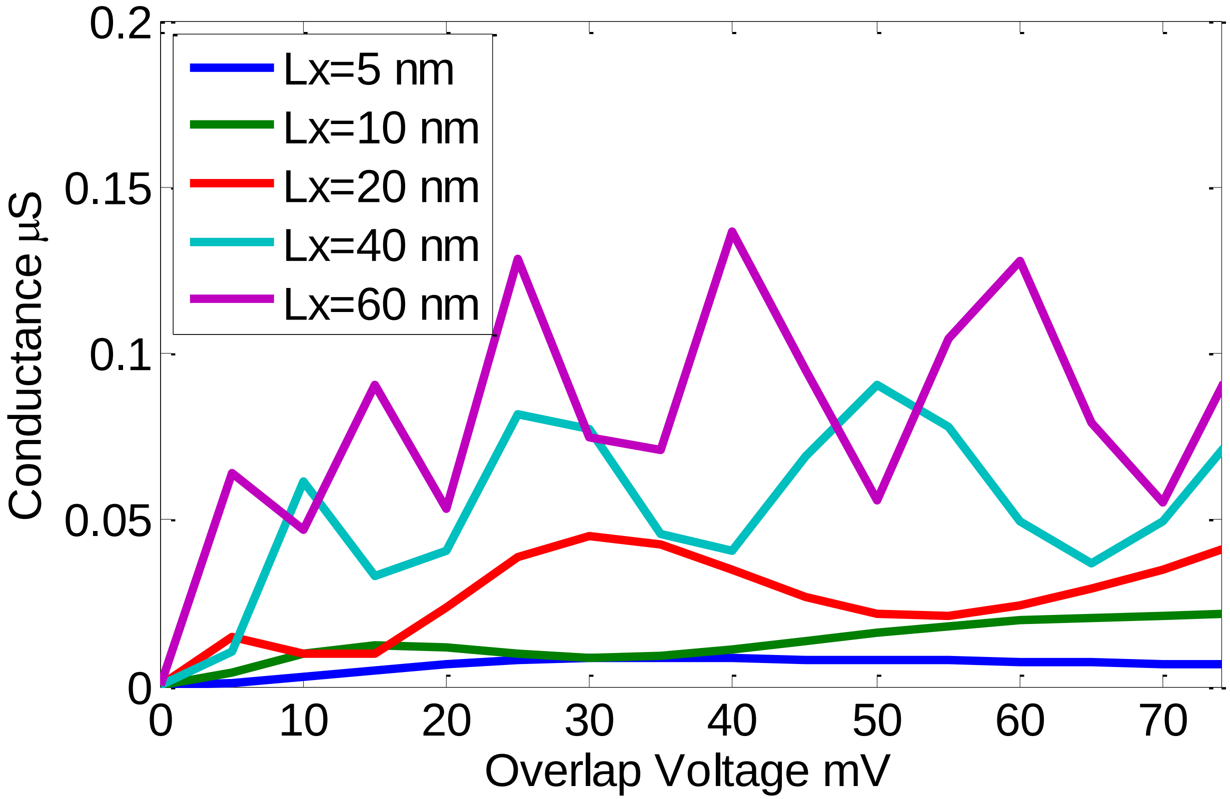


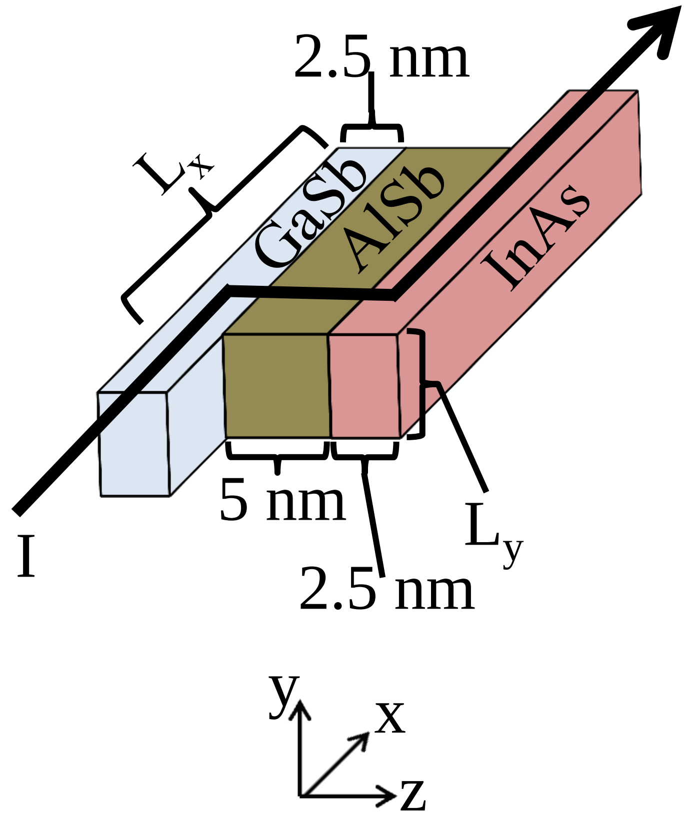




Need to account for discrete transverse states

What Happens When the Overlap is Increased?





Assumed $k_y=0$

Define a Hamiltonian for the System

- Start with an 8 band k.p Hamiltonian

$$H = \begin{bmatrix} H_{\mathrm{int}} & 0 \\ 0 & H_{\mathrm{int}} \end{bmatrix} + H_{S.O.} \quad H_{\mathrm{int}} = \begin{bmatrix} E_C + \frac{\hbar^2 k^2}{2m_o} & +iP_o k_x & +iP_o k_y & +iP_o k_z \\ -iP_o k_x & \begin{matrix} E_V + \hbar^2 k^2/2m_o \\ +M(k_y^2 + k_z^2) + L' k_x^2 \end{matrix} & N' k_x k_y & N' k_x k_z \\ -iP_o k_y & N' k_x k_y & \begin{matrix} E_V + \hbar^2 k^2/2m_o \\ +M(k_x^2 + k_z^2) + L' k_y^2 \end{matrix} & N' k_y k_z \\ -iP_o k_z & N' k_x k_z & N' k_y k_z & \begin{matrix} E_V + \hbar^2 k^2/2m_o \\ +M(k_x^2 + k_y^2) + L' k_z^2 \end{matrix} \end{bmatrix}$$

- Convert k to a discrete spatial derivative

$$k_x x_n = -i \frac{\partial}{\partial x} x_n = \frac{-i}{2a}(x_{nx+1} - x_{nx-1})$$

- Write Hamiltonian for each grid point to get spatial variation

$$H_{S.O.} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & -i & 0 & 0 & 0 & 0 & 1 \\ 0 & i & -1 & 0 & 0 & 0 & 0 & -i \\ 0 & 0 & 0 & -1 & 0 & -1 & i & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & -1 & i & 0 \\ 0 & 0 & 0 & -i & 0 & -i & -1 & 0 \\ 0 & 1 & i & 0 & 0 & 0 & 0 & -1 \end{bmatrix}$$

Principles Behind NEGF Calculation

Electron density is given by a sum of delta functions

$$D(E) = \sum_{\alpha} \delta(E - \varepsilon_{\alpha})$$

Write the delta function as a limit

$$2\pi \times \delta(E - \varepsilon_{\alpha}) = \left. \frac{2\eta}{(E - \varepsilon_{\alpha})^2} \right|_{\eta \to 0^+}$$

$$= i \left[\frac{1}{E - \varepsilon_{\alpha} + i\eta} - \frac{1}{E - \varepsilon_{\alpha} - i\eta} \right]_{\eta \to 0^+}$$

Converting this to a matrix gives the spectral density function, A

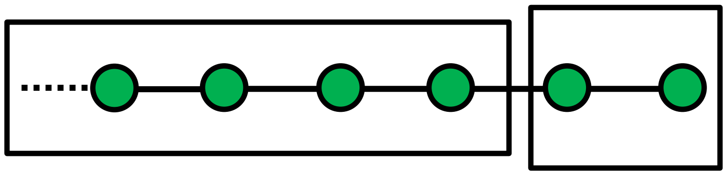
-Consider the eigenstates of H as the basis

$$A = i\left[G(E) - G^{+}(E)\right]$$

$$\text{where } G(E) = \frac{1}{E - \varepsilon_{\alpha} + i\eta}$$

Thus we have defined the Green's function as a convenient way to express a delta function

How to deal with an infinite contact?



Contact/ Reservoir

Channel

Channel Hamiltonian (Size d X d) ⟵ Small

$$\overline{H} = \begin{bmatrix} H & \tau \\ \tau^{+} & H_R \end{bmatrix}$$

Coupling between channel and contact (Size d X R)

Contact Hamiltonian (Size R X R) ⟵ Huge!!

$$\overline{G} = \left[(E+i0^{+})I - \overline{H}\right]^{-1} = \begin{bmatrix} (E+i0^{+})I - H & -\tau \\ -\tau^{+} & (E+i0^{+})I - H_R \end{bmatrix}^{-1}$$

$$= \begin{bmatrix} A & B \\ C & D \end{bmatrix}^{-1} = \begin{bmatrix} G & G_{dR} \\ G_{Rd} & G_{RR} \end{bmatrix}^{-1}$$

Only care about the electron density in the channel and thus G

$$G = (A - BD^{-1}C)^{-1}$$

$$= \Big(\underbrace{(E+i0^{+})I - H}_{\text{Invert the channel part}} - \Sigma\Big)^{-1}$$

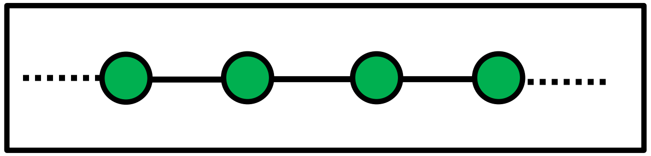
where $\Sigma = \tau G_R \tau^{+}, G_R = \left[(E+i0^{+})I - H_R\right]^{-1}$

Invert the channel part

Subtract our the effect of the contact/reservoir

If we know the self energy, Σ, finding G is easy

Trick to finding Σ



In the contact adjacent atoms are identical and have the same electron density

$$G = \left[(E + i0^+)I - H - \Sigma\right]^{-1}$$

$$\Sigma = \tau G_R \tau^+$$

$$G_R = \left[(E + i0^+)I - H_R\right]^{-1}$$

$G=G_R$

Solve the equation self consistently for G

How to Find Current

Weight the electron density from the left contact by f_1 and the electron density from the right contact by f_2

$$\text{Evaluate } I = \frac{d}{dt}\psi^{+}\psi$$

$$\text{using } i\hbar\frac{d\{\psi\}}{dt} = [H]\{\psi\}$$

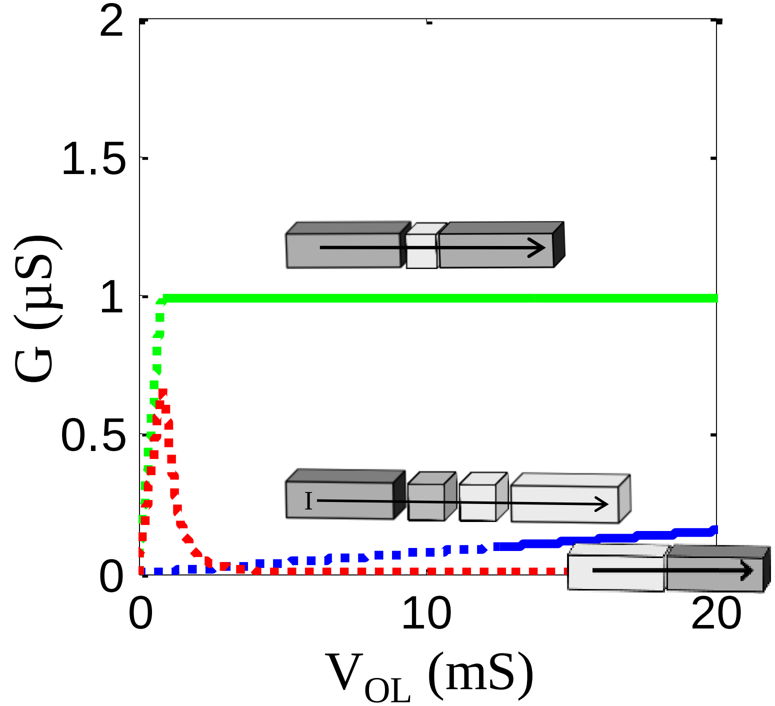
Sandia National Laboratories

What do We Know So Far

- Need a steep density of states to get a steep subthreshold swing
  - Must eliminate doping: Use bilayer or double gate lateral FET
  - Vertical FET needs doping and so it will not work
- Lateral FET has a gate efficiency ~1
- Bilayer has a gate efficiency ~ 0.5
- Bilayer has a higher I_{ON} and lower overdrive voltage

Can we Improve the Lateral Structure?

- Increase T from ~1% to 50%
  - How?
  - Would reduce the required overdrive voltage and increase I_{ON}
- If we can't increase T, use quantum confinement in a lateral structure I-V is a delta function



Gate Controls Band Overlap