NEEDS
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CICC Seminar, San Jose, Sept 30, 2015

PURDUE ENGINEERING

Physics-based Compact Models for Biosensors, Landau Transistors, & Thin-Film Solar Cells

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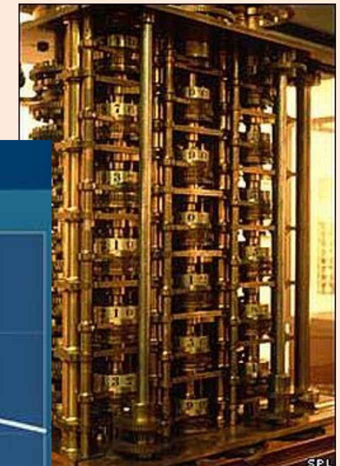
Outline

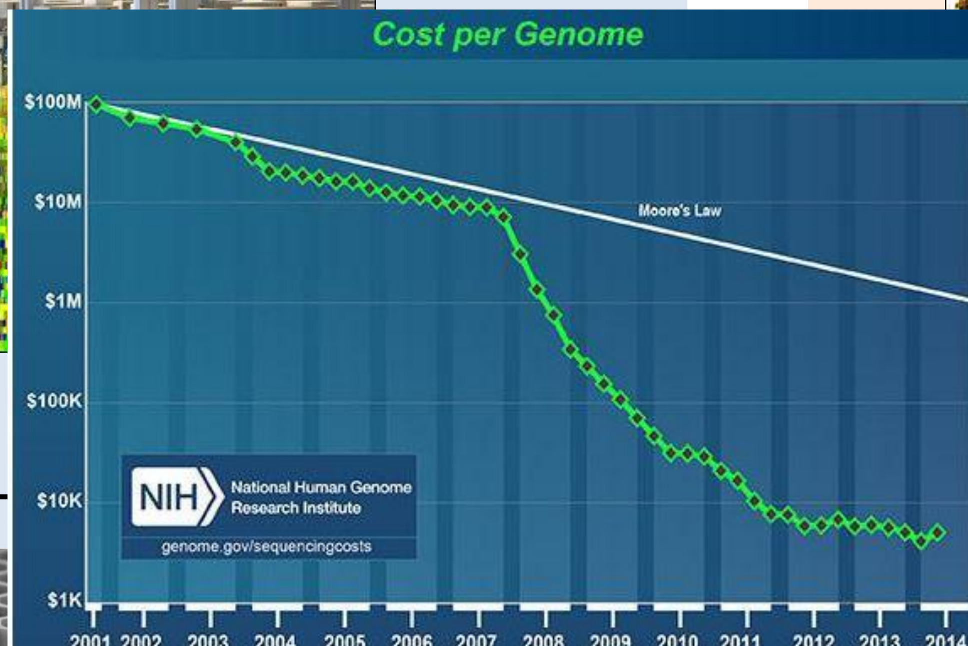
- Is there a life after Moore's Law?
- Power sources: Harvesters, solar cells, etc.
- Implantable and clinical nanobiosensors
- Low-power Landau switches
- The challenges of integrated simulation
- Conclusions

Life after Moore's law: The Transistor is Dead, Long live The Transistor

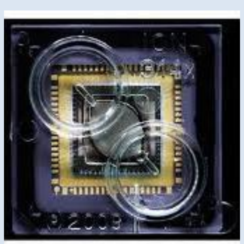
Sanger method (1990s)

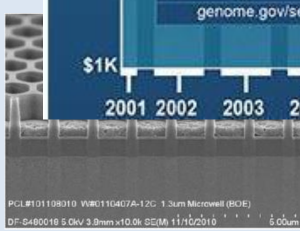
Babbage computer (~1830s)





Ion-

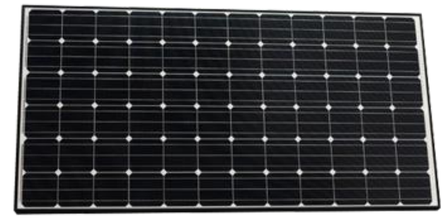




tel Chip Today

Live After Moore's law: End-to-end modeling of solar cells

Scaling up can induce efficiency gap



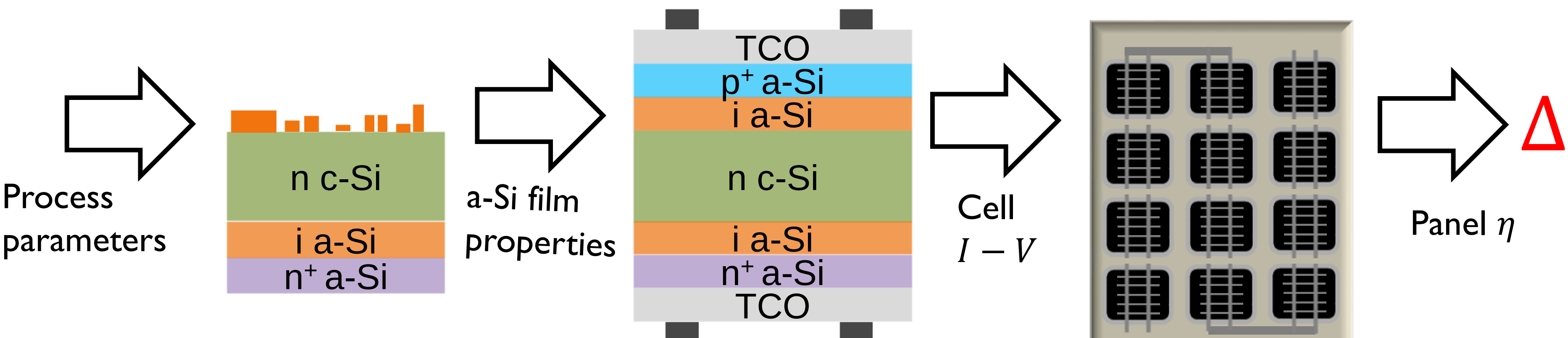
Record cell efficiency >22%

State-of-the-art commercial panels: 19.4%

Process variations

Contacts and shunts

Grid resistance, shading etc.



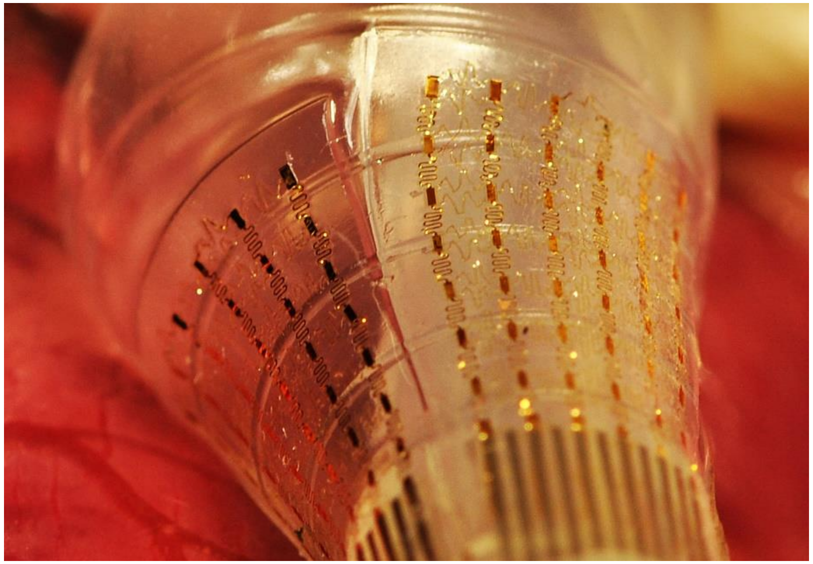
Process stage

Device stage

Panel stage

ITRPV, 2013, Panasonic, N-285 series,, Ballif, *et al.*, 2014

Life after Moore's Law: Heterogeneous integration on active substrate

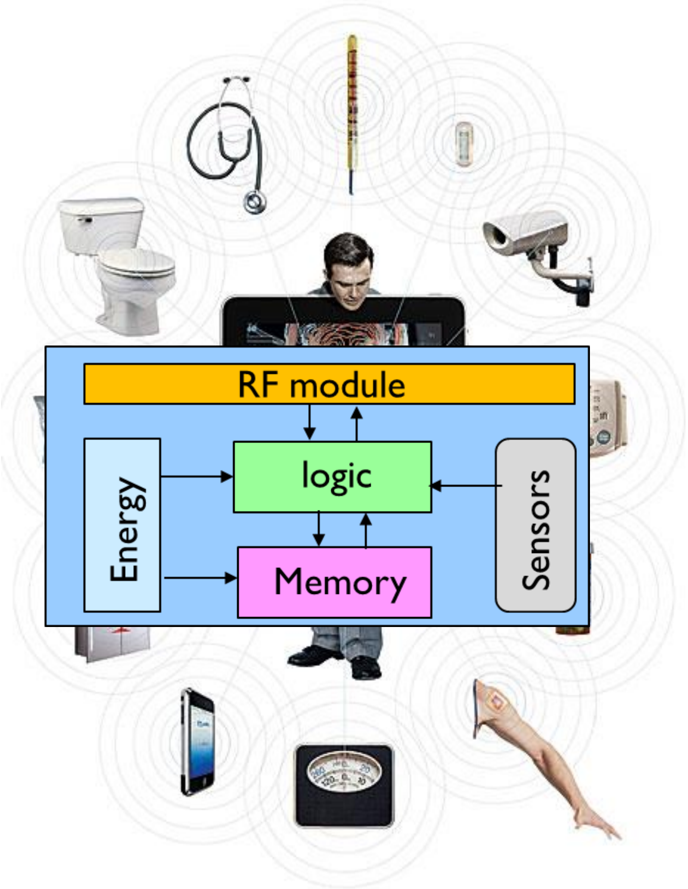


Reliability in fluids
Energy harvesting
Noise immunity
Biofouling

M.A. Alam, Purdue University, 2015

Life after Moore's Law: Internet of (too many?) things …

Lab-on-a-phone
(nano+biotechnology)



Always on sensor network
(nanotechnology + biotechnology + wireless technology)

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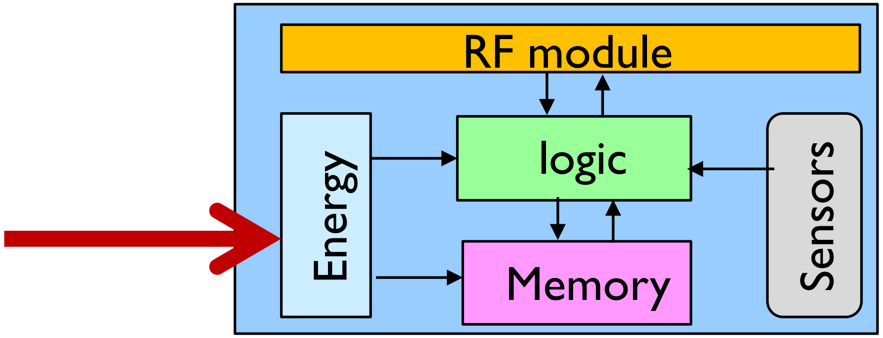
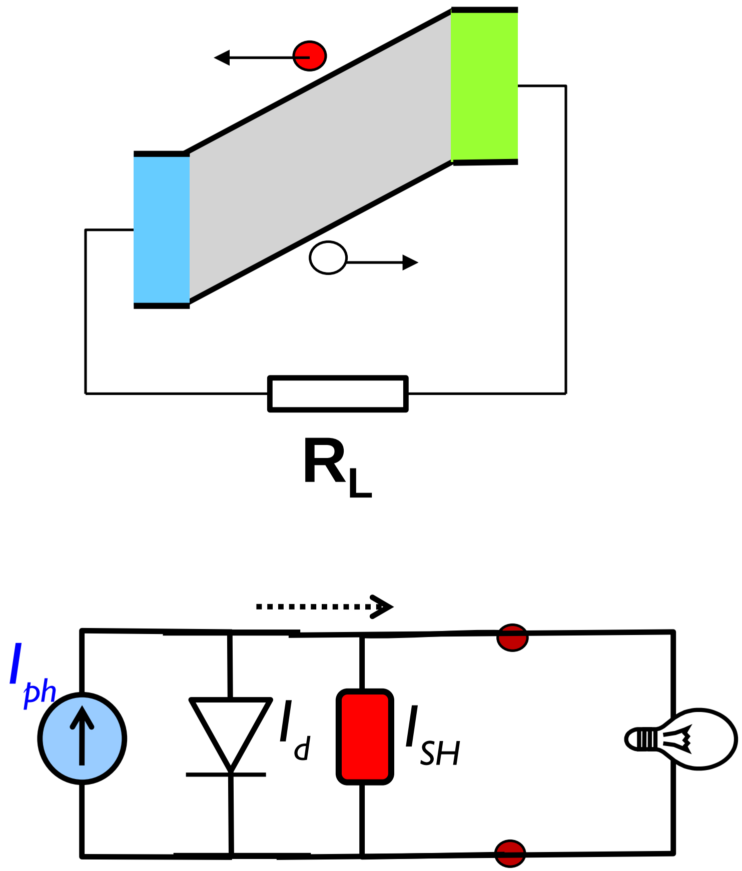
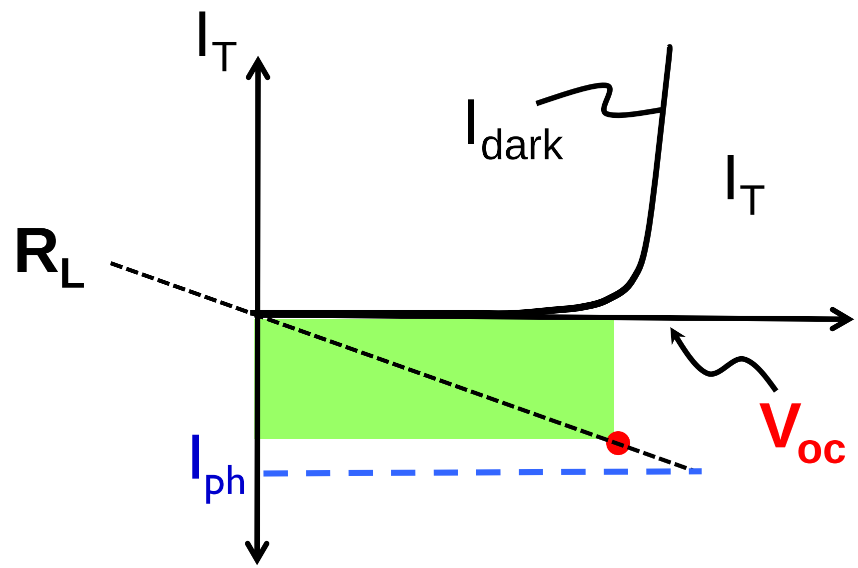


Basics of solar cell operation

Alam, Proc. IRPS, p. 312, 2010.

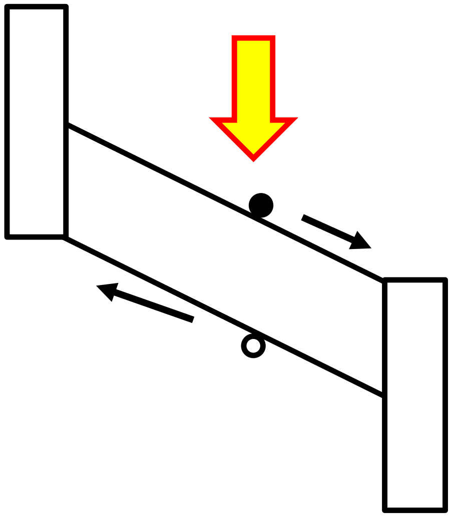




Voltage independent photocurrent
Good for c-Si, but almost nothing else

Technology-agnostic end-to-end modeling

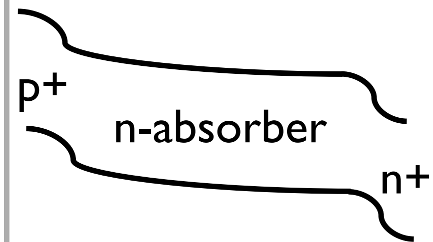
Ideal solar cell



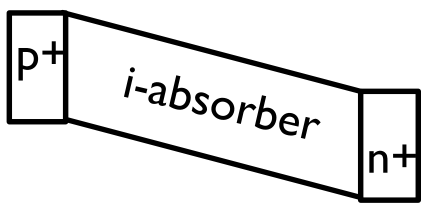
- Photo-generation in absorber layer only
- Strong electric field to push carriers to contacts
- Carrier selective contacts to minimize recombination

Reality

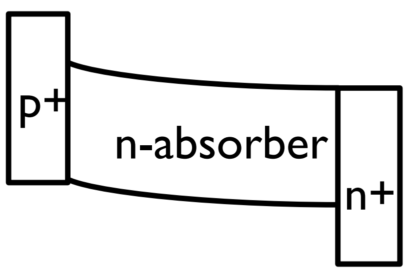
p-n homojunction



p-i-n homojunction

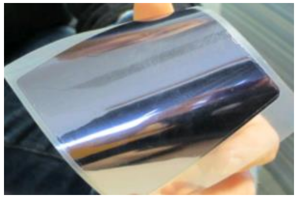


P-n heterojunction



Technologies

High Performance & High Costs



GaAs

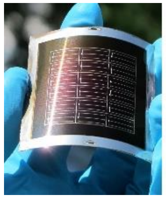
c-Si

Low Performance & Low Costs

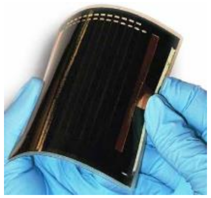
a-Si cell

High Performance & Low Costs

HIT cell



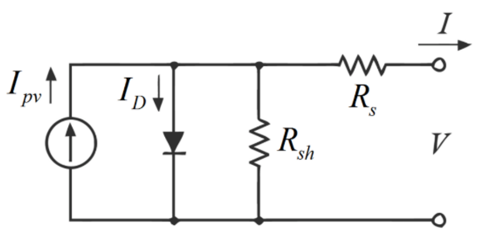
CdTe

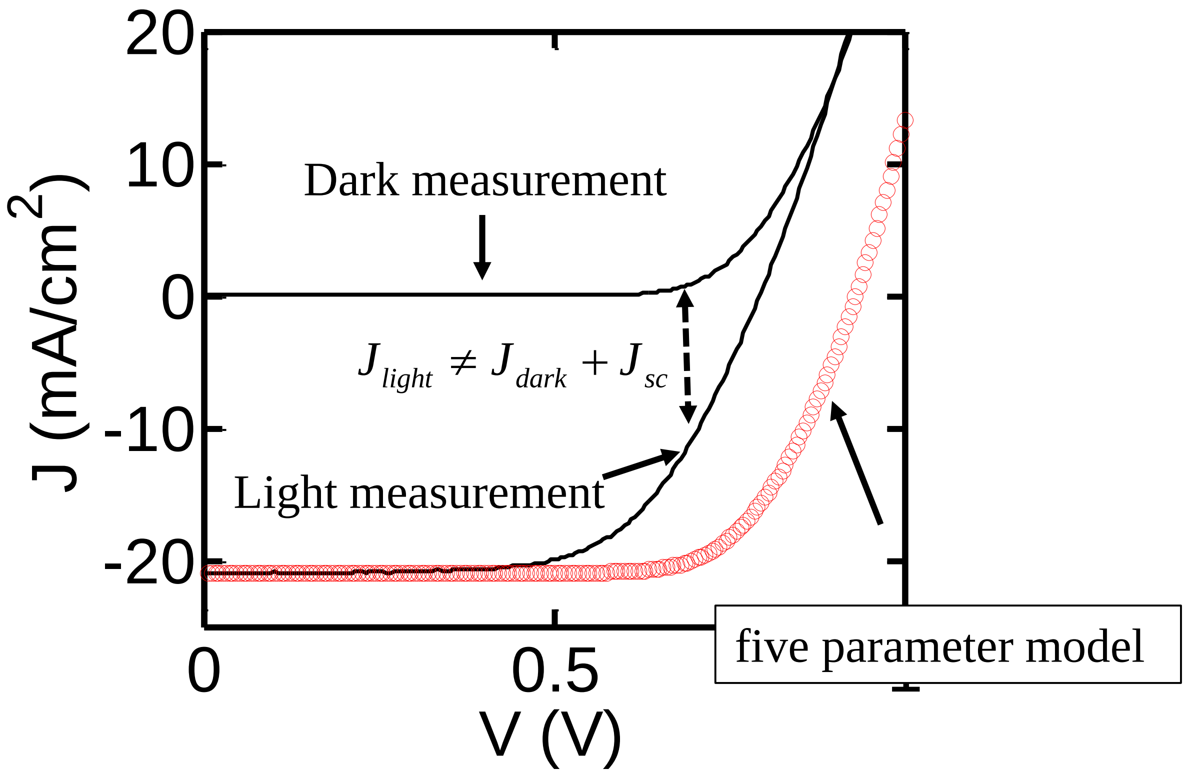


CIGS

*Google Images

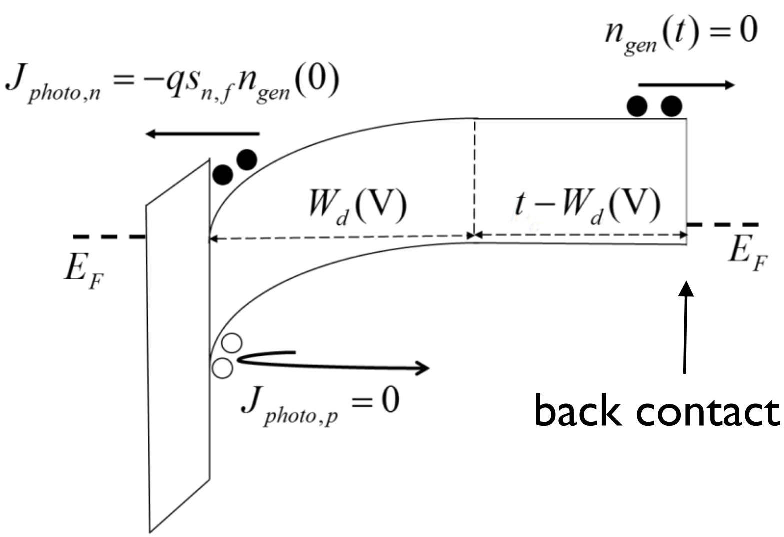
Si Compact Model .. Not appropriate for Thin-Film HJ Cells





Temperature dependence is completely wrong!

A new compact model for HJ Cells



we solve the electron continuity equation **ONLY** considering the **generated** carriers

$$D\frac{\partial^2 n_{gen}(x)}{\partial x^2} + \mu E(x)\frac{\partial n_{gen}(x)}{\partial x} + G(x) = 0$$

$$J_{photo,n} = q\mu E(x)n_{gen}(x) - qD\frac{\partial n_{gen}(x)}{\partial x}$$

$$J_{photo} = \frac{J_{tot}\left(1 - e^{-\chi\sqrt{\frac{V_{bi}-V}{V}}}\right)}{1 + \alpha_c e^{\beta\frac{q(V-V_{bi})}{kT}}}$$

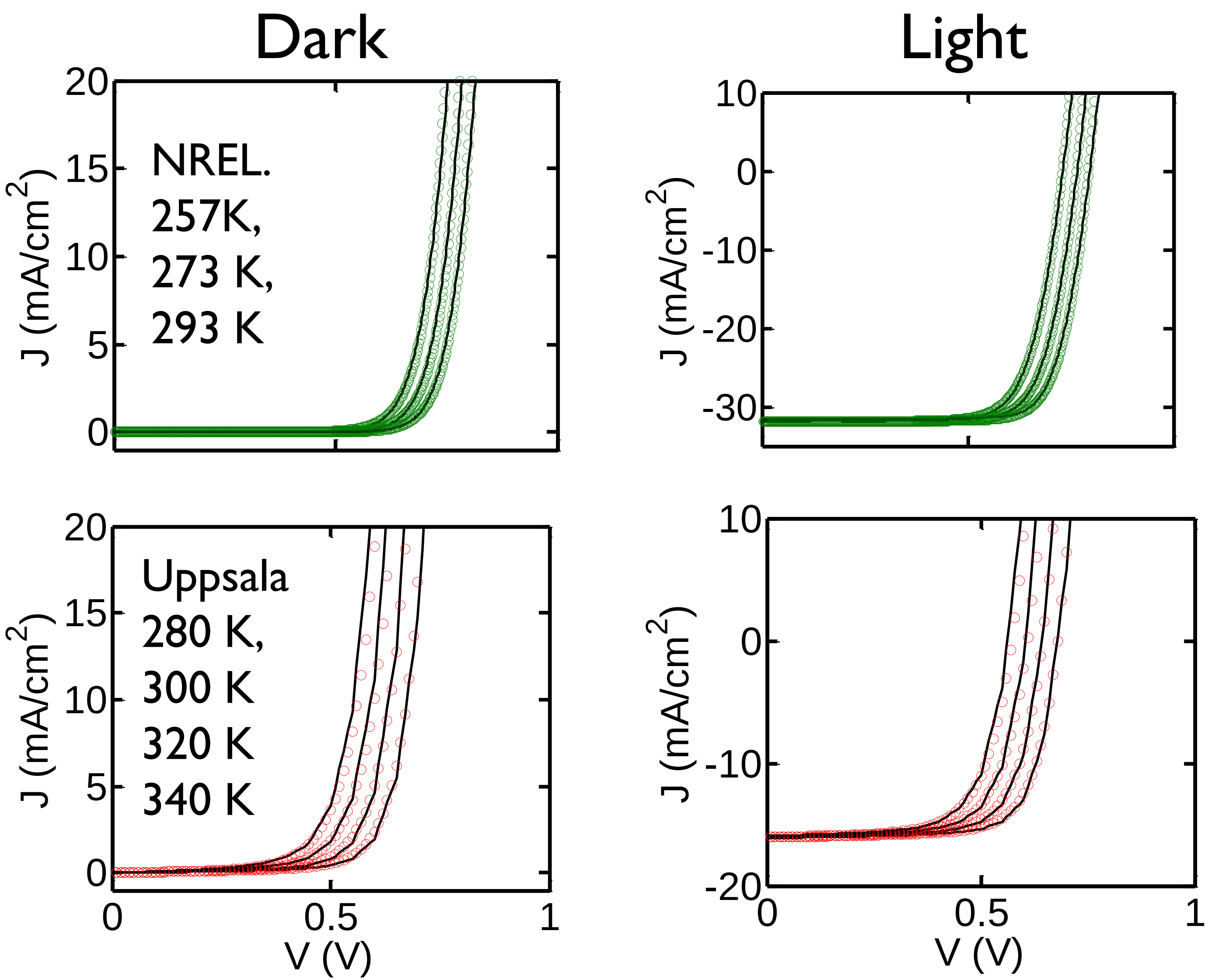
$$J_{dark} = J_0\left(\exp\left(\frac{qV}{NkT}\right) - 1\right)$$

$$\chi = \frac{W_{delp}(0V)}{\lambda_{ave}}$$

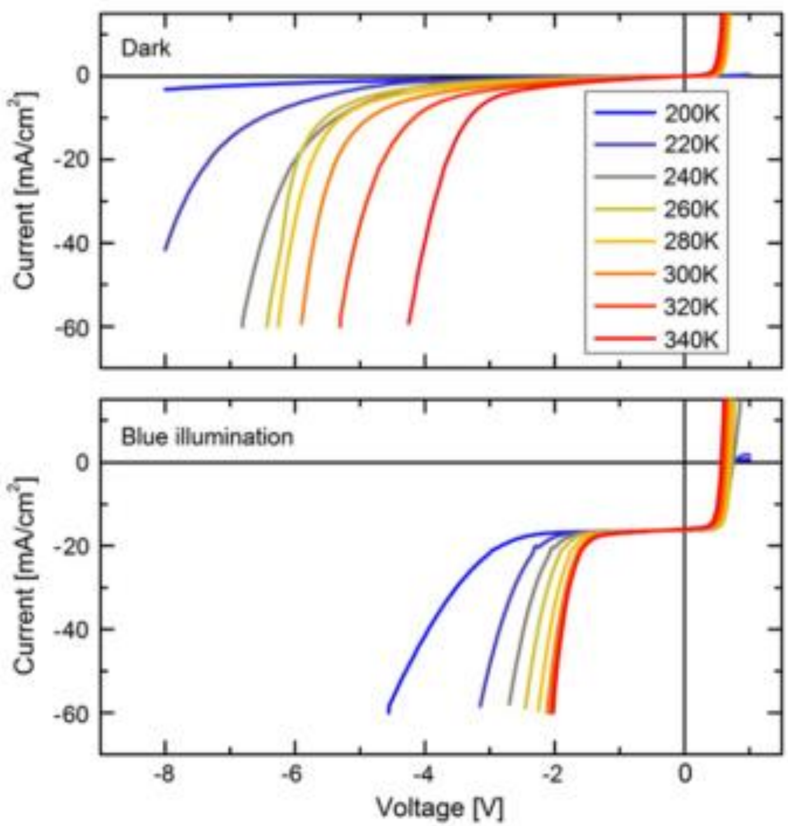
$$\alpha_c = \frac{s_{n,b}}{s_{n,f}}$$

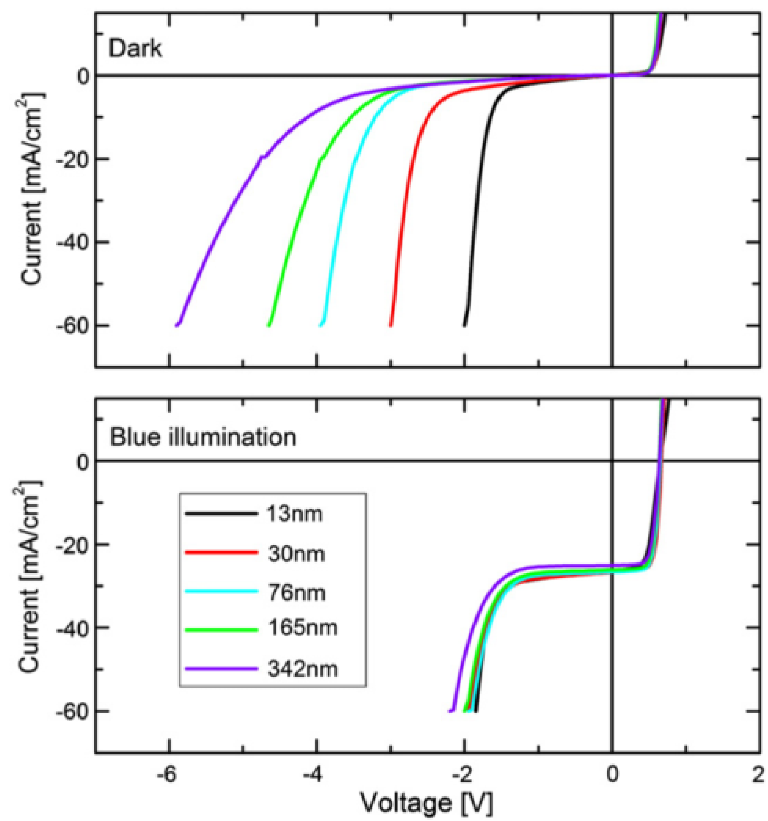
Silverman et al., JPV, 2015.

Model Captures CIGS Response



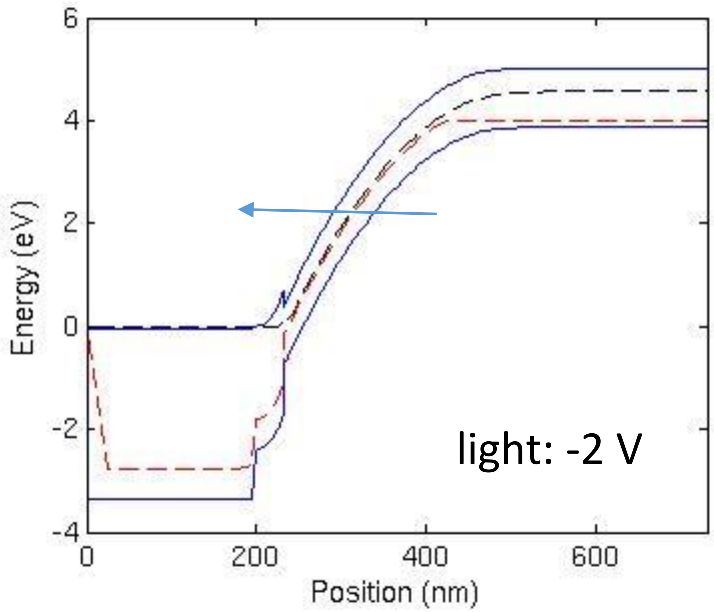
Model Captures Light Enhanced Breakdown

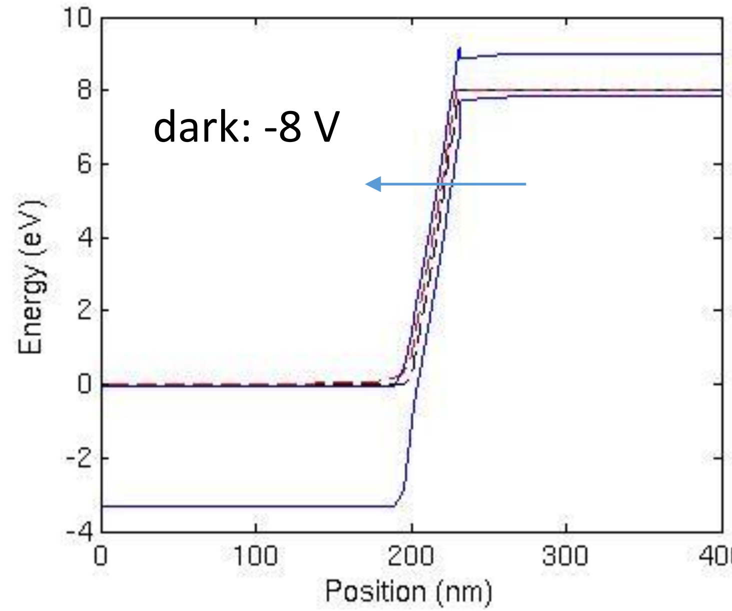




P. Szaniawski, J. Lindahl, T. Törndahl, U. Zimmermann, and M. Edoff, "Light-enhanced reverse breakdown in Cu(In,Ga)Se2 solar cells," *Thin Solid Films*, vol. 535, pp. 326–330, May 2013.

A very strange diode in Reverse Bias

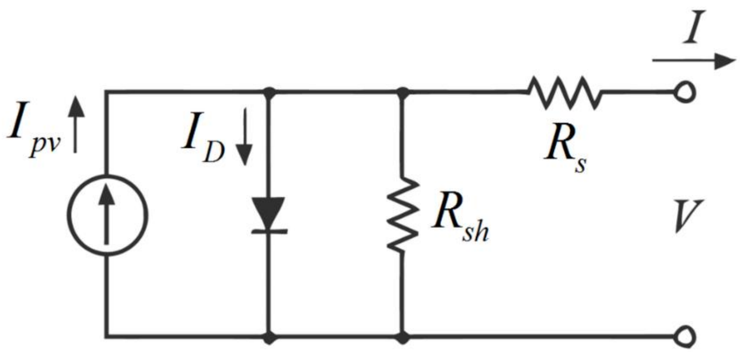


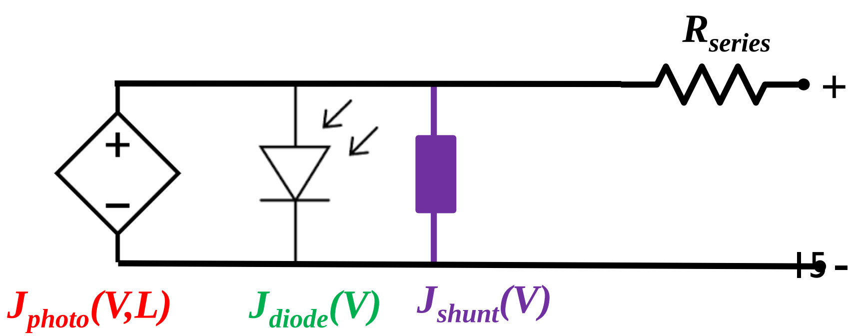


$$J_{FP} = J_0 \frac{V}{t} \exp\left(\frac{q}{kT}\sqrt{\frac{q}{\pi \varepsilon_o \varepsilon_{buffer}}}\sqrt{\frac{V}{t}}\right)$$

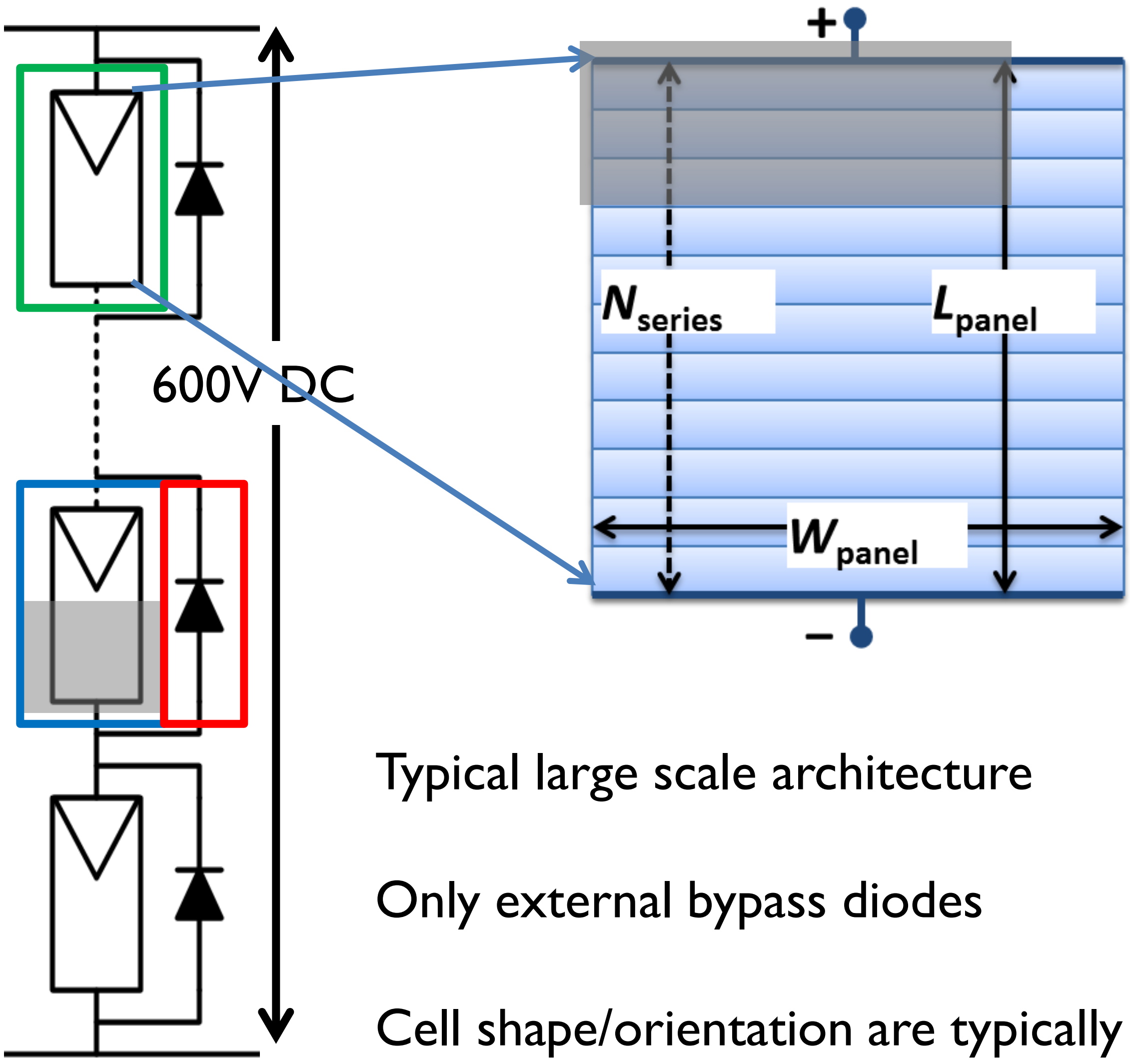
$$J_0 \sim exp(-\frac{q\Phi_{defect}}{kT})$$

New Compact Model





Partial shading in string architecture

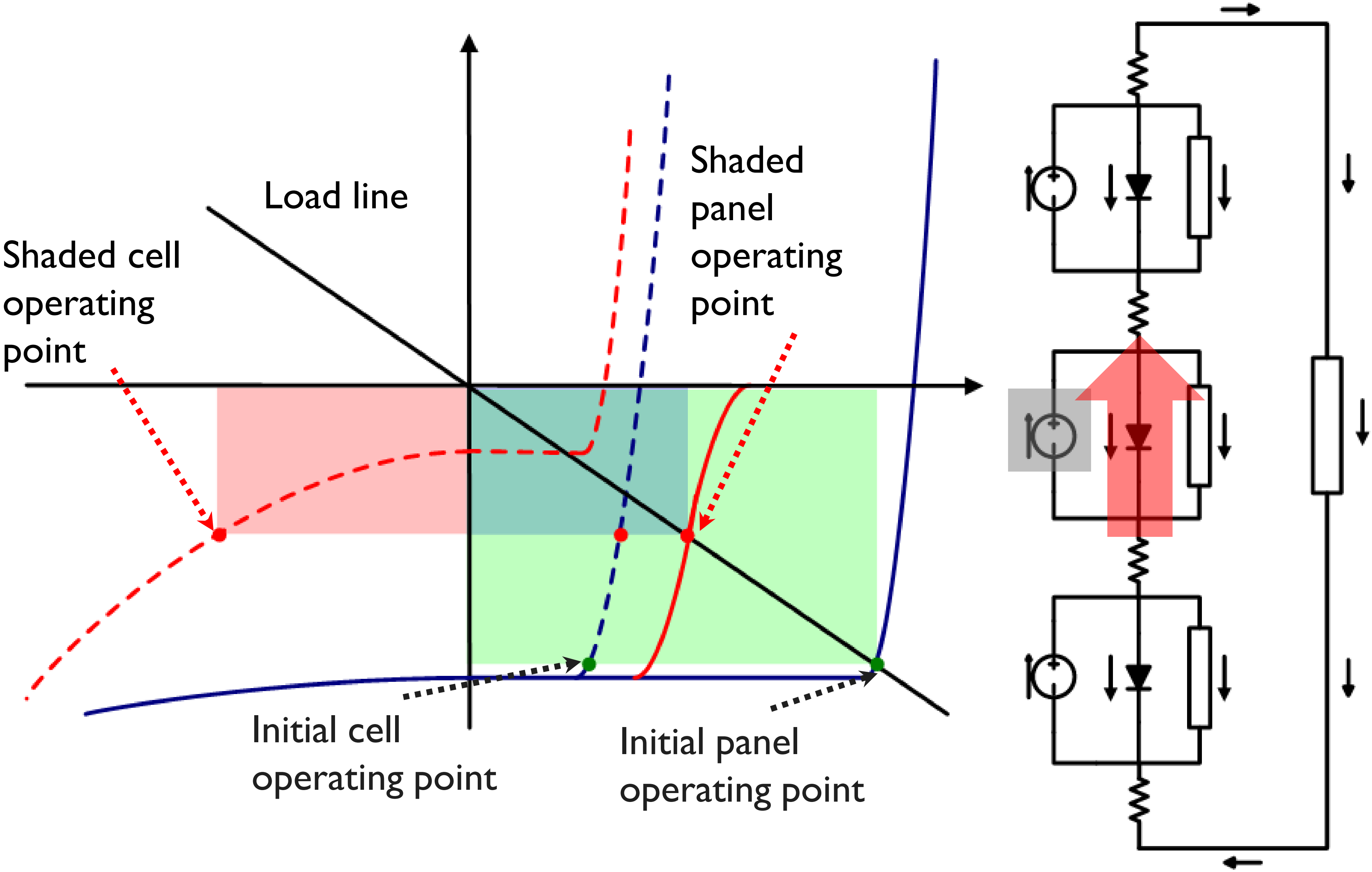


Typical large scale architecture

Only external bypass diodes

Cell shape/orientation are typically not considered

Being in shadow stresses the device

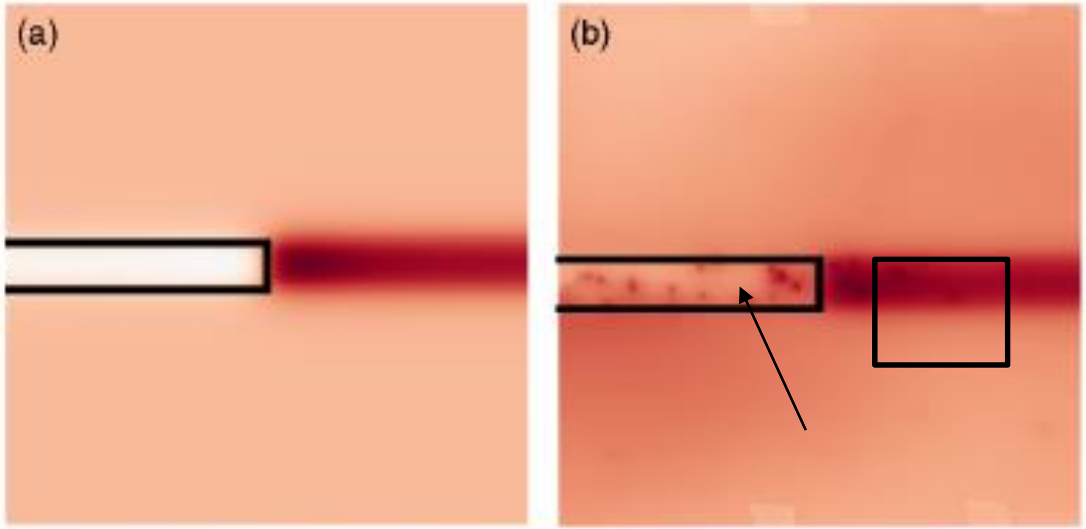


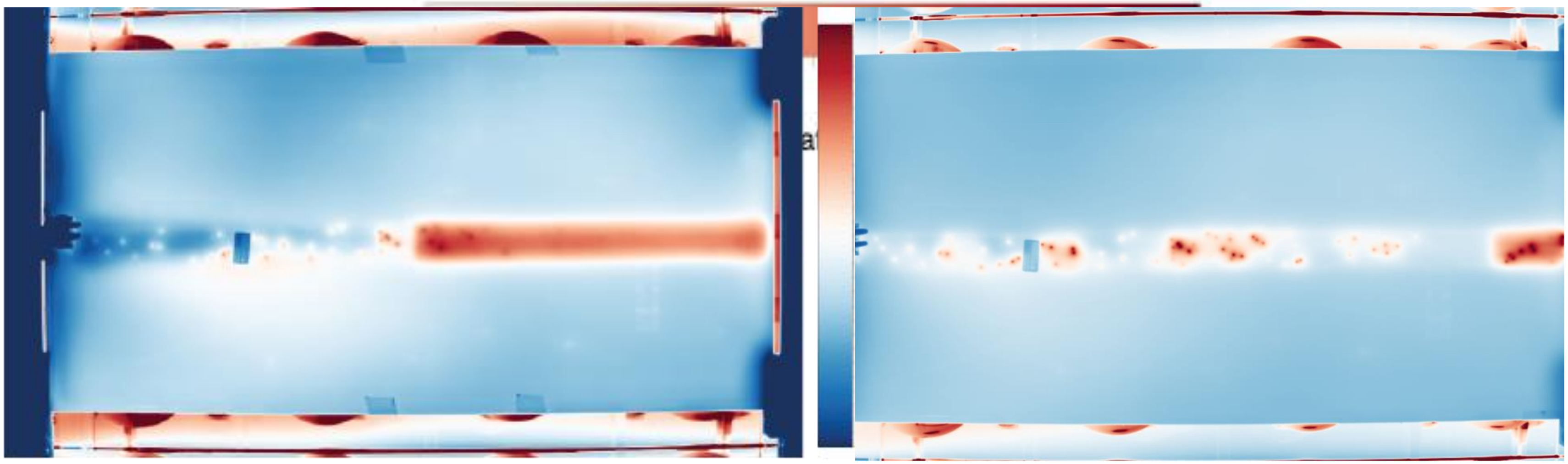
Shaded cells can get reverse biased!

Simulation reproduces experiments

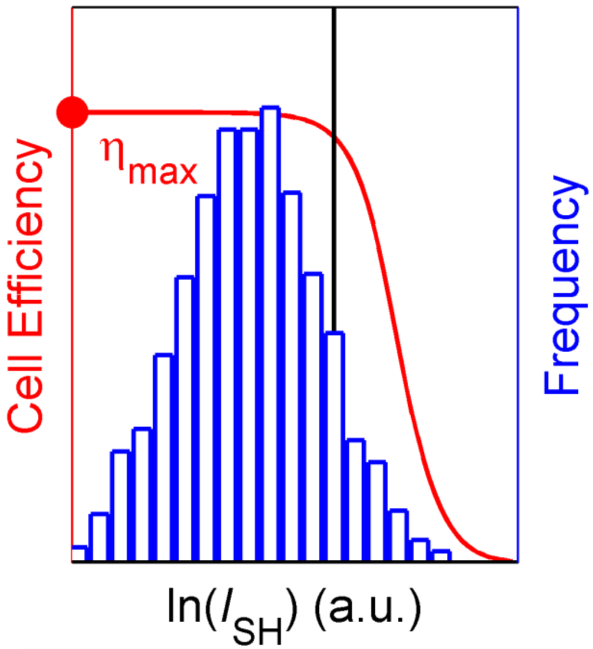
Simulation

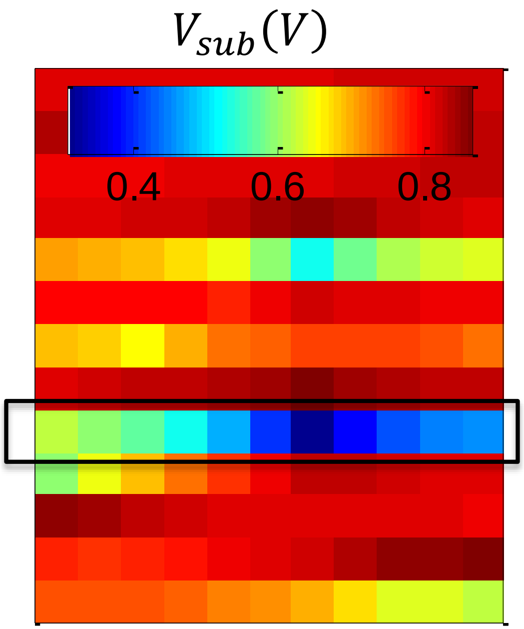
IR image

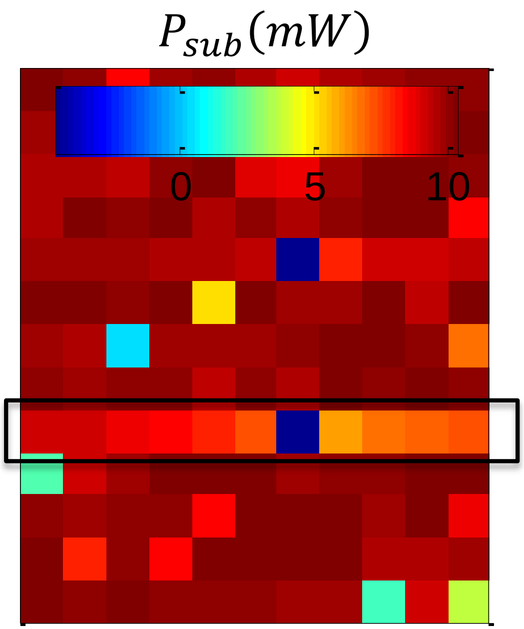




Impact of heavy tailed shunt distribution







Heavy tail of shunt distribution determines the number of low efficiency shunted cells

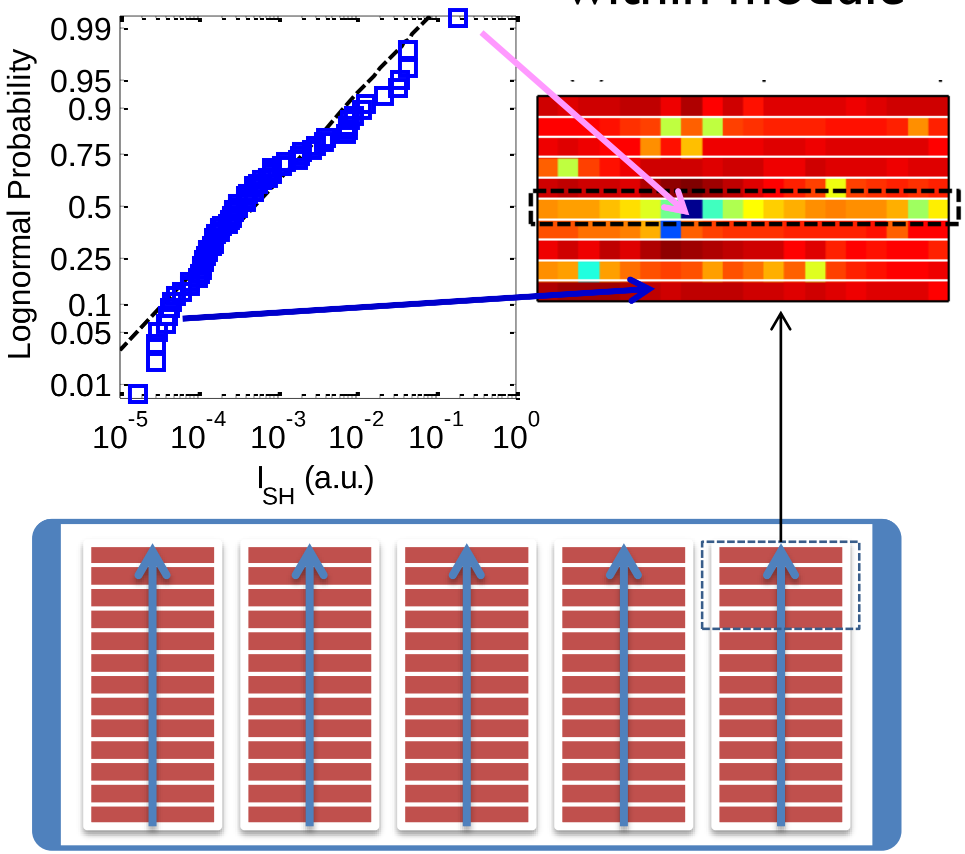
Shunted cells modify the bias of entire row, affecting the power output of their neighbors

Shunted cells drain the power output of neighbors, with disproportionate impact on module output

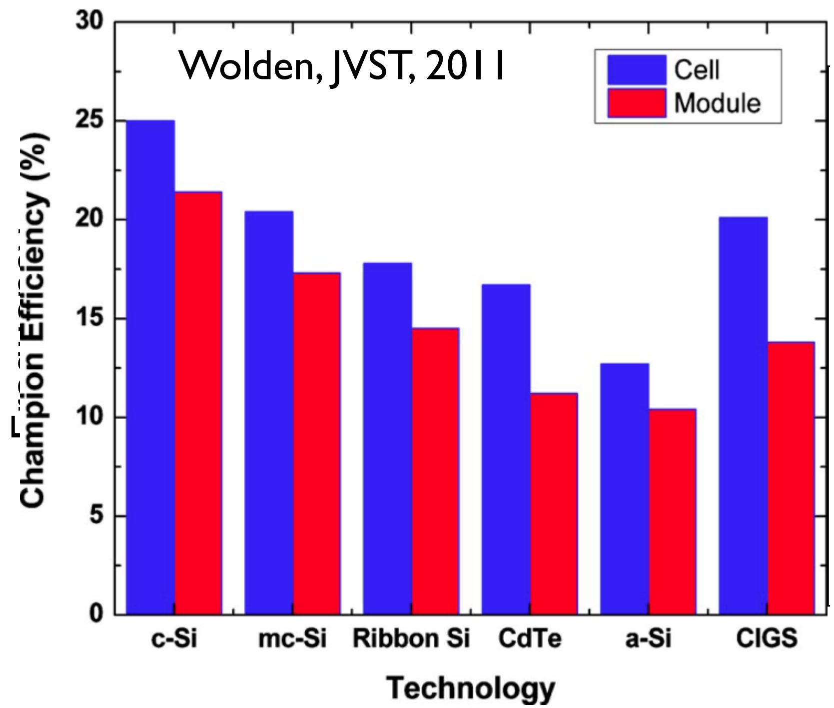
Long range interaction between sub-cells determines module performance loss

Panel vs. Cell Efficiency Gap Universal ?!

Shunts distributed within module



shunt and series resistance explain the gap



Cell/panel gap is essentially technology agnostic

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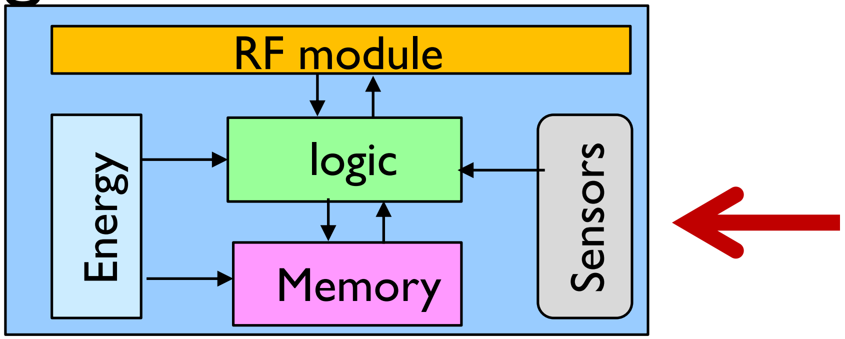
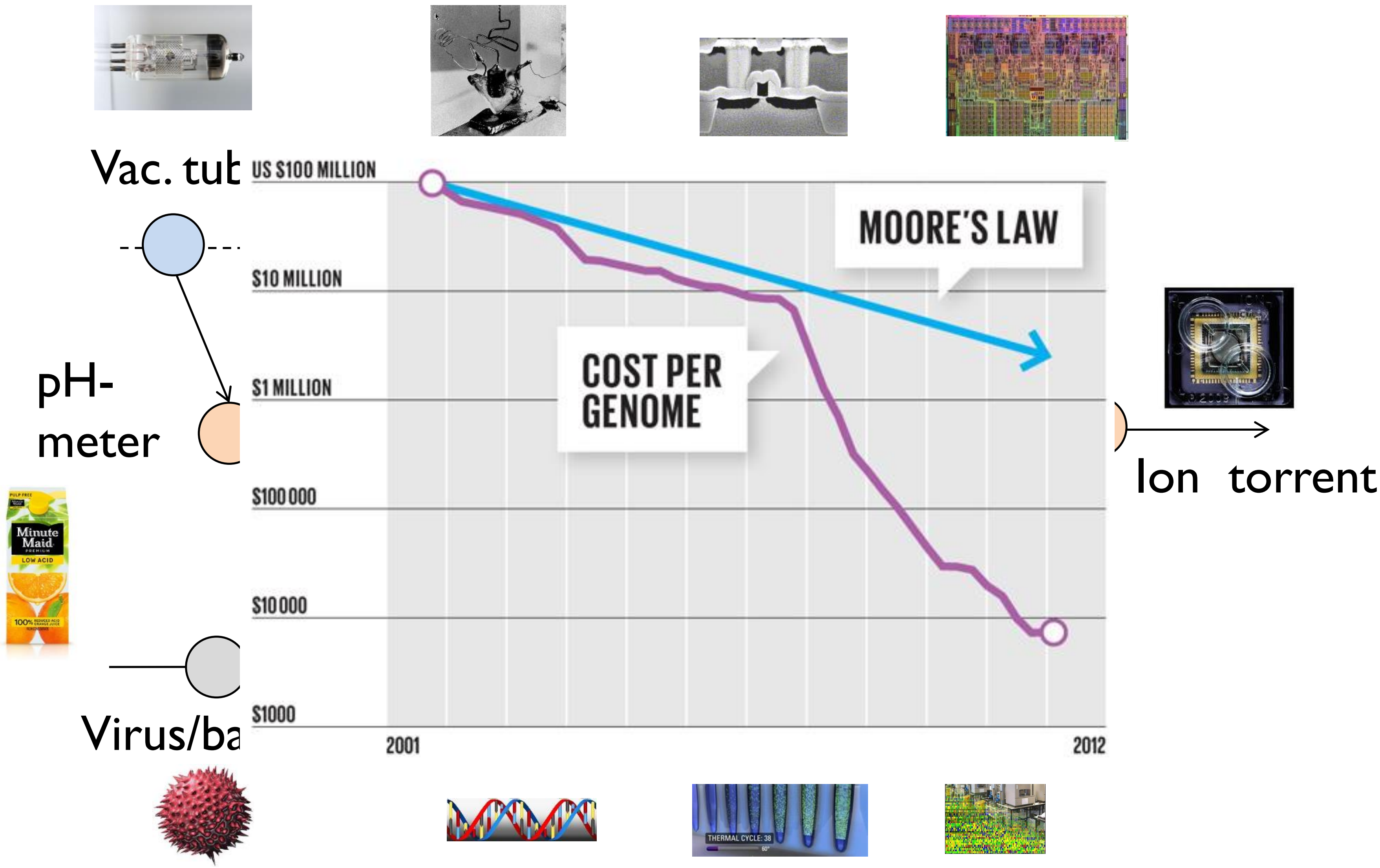
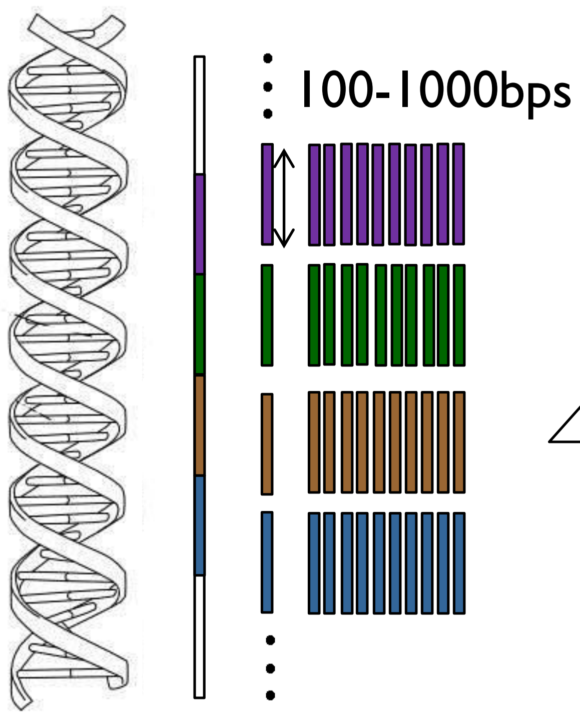
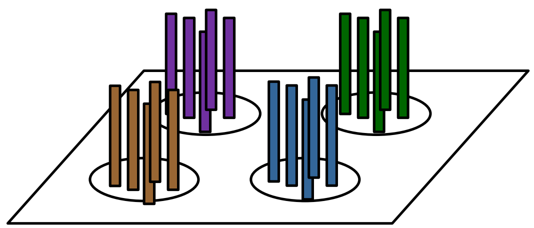


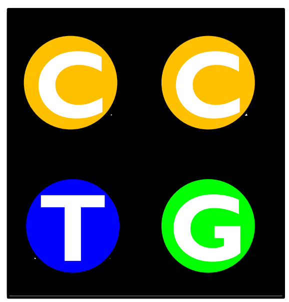
Back-story: A Century-long Convergence

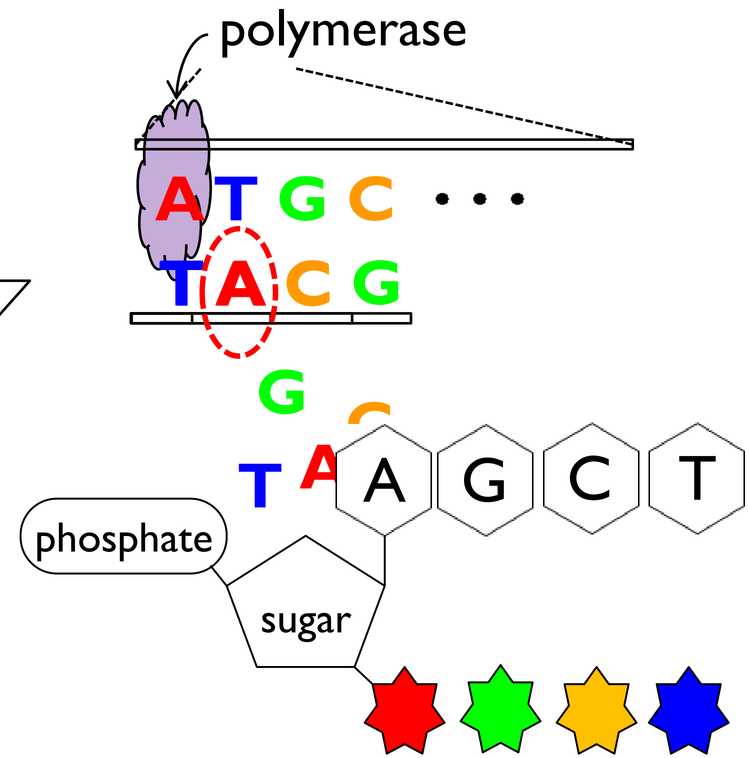


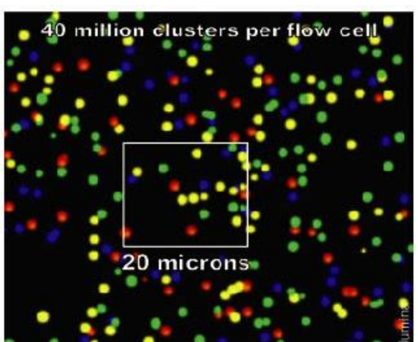
Conventional Sequence-by-Synthesis











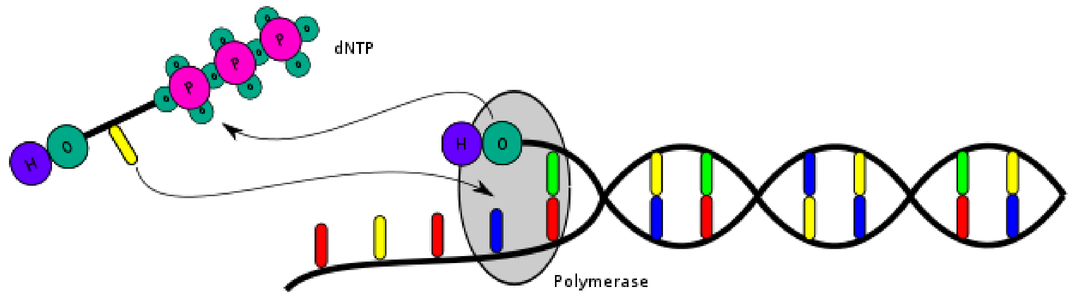
Courtesy of Illumina

Optical detection scheme expensive, because

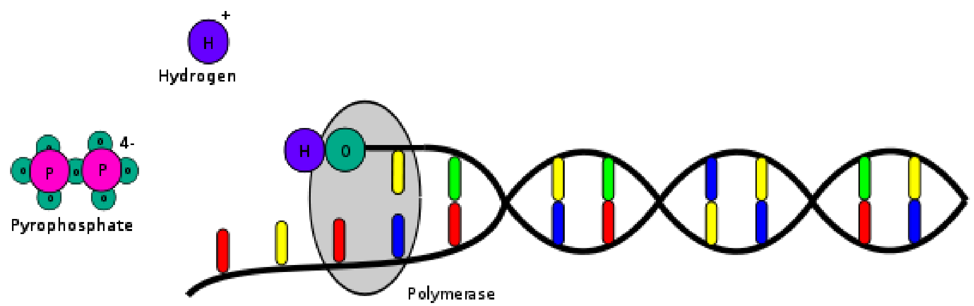
- tagging of bases with fluorescent dye
- bulky and expensive optical detector
- processing costs of high volume images

DNA Synthesis releases Proton

deoxyribonucleotide triphosphate (dNTP)



Polymerase integrates a nucleotide.



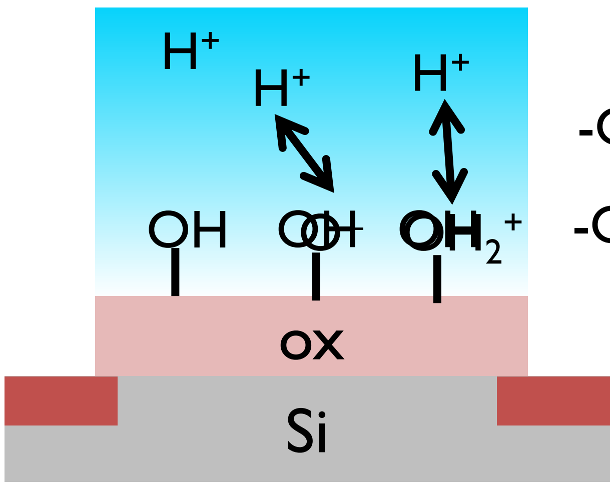
Hydrogen and pyrophosphate are released.

Source: Wikipedia

ISFET: Theory of pH-sensing

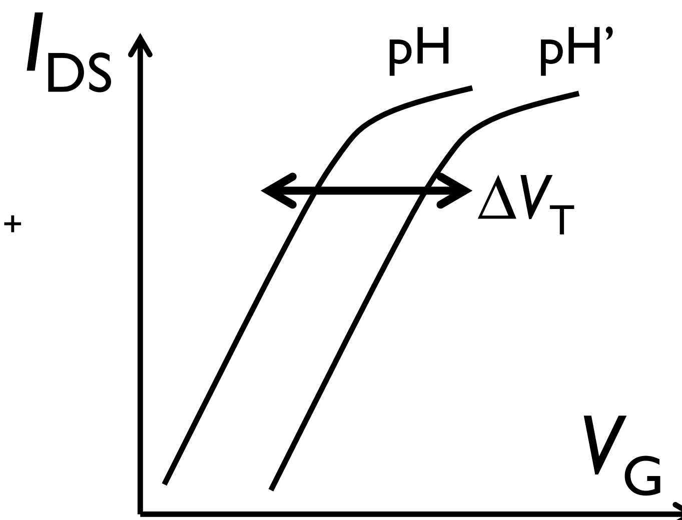
$$\mathrm{pH} = -\log_{10}\left[\mathrm{H}^{+}\right]_{\mathrm{B}}$$

$$\left[\mathrm{H}^{+}\right]_{\mathrm{B}} = 10^{-7}\,\mathrm{M} \Rightarrow \mathrm{pH} = 7$$



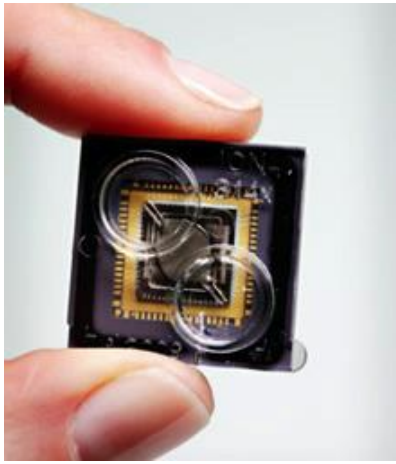
$-\mathrm{OH} \longleftrightarrow -\mathrm{O}^{-} + \mathrm{H}^{+}$

$-\mathrm{OH}_2^{+} \longleftrightarrow -\mathrm{OH} + \mathrm{H}^{+}$

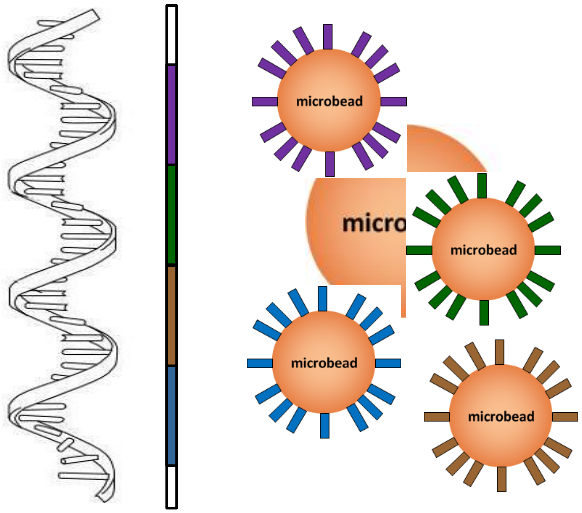


pH sensitivity ≡ $\Delta V_T / \Delta\mathrm{pH} < 59\,\mathrm{mV/pH}$ (Nernst limit)

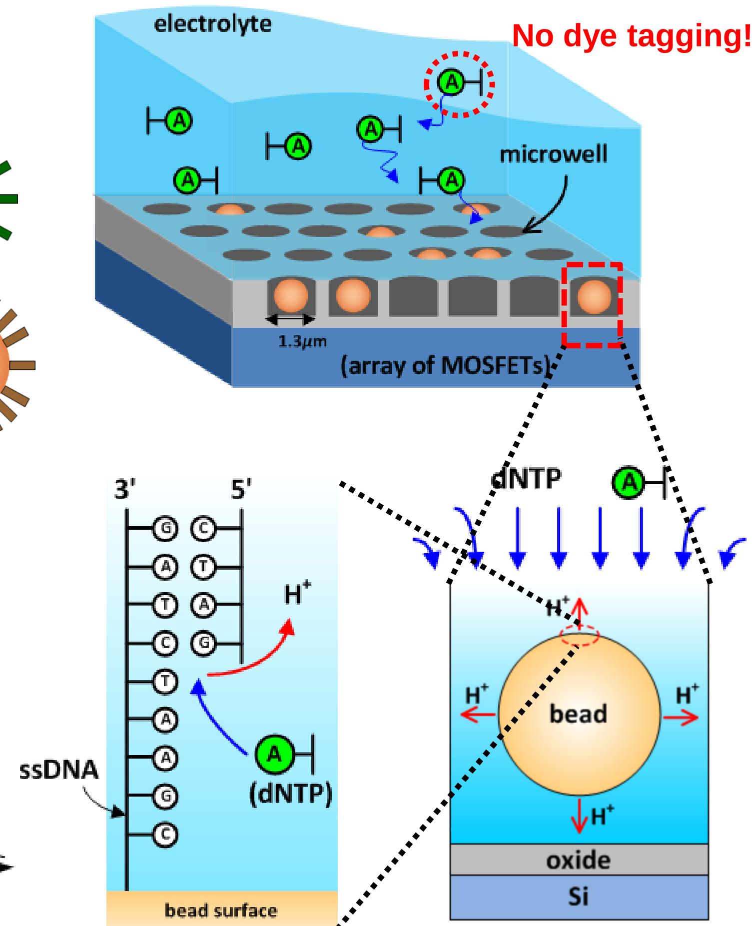
pH-based Genome Sequencers

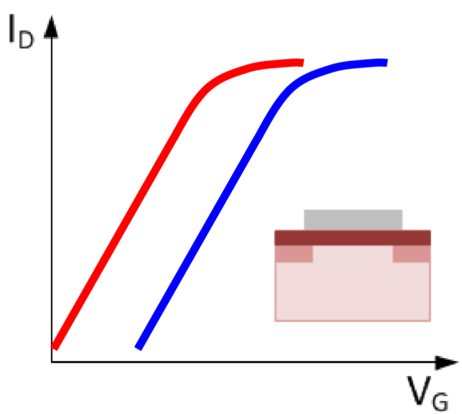


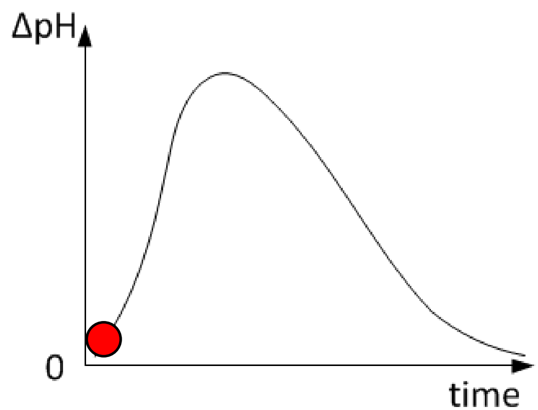
Courtesy of Ion Torrent



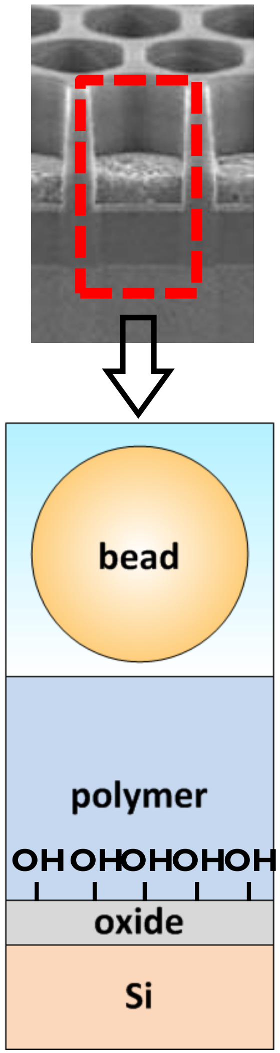
Reference: Rothberg et al., Nature 2011







Modeling Approaches (Go, JAP, 2013)



- Proton diffusion:

$$\frac{\partial(\Delta\rho_H)}{\partial t} = D_H \nabla^2 (\Delta\rho_H)$$

- ISFET electrostatics

$$-\nabla \bullet (\varepsilon \nabla \Psi) = \rho$$

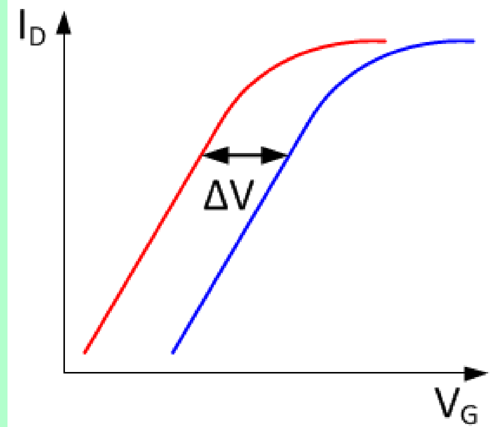
- Reaction of OH groups[1]

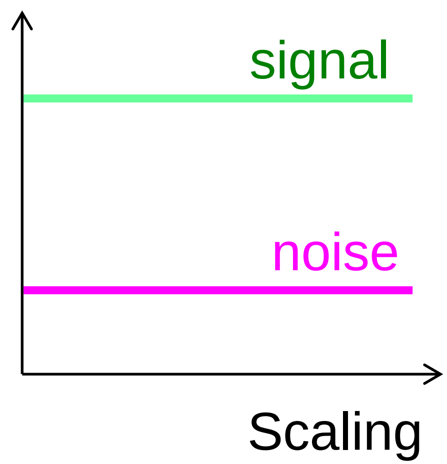
$$\sigma_{\mathrm{OH}} = qN_s \frac{10^{pK_a - \mathrm{pH}_S} - 10^{\mathrm{pH}_S - pK_b}}{1 + 10^{pK_a - \mathrm{pH}_S} + 10^{\mathrm{pH}_S - pK_b}}$$

[1] Landheer at al., JAP 2005

- 1/f noise of ISFET[2]

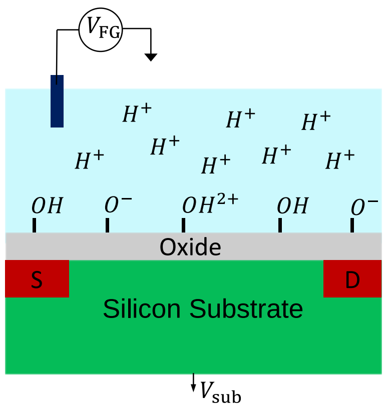
$$\delta V_G = \sqrt{\frac{q^2 k_B T N_t \lambda}{WLC_{eff}^2}} \left[1 + \left(\alpha \mu_{eff} C_{eff} \frac{I_{DS}}{g_m} \right) \right] \log\left(\frac{f_2}{f_1} \right)$$

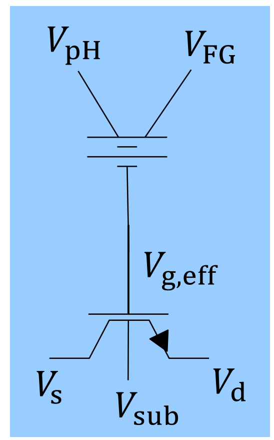


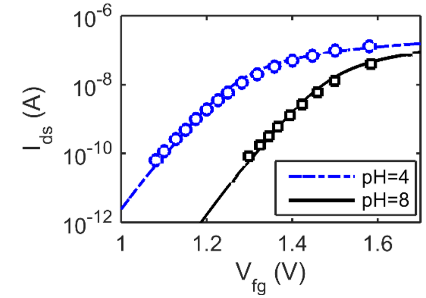


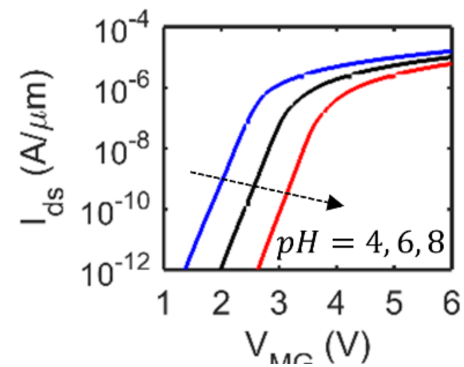
[2] Deen at al., JAP 2006

A Physics-based Compact Model

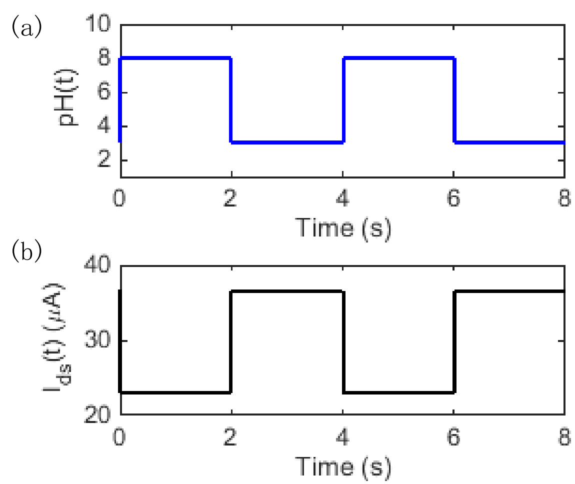


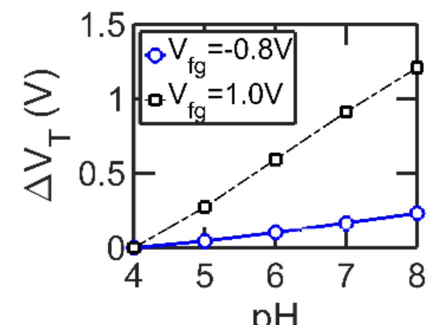






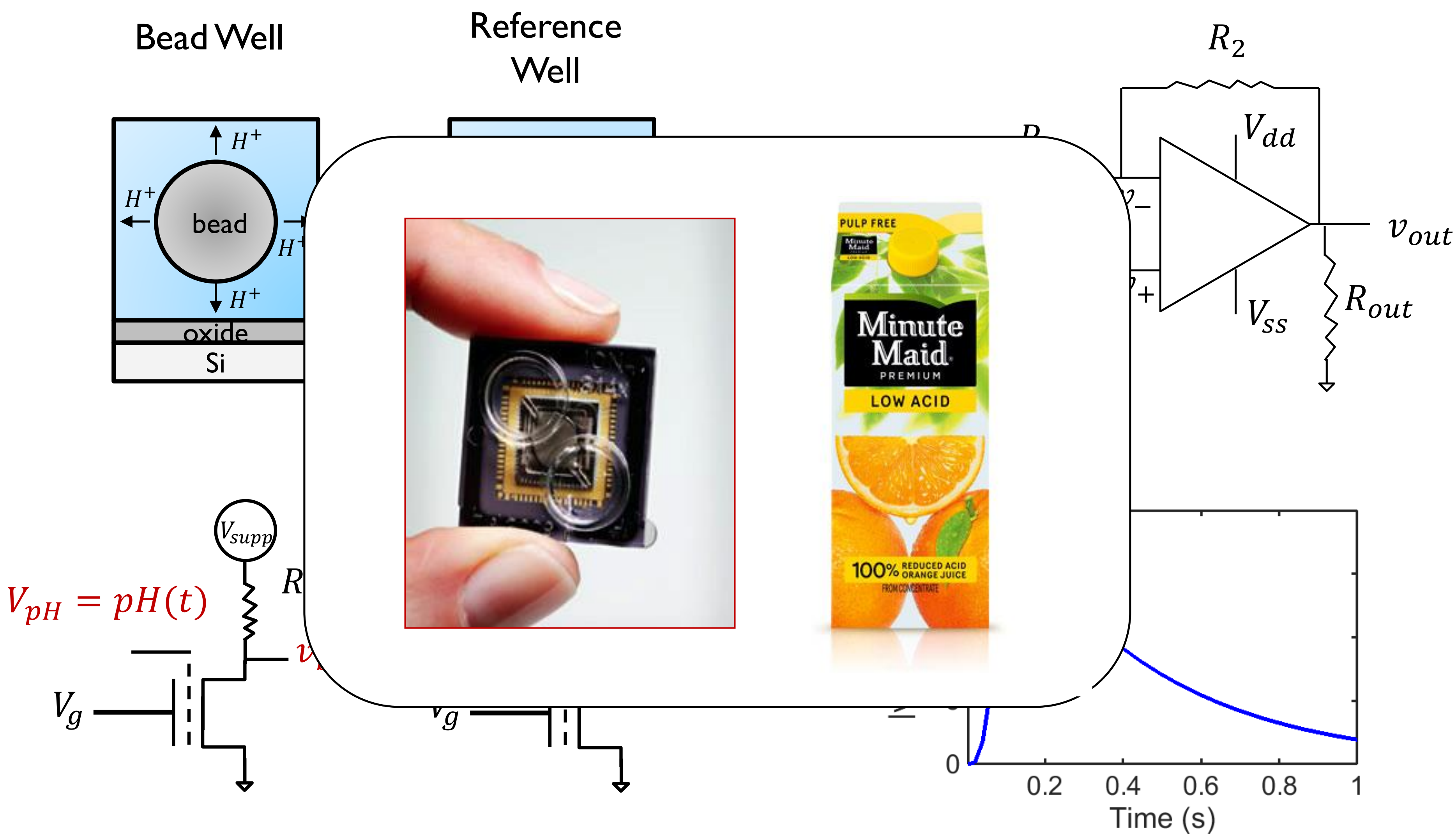
$\sigma_{dl} + \sigma_{OH} + \sigma_{mos} = 0$		(1)
$\mathrm{AOH_2^+} \rightleftarrows \mathrm{AOH} + \mathrm{H_s^+}$	K_a	(2)
$\mathrm{AOH} \rightleftarrows \mathrm{AO^-} + \mathrm{H_s^+}$	K_b	(3)
$\sigma_{OH} = q([\mathrm{AOH_2^+}] - [AO^-])$ $= -2qN_s \dfrac{(\tanh(q\psi_e/kT + 2.3\,\Delta pH))}{(10^{\Delta pK/2}\,\mathrm{sech}(q\psi_e/kT + 2.3\,\Delta pH)}$		(4)
$\psi_e = \psi_0 + \sigma_{OH}/C_{stern}$		(5)
$\sigma_{dl} = -\sqrt{8kT\varepsilon_w n_0}\,\sinh\left(\dfrac{q\psi_0}{2kT}\right)$		(6)
$\psi_e = \dfrac{2kT}{q}\,\mathrm{asinh}\left(\dfrac{\sigma_{OH}}{\sqrt{8kT\varepsilon_w n_0}}\right) + \dfrac{\sigma_{OH}}{C_{stern}}$		(7)
$V_{g,eff} = V_{fg+\psi_e}$		(8)
$\Delta pH = pH - (pK_a + pK_b)/2$		(9)
$\Delta pK = pK_b - pK_a$		
$pK_a = -\log_{10}(K_a),\ \ pK_b = -\log_{10}(K_b)$		(10)





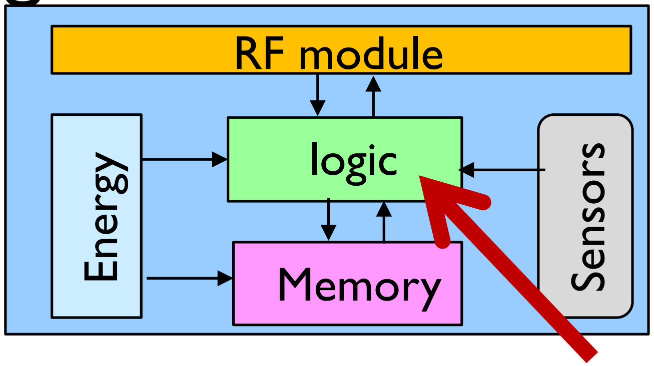
M.A. Alam, Purdue University, 2015

Differential Amplifier Circuit Used

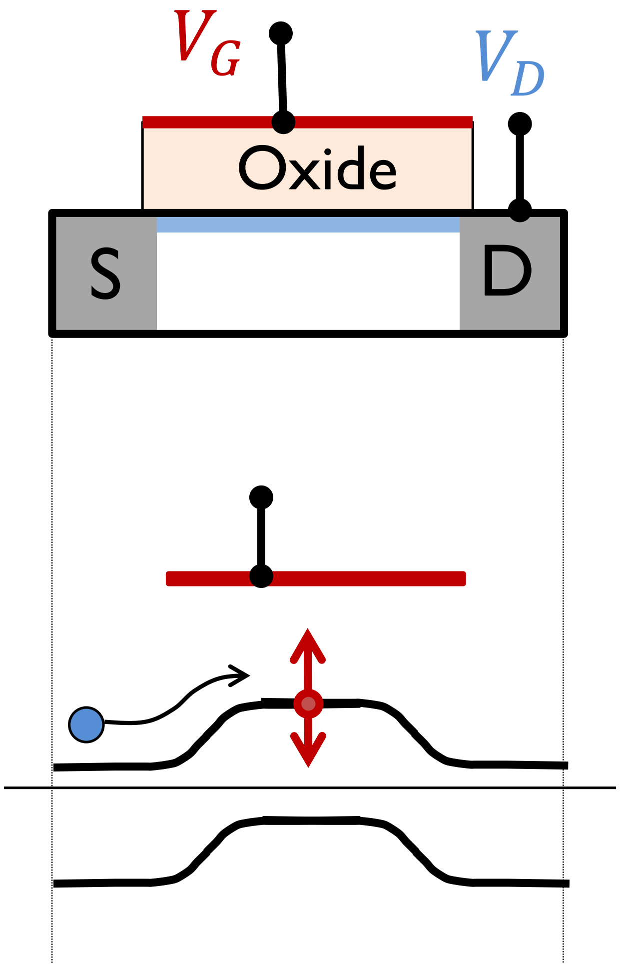


Outline

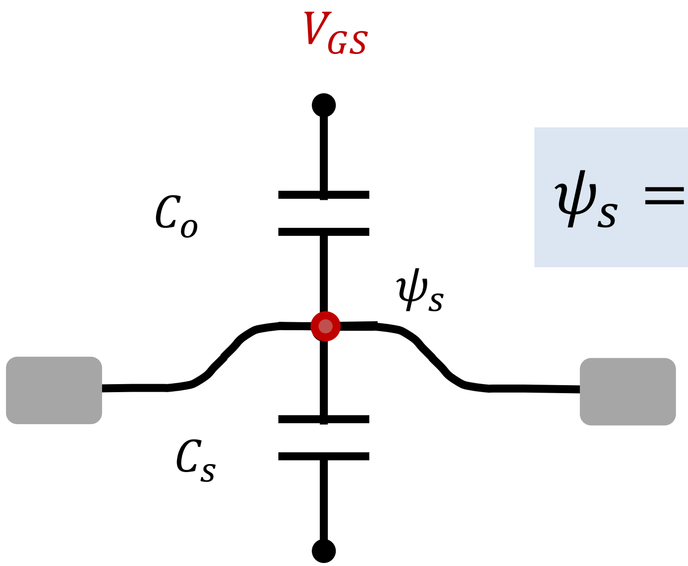
- Is there a life after Moore's Law
- Power sources: Harvesters, solar cells, etc.
- Implantable and clinical nanobiosensors
- Low-power Landau switches
- The challenges of integrated simulation
- Conclusions



Capacitors control MOSFET Operation



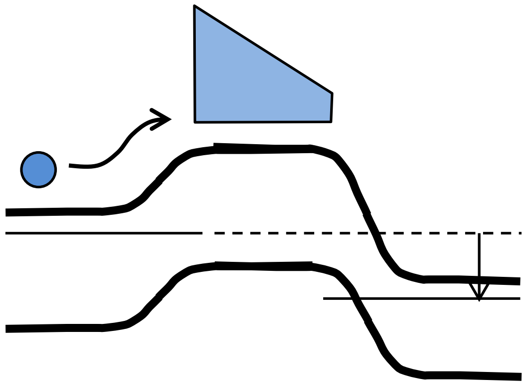
$$m = \frac{dV_G}{d\psi_s} = 1 + \frac{C_s}{C_0}$$

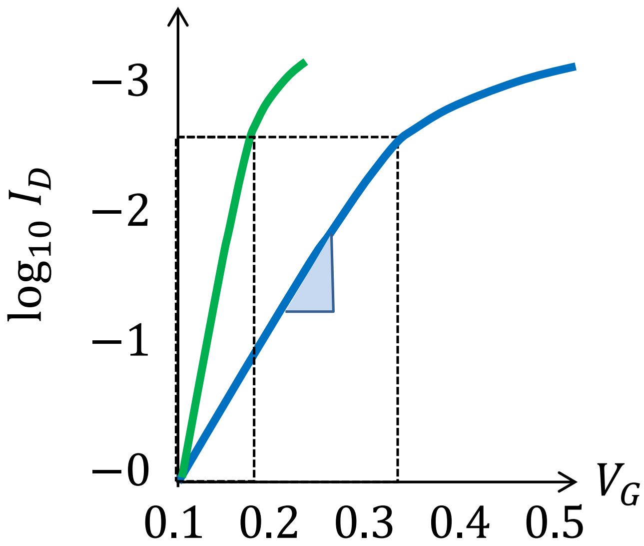


$$\psi_s = \frac{C_o}{C_s + C_o} V_G$$

Subthreshold Slope describes Transistors Performance

$$I_D = I_0\, e^{\frac{q\psi_S}{kT}}\left(1 - e^{-\frac{qV_D}{kT}}\right) \sim I_0\, e^{\frac{q\psi_S}{kT}} = I_0\, e^{qV_G/mkT}$$

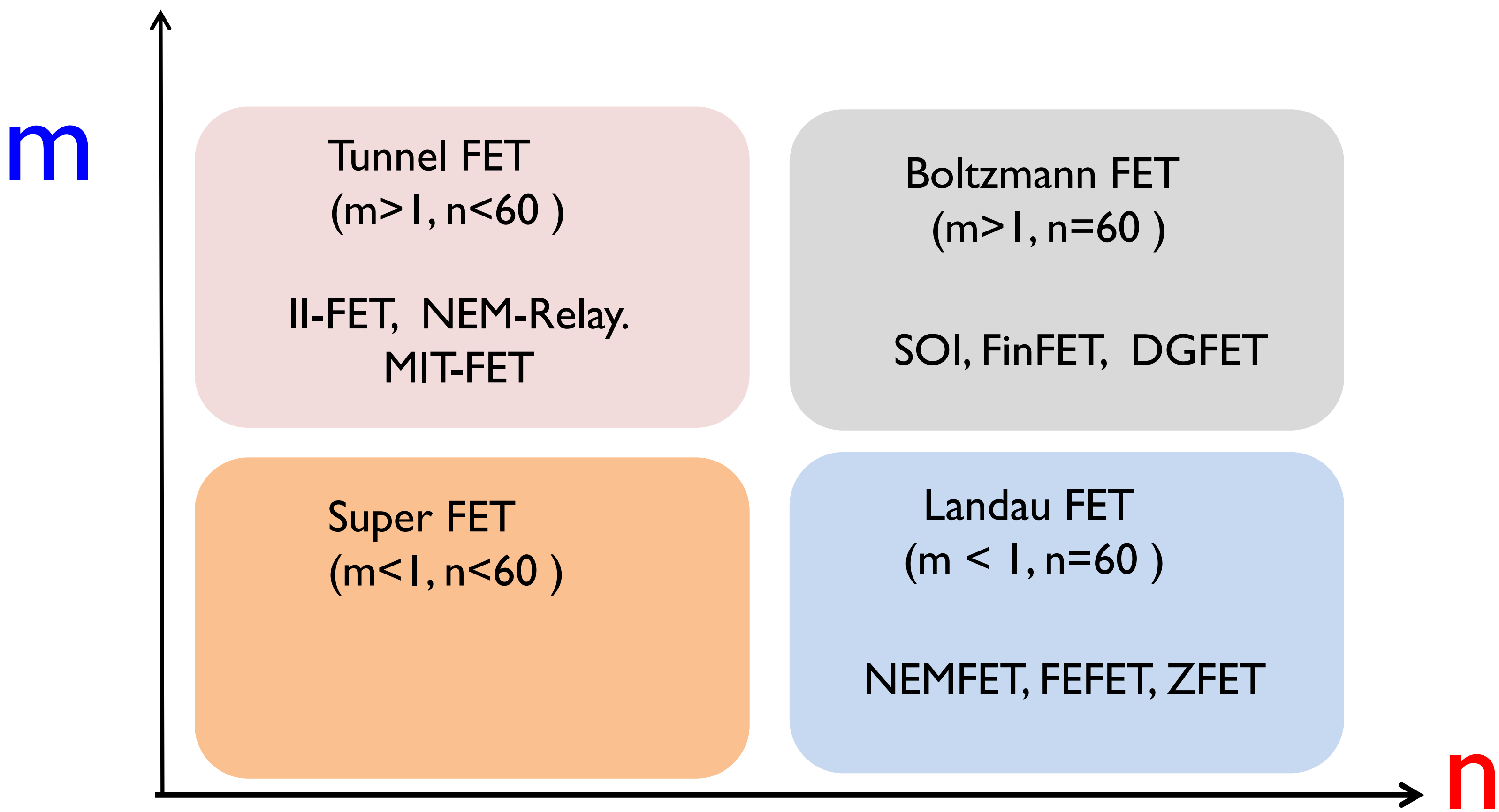




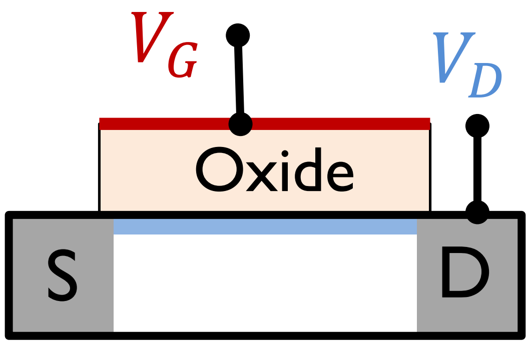
$$S \equiv \left[\frac{d\log_{10}(I_{DS})}{dV_G}\right]^{-1} = \left[\left(\frac{d\psi_s}{dV_G}\right)\left(\frac{d\log_{10}(I_{DS})}{d\psi_s}\right)\right]^{-1} = m\times n \quad = m\times 60\ \text{mV/dec}$$

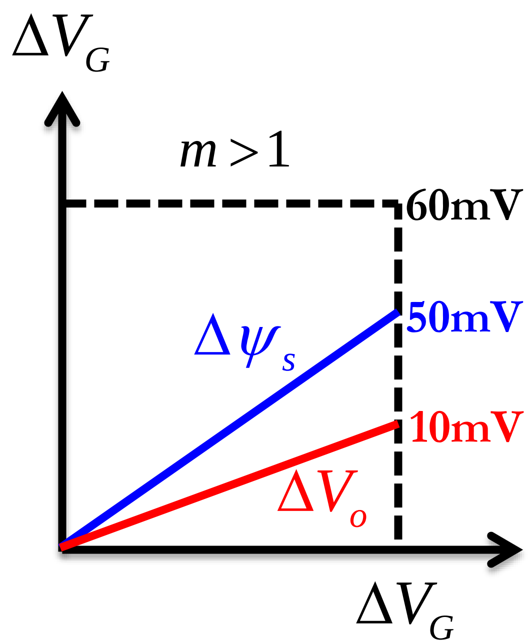
Phase Space of FET

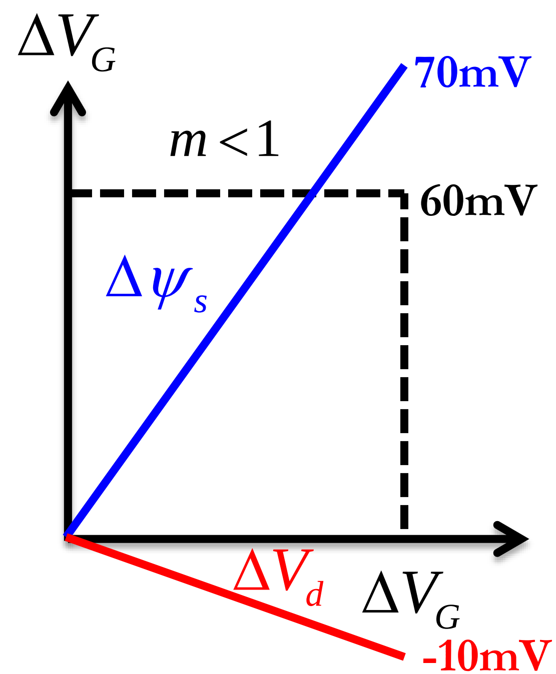
$$S \equiv \left[\left(\frac{d\psi_s}{dV_G} \right) \left(\frac{d \log_{10}(I_{DS})}{d\psi_s} \right) \right]^{-1} = m \times n$$

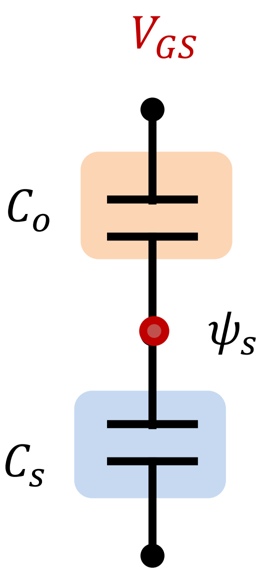


S<60 mV/dec switching?





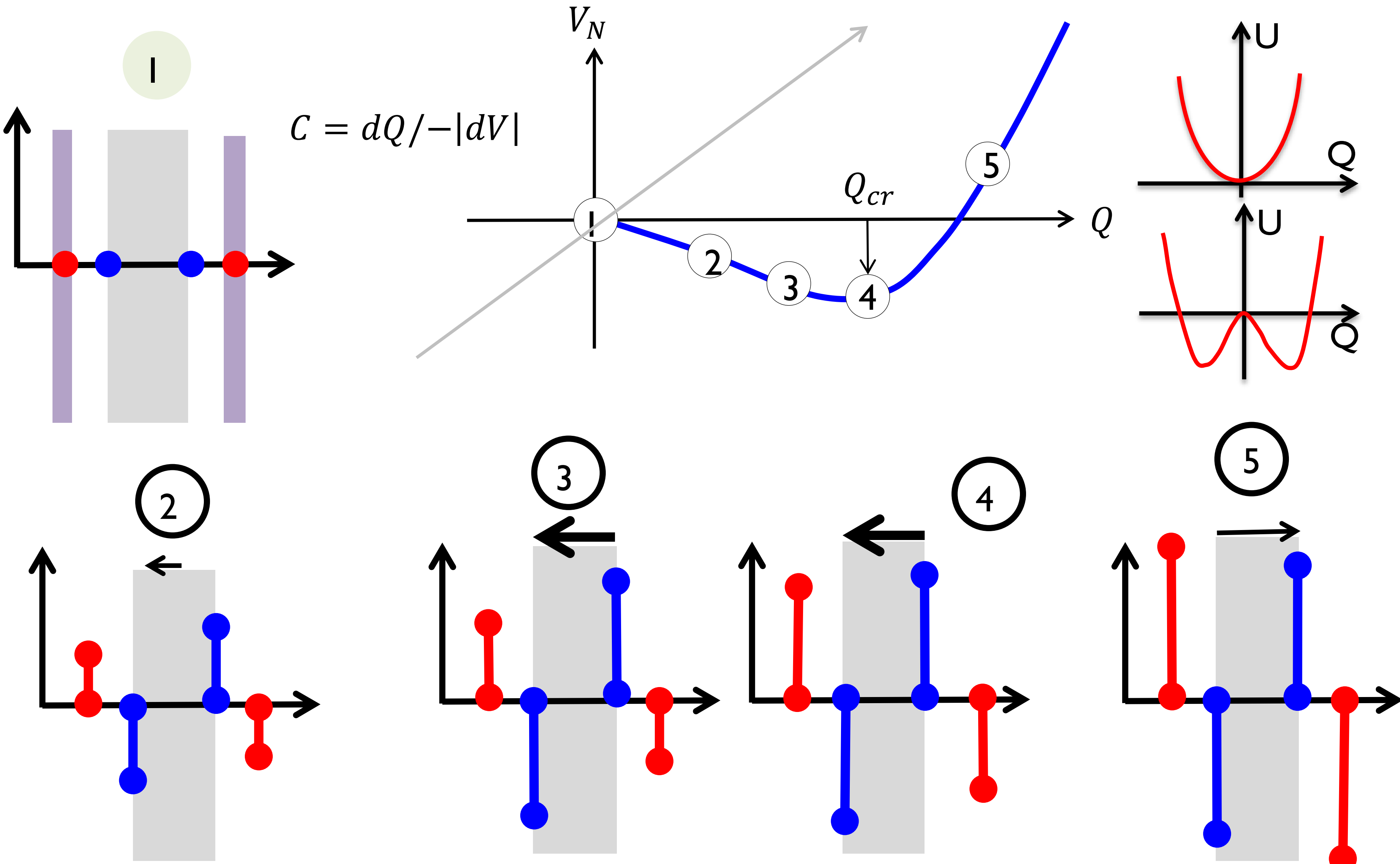




$$S = m \times 60 \text{ mV/dec}$$

$$m = \frac{dV_G}{d\psi_s} = 1 + \frac{C_S}{C_0}$$

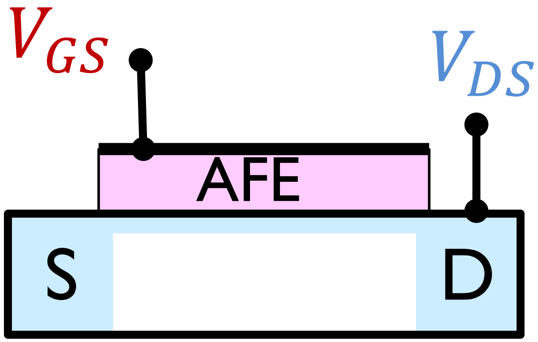
Single ferroelectric charge profile

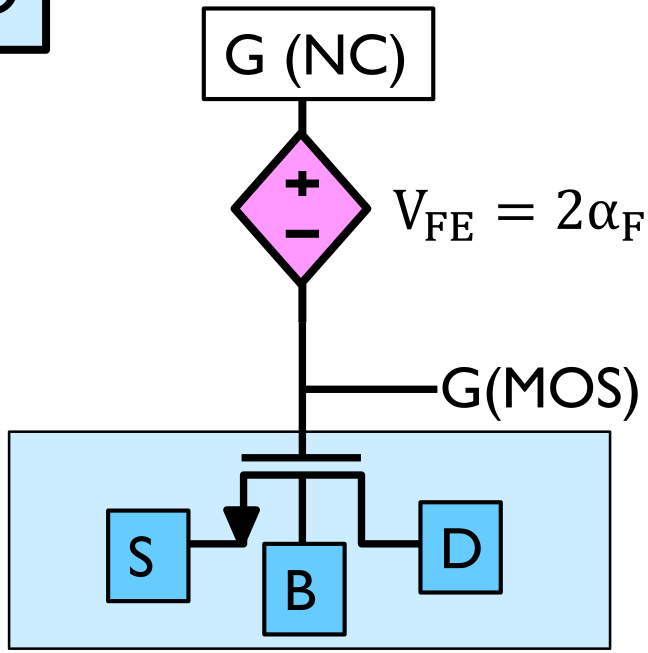


$$C = dQ/-|dV|$$

$$dV_3 = dV_4$$

Coupling of Capacitors: Algorithm





$$V_{FE} = 2\alpha_{FE} t_{FE} Q_G + 4\beta_{FE} t_{FE} Q_G^3$$

M. A. Alam, Purdue University, 2015

MVS-compact model

$$I_D/W = Q_{ix_o} v_{x_o} F_s$$

$$F_s = \frac{V'_{DS}/V_{\mathrm{DSAT}}}{\left(1+(V'_{DS}/V_{\mathrm{DSAT}})^{\beta}\right)^{1/\beta}}.$$

$\beta \rightarrow$ saturation-transition-fitting parameter

$$Q_{ix_o} = C_{\mathrm{inv}} n\phi_t \ln\left(1+\exp\frac{V'_{GS}-(V_T-\alpha\phi_t F_f)}{n\phi_t}\right)$$

$n \rightarrow$ sub-threshold coefficient

$\alpha \rightarrow$ fitting parameter

$$V_T = V_{T0} - \delta V'_{DS}$$

$\delta \rightarrow$ DIBL coefficient

$$V_{\mathrm{DSAT}} = V_{\mathrm{DSAT}s}(1-F_f)+\phi_t F_f$$

$$V_{\mathrm{DSAT}s} = \frac{v_{x_o} L_C}{\mu}$$

$v_{xo} \rightarrow$ sort of saturation velocity

$\mu \rightarrow$ sort of low field mobility

$$F_f = \frac{1}{1+\exp\left(\frac{V'_{GS}-(V_T-\alpha\phi_t/2)}{\alpha\phi_t}\right)}$$

$F_f \rightarrow$ Fermi function for smooth transition

$$\gamma = \sqrt{2q\varepsilon_{\mathrm{Si}}N}/C_g$$

$\gamma \rightarrow$ body factor

$$V'_{DS} = V_{DS} - I_D(R_S+R_D)$$

Voltage drop in R_S and R_D

$$I_D = I_D + I_D(V_{GS}=0)$$

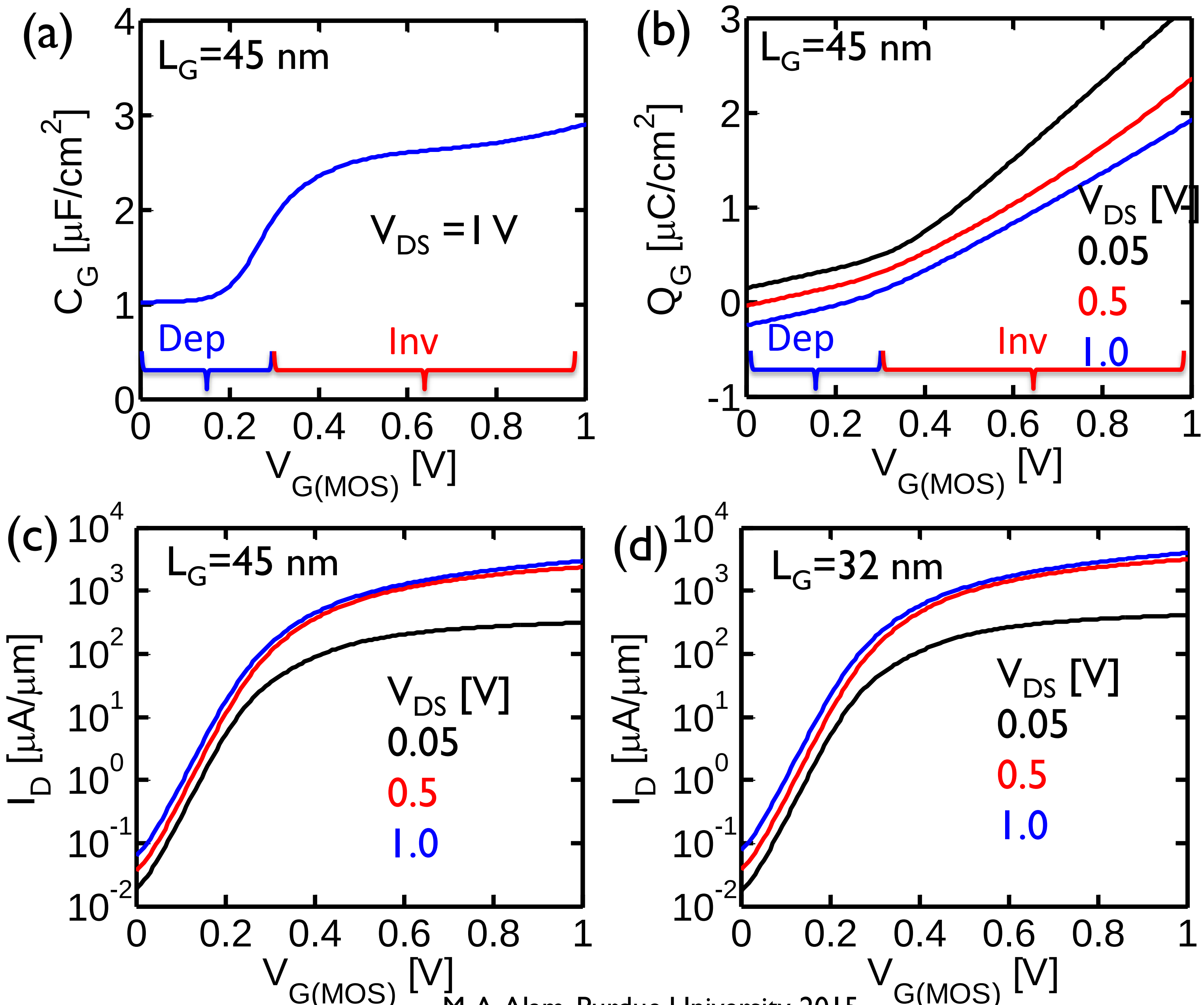
Current saturation in depletion/accumulation edge

Khakifirooz, *TED*, 56 (2009) 1674

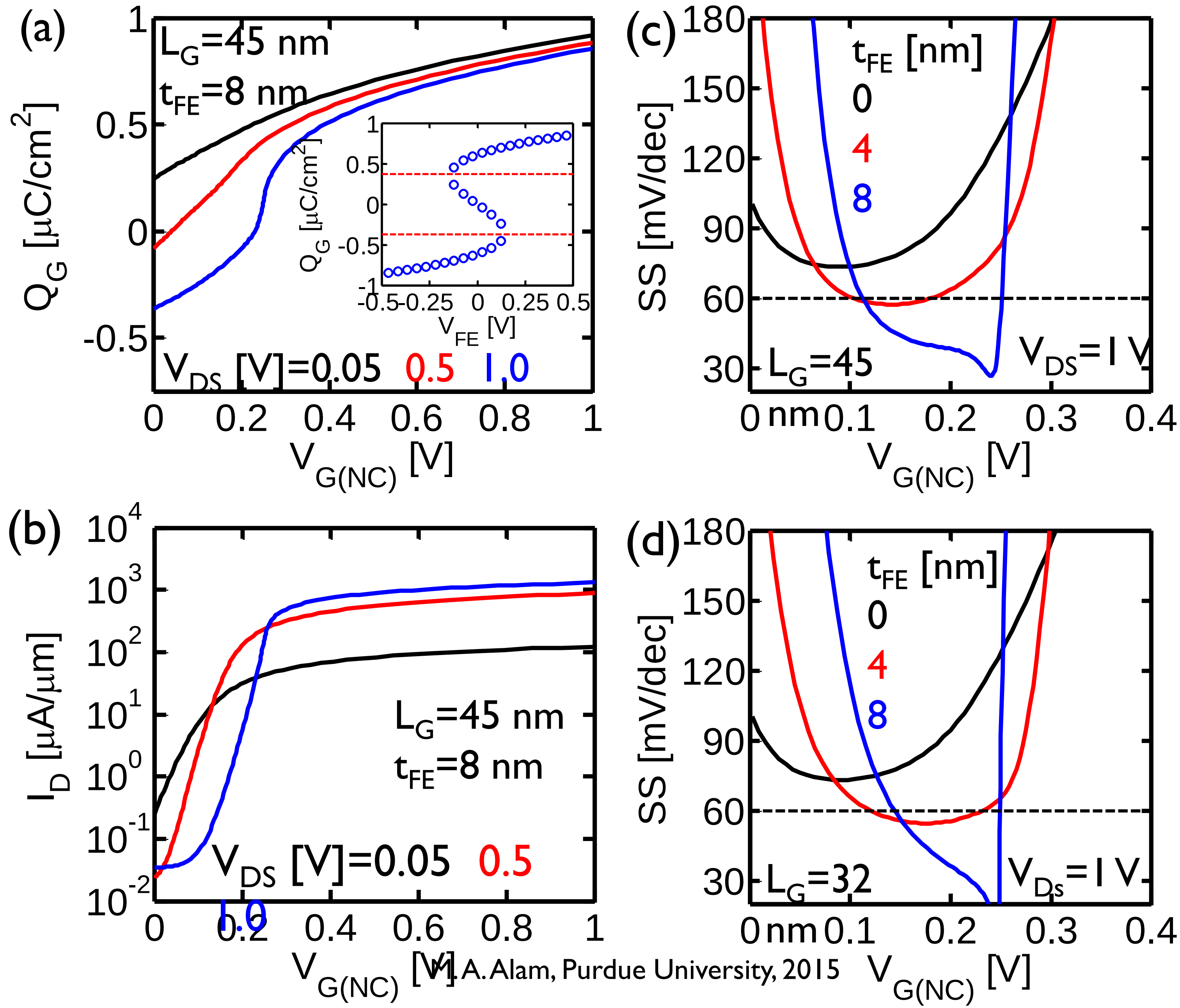
Wei, TED, 59 (2012): 1263

Rakheja, nanoHUB.

doi:10.4231/D3H12V82S



(a)
L_G=45 nm
V_{DS} =1 V
Dep
Inv
C_G [μF/cm^2]
$V_{G(MOS)}$ [V]
(b)
L_G=45 nm
V_{DS} [V]
0.05
0.5
1.0
Dep
Inv
Q_G [μC/cm^2]
$V_{G(MOS)}$ [V]
(c)
L_G=45 nm
V_{DS} [V]
0.05
0.5
1.0
I_D [μA/μm]
$V_{G(MOS)}$ [V]
(d)
L_G=32 nm
V_{DS} [V]
0.05
0.5
1.0
I_D [μA/μm]
$V_{G(MOS)}$ [V]



(a)
L_G=45 nm
t_{FE}=8 nm
Q_G [μC/cm^2]
V_{DS} [V]=0.05 0.5 1.0
$V_{G(NC)}$ [V]
V_{FE} [V]
(b)
I_D [μA/μm]
L_G=45 nm
t_{FE}=8 nm
V_{DS} [V]=0.05 0.5 1.0
$V_{G(NC)}$ [V]
(c)
t_{FE} [nm]
0
4
8
SS [mV/dec]
L_G=45 nm
V_{DS}=1 V
$V_{G(NC)}$ [V]
(d)
t_{FE} [nm]
0
4
8
SS [mV/dec]
L_G=32 nm
V_{Ds}=1 V
$V_{G(NC)}$ [V]

Conclusions

- There is (different) life after Moore's law.
- Power sources: Significant progress in terms of physics-based compact modeling of energy harvesters (e.g. solar cells).
- Biosensors can be transformative. Physics-based modeling is already playing a role in sequencing.
- Landau switches may obviate sub-threshold logic.

Acknowledgement: NEEDS

Goal: To advance the science of nano-devices and enable new applications.

Focus:

1) Physics-based compact models for emerging devices

2) Infrastructure to support the NEEDS team and the broader community.

NEEDS

needs.nanoHUB.org

Specific Infrastructure Objectives

1) Develop a suite of open-source, **physics-based** compact models for emerging nanodevices.

2) Develop **tools and processes** for creating, testing, and publishing “simulation-ready” compact models.

3) Develop **educational resources** to help beginners develop compact models and to convey the physical principles of new nano-devices.

4) Leverage **nanoHUB.org** to to engage a broad community of materials and device researchers and circuit and system designers.

Nano-Engineered Electronic Device Simulation Node

NEEDS has a vision for a new era of electronics that couples the power of billion-transistor CMOS technology with the new capabilities of emerging nano-devices and a charter to create high-quality models and a complete development environment that enables a community of compact model developers.

NEEDS Team: Purdue, MIT, U.C. Berkeley, and Stanford.

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NEWEST COMPACT MODEL RELEASE: UCSB 2D Transition-Metal-Dichalcogenide (TMD) FET model 1.0.0. See Compact Models Page

NEEDS announces the public release of Berkeley MAPP, a MATLAB-based platform for prototyping compact models and simulation algorithms.

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NANOSCIENCE TO SYSTEMS

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FOR DEVELOPERS

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