COMSOL Multiphysics® Software and Photovoltaics: A Unified Platform for Numerical Simulation of Solar Cells and Modules

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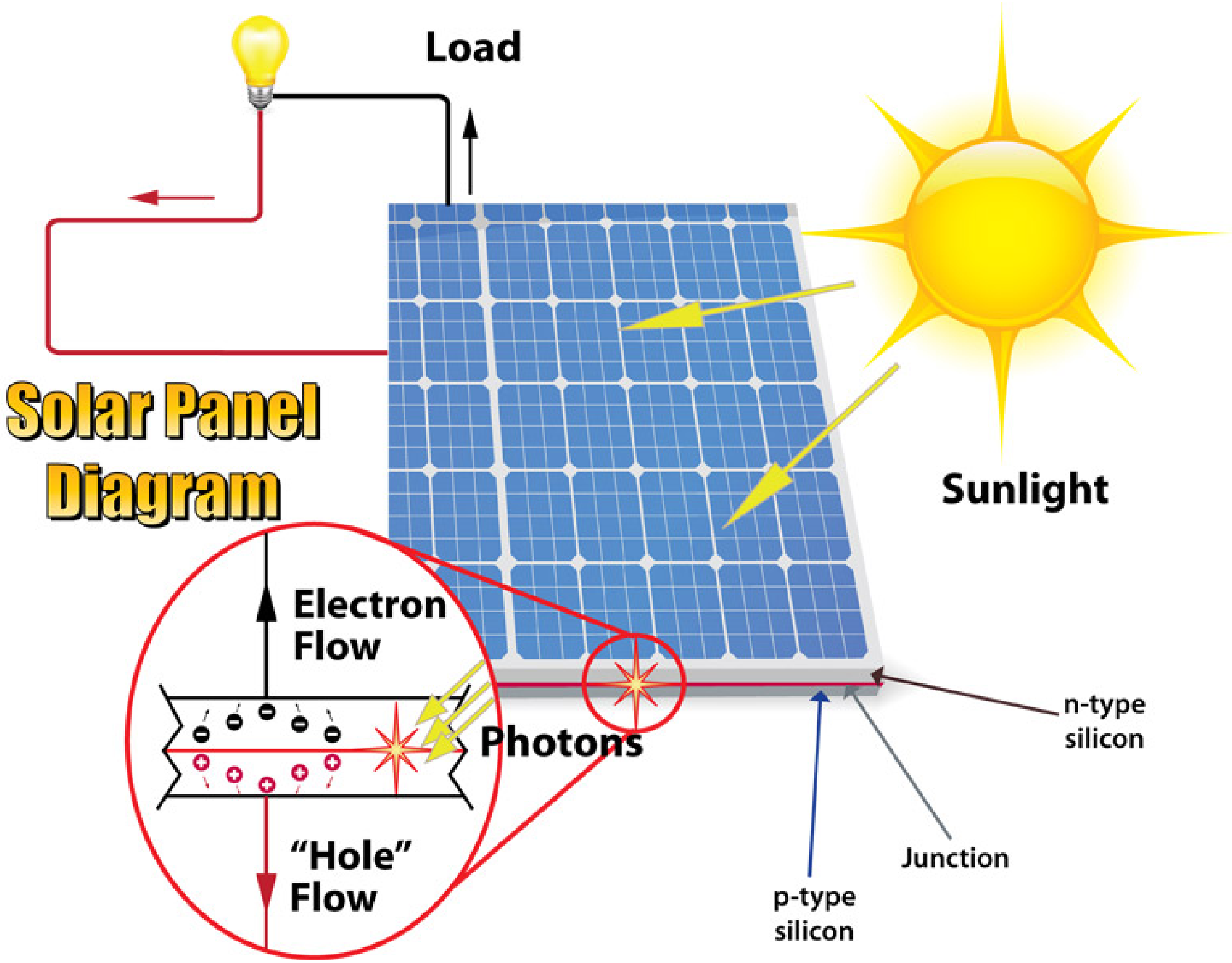
COMSOL CONFERENCE
2015 BOSTON

Photovoltaics (PV)

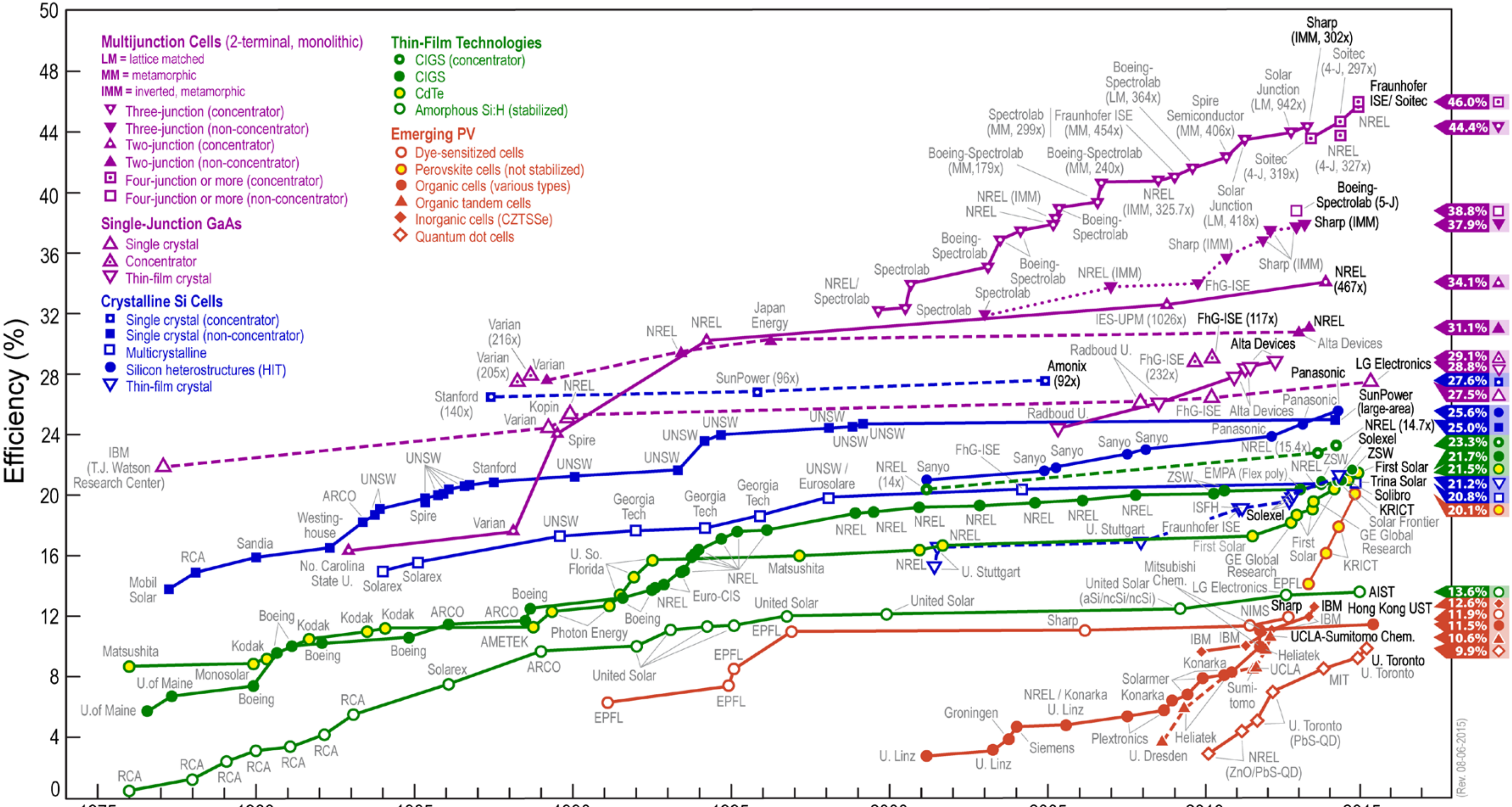


http://etap.com/renewable-energy/photovoltaic-101.htm

Outline

- Fundamental Equations
- Key Outputs
- Advantages of using COMSOL Multiphysics
- Challenges, Tips, and Tricks

Best Research-Cell Efficiencies



National Renewable Energy Lab http://www.nrel.gov/ncpv/

Fundamental Equations

Semiconductor Physics

$$\nabla \cdot (\varepsilon_s \nabla \phi) = -\rho \quad \Rightarrow \quad \rho = q(n - p + N_A - N_D)$$

$$\frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot \boldsymbol{J}_n - U_n + G_n \quad \Rightarrow \quad \boldsymbol{J}_n = -q\mu_n n \nabla \phi + qD_n \nabla n$$

$$\frac{\partial p}{\partial t} = \frac{1}{q} \nabla \cdot \boldsymbol{J}_p - U_p + G_p \quad \Rightarrow \quad \boldsymbol{J}_p = -q\mu_p n \nabla \phi - qD_n \nabla p$$

Dependent Variables:

ϕ – electrostatic potential
n – electron concentration
p – hole concentration

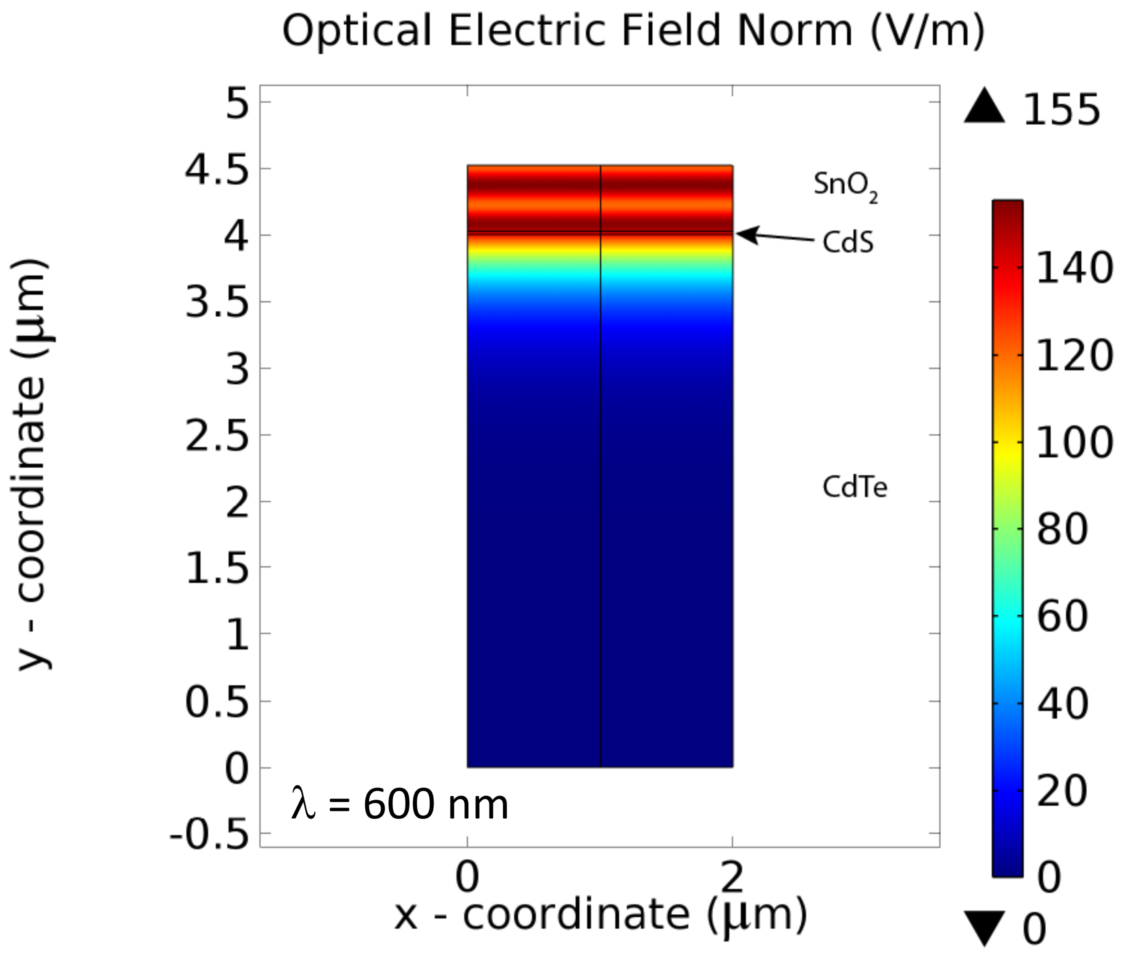
Fundamental Equations

Optical Physics

$$\nabla \times (\nabla \times \boldsymbol{E}) - k_0^2 \varepsilon_r \boldsymbol{E} = 0$$

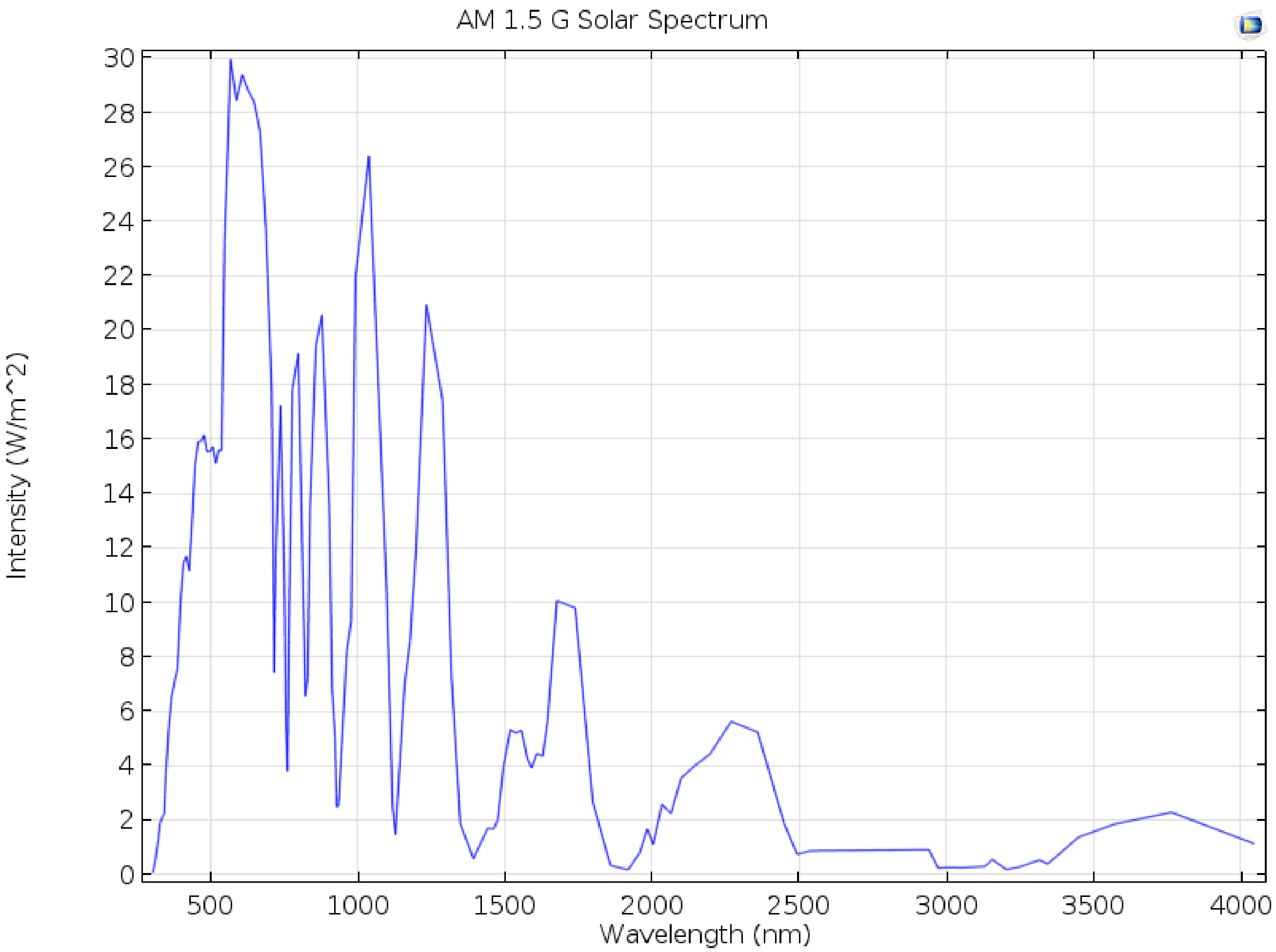
- ***E*** used to calculate power dissipation, *Q*
- Photo-generation rate given by:

$$\mathrm{G} = \frac{Qc}{h\lambda}$$



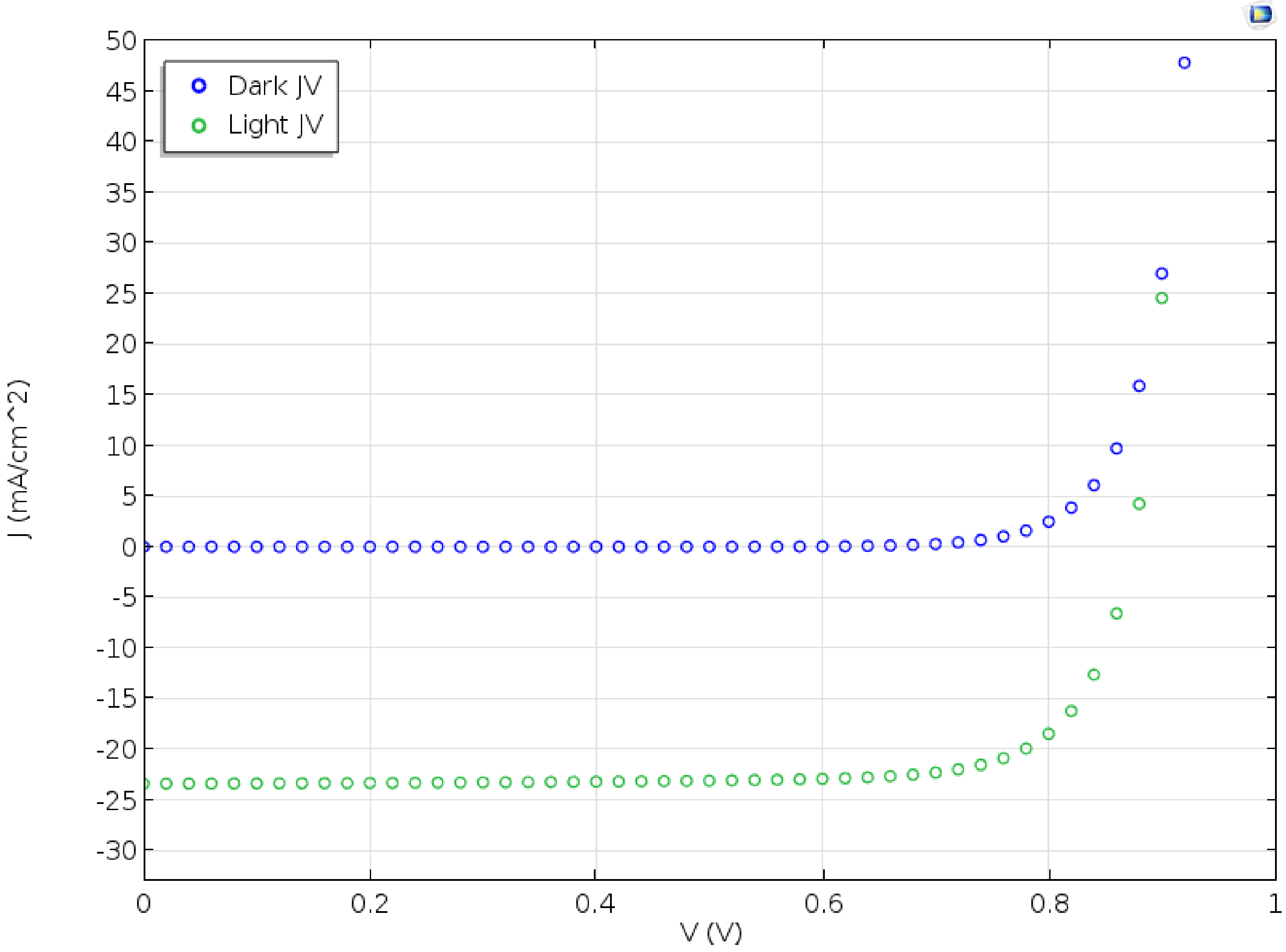
Fundamental Equations

Optical Physics – Solar Spectrum



Key Outputs

Current-Voltage Characteristics (Voltage Sweep)



Independent Variables

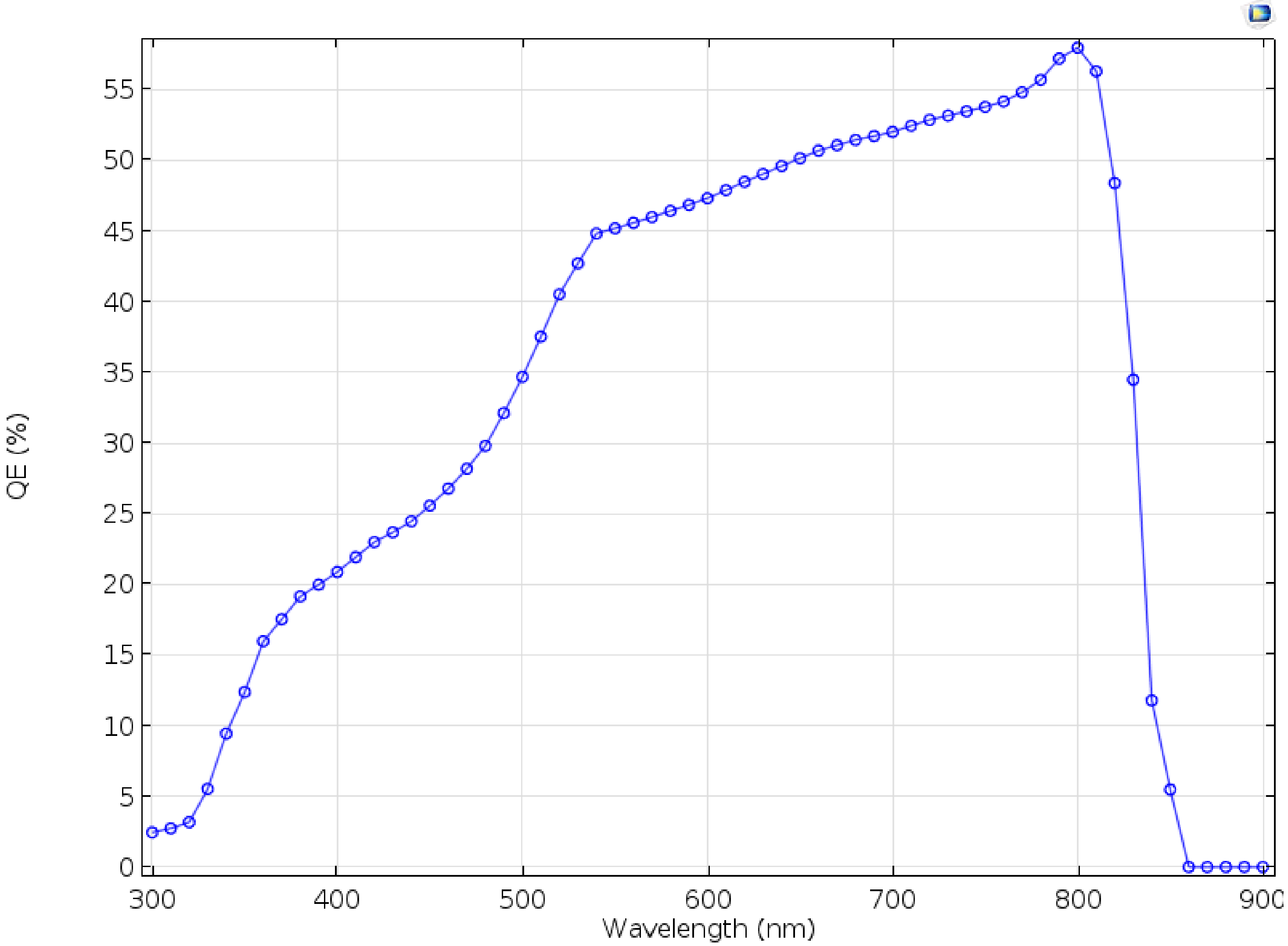
1. Light Intensity
2. Temperature
3. Voltage Bias

Key Metrics

1. Efficiency
2. Open-circuit voltage
3. Short-circuit current
4. Fill factor

Key Outputs

Quantum Efficiency (Light Frequency Sweep)

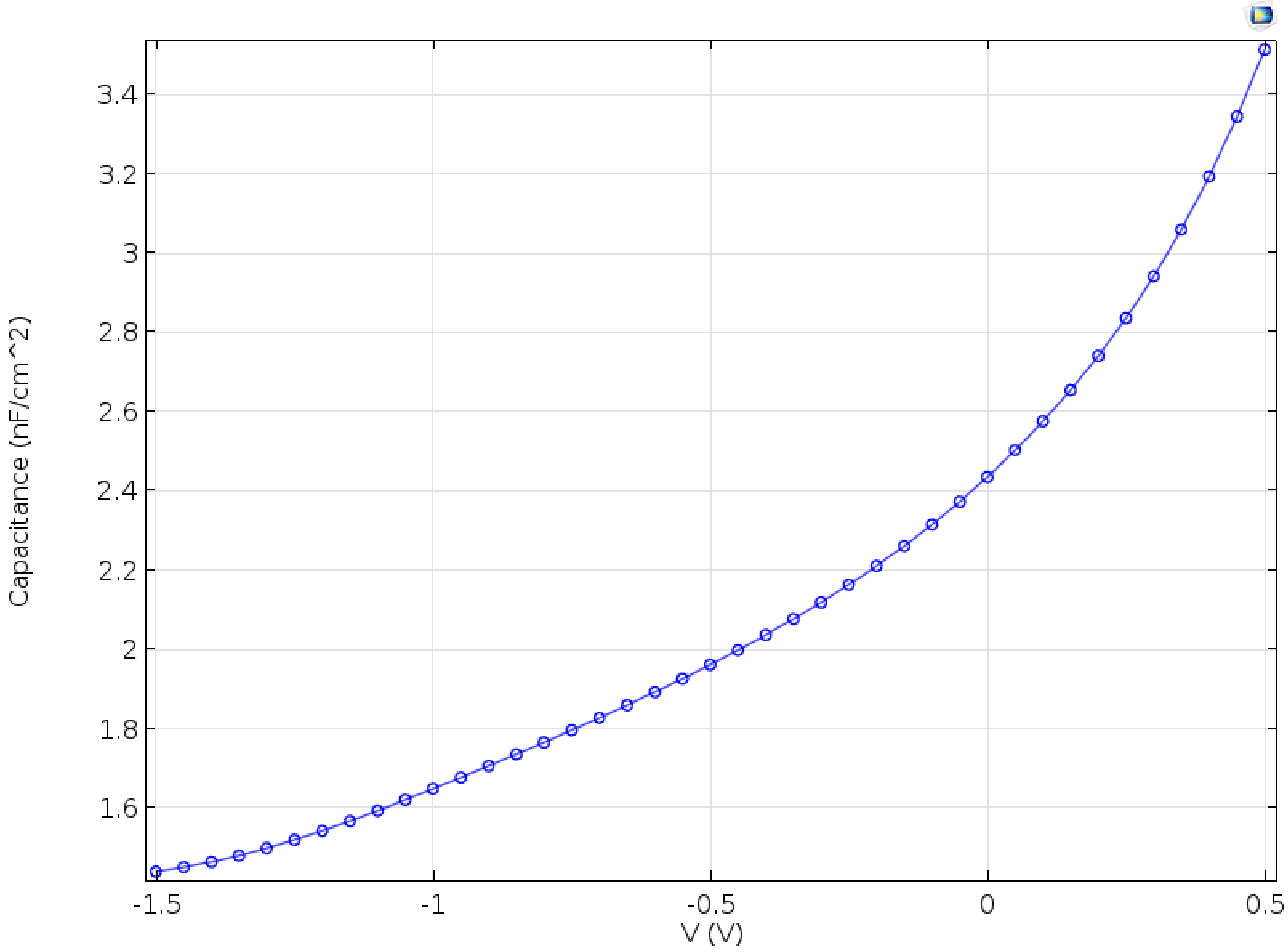


Quantum Efficiency:

1. Efficiency of converting photons to electrons
2. Depends on light wavelength

Key Outputs

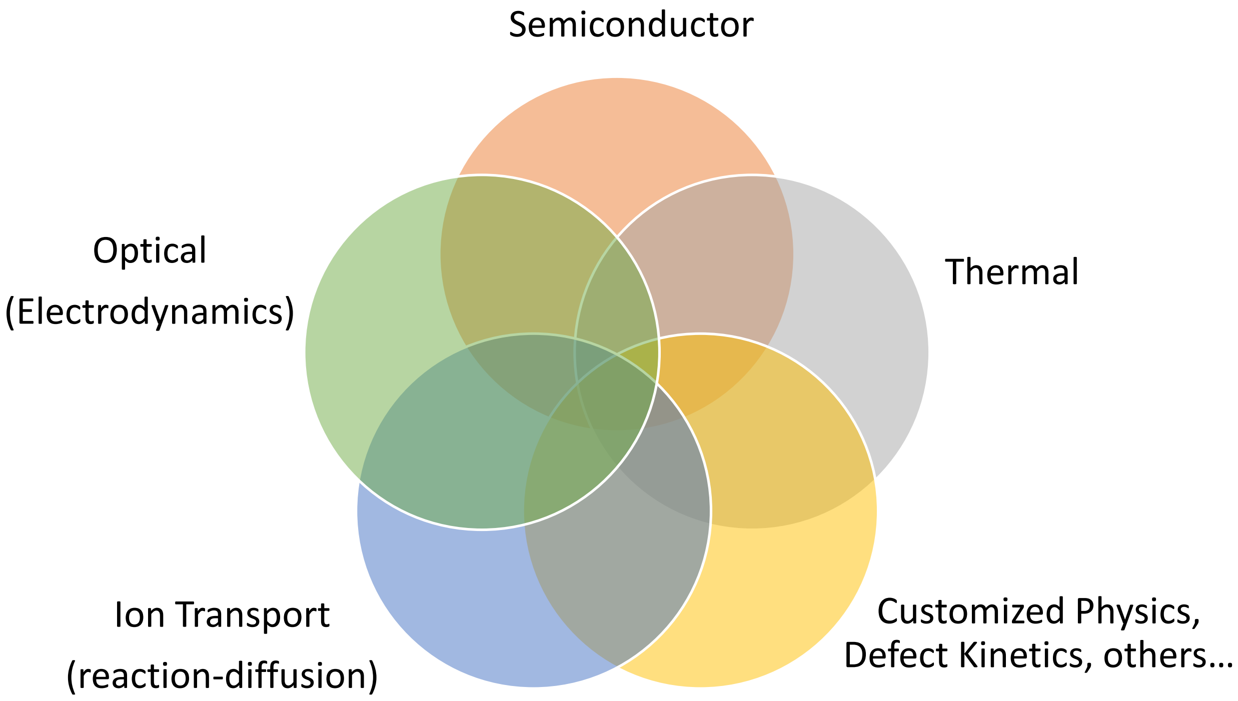
Capacitance-Voltage Characteristics (Voltage Sweep – Small Signal Analysis)



Capacitance-Voltage:

1. Provides information on charge distribution

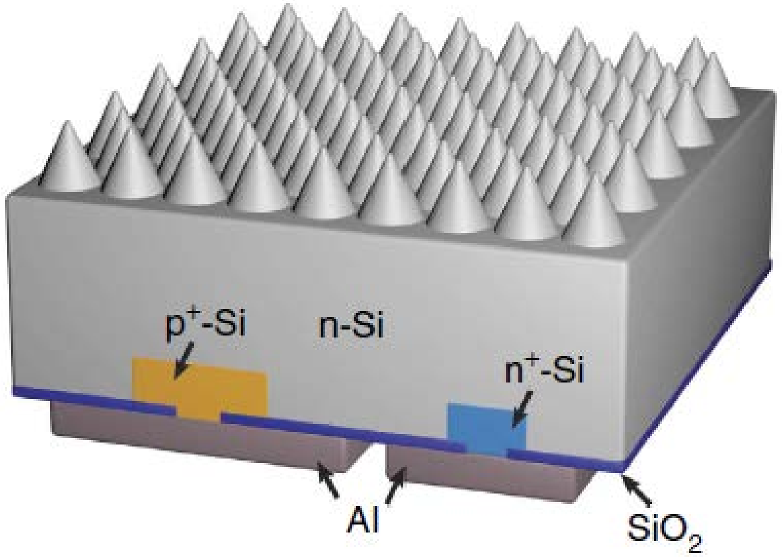
Unified Platform: COMSOL Multiphysics®



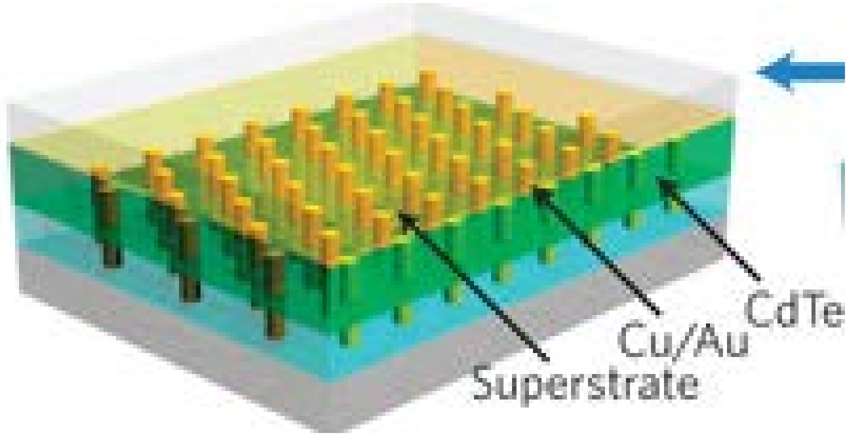
- Multi-physics
- Multi-dimensional
  - 2D, 3D, time-dependent capabilities
- Multi-scale
  - Micro-diodes to modules
- Customizable equations
- LiveLink® with MatLab®

Multi-dimensional

- 2D and 3D design features



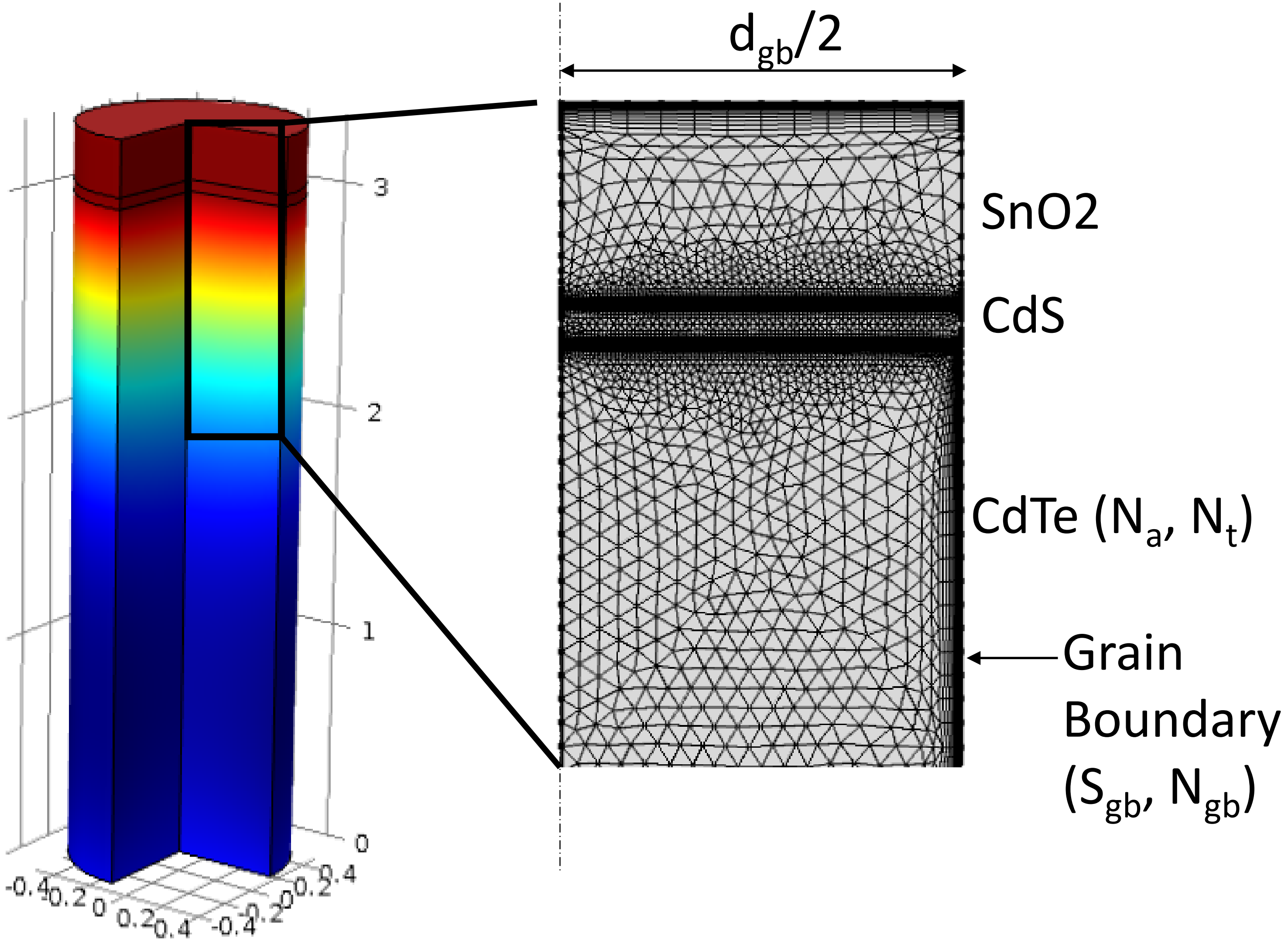
S. Jeong, M. D. McGehee, Y. Cui, Nat. Comm. **4**, 2950 (2013).



Z. Fan et. al. *Nature Materials* **8**, 648 - 653 (2009)

Multi-dimensional

Grain Boundary Effects

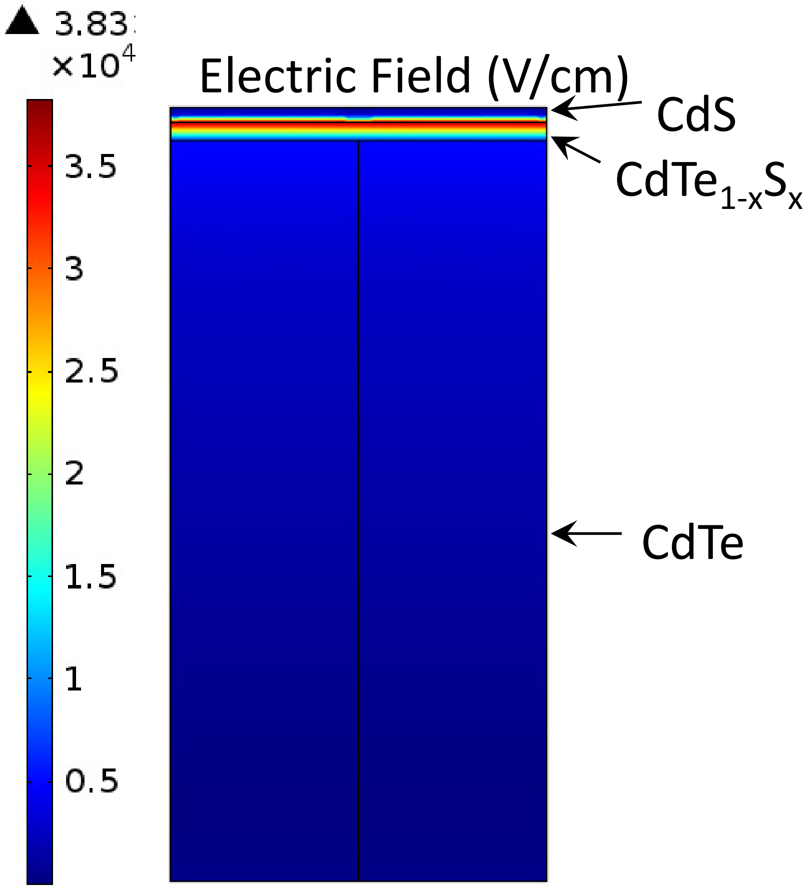


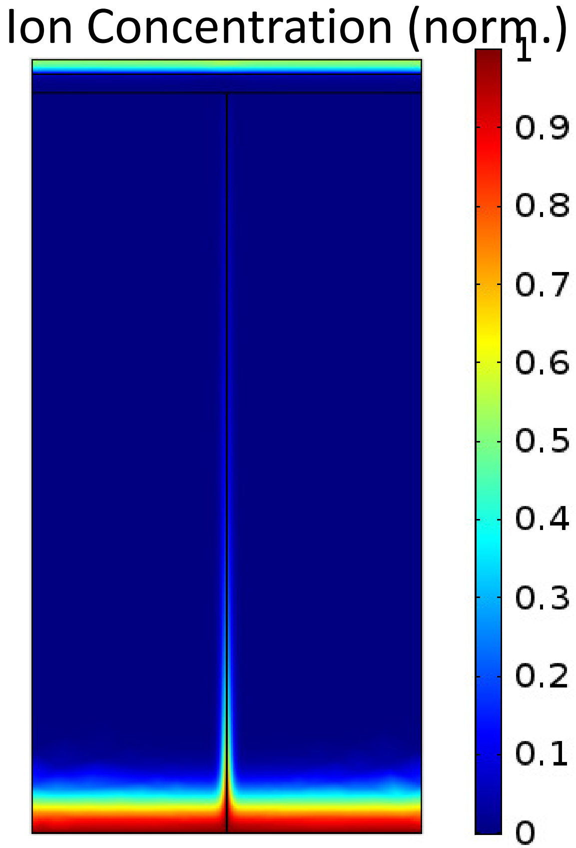
Variable	Definition
N_a (1/cm^3)	Bulk/grain acceptor doping concentration
N_t (1/cm^3)	Bulk/grain deep gap state concentration
N_{gb} (1/cm^2)	Grain boundary surface charge density (+/-)
S_{gb} (cm/s)	Grain boundary surface recombination velocity
d_{gb} (μm)	Grain boundary diameter

Multi-physics

Ion Migration

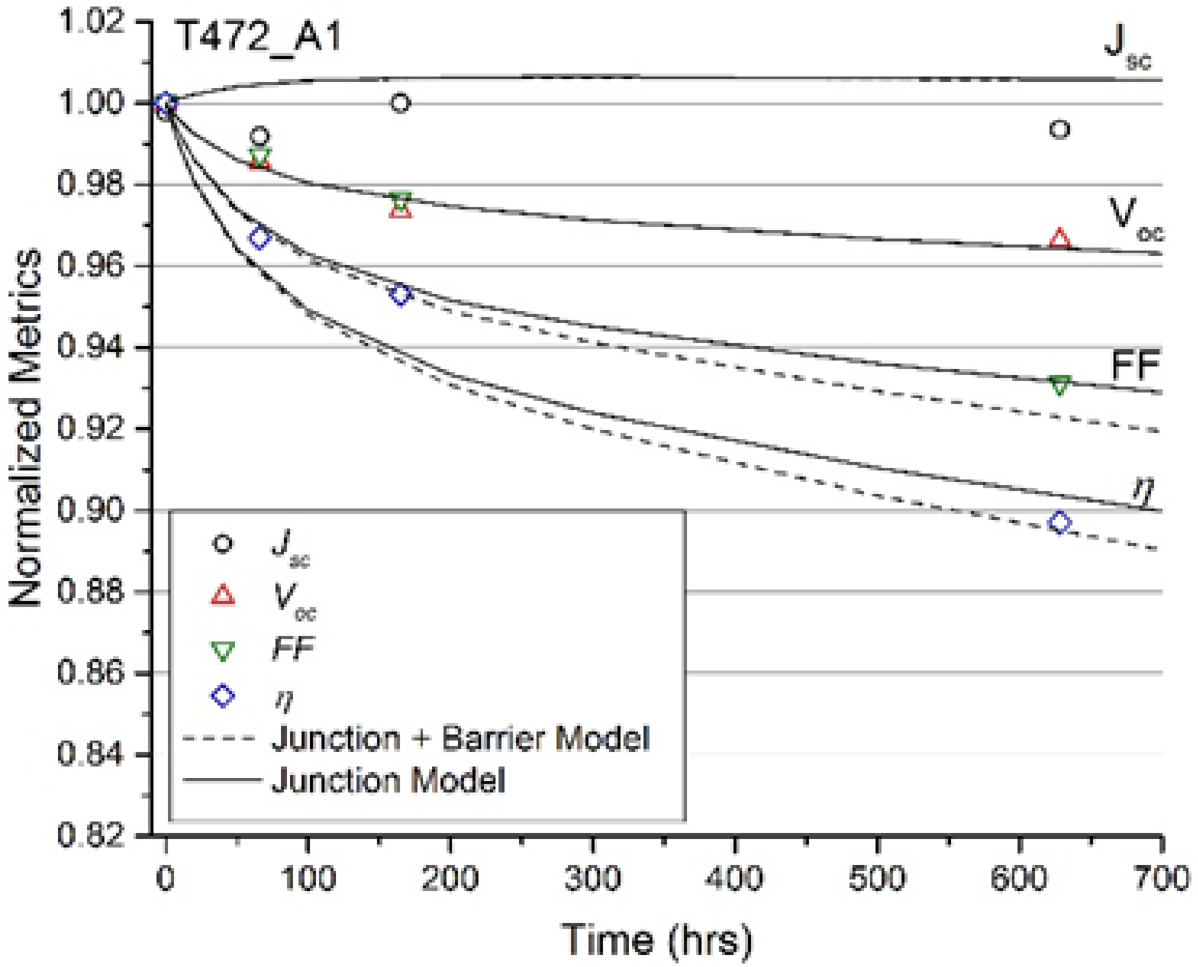
$$\frac{\partial c}{\partial t} = \nabla \cdot (D \nabla c) - \nabla \cdot \left(c \mu \vec{E}\right) + R$$





Time Dependence and Custom Physics

Studying Device Degradation



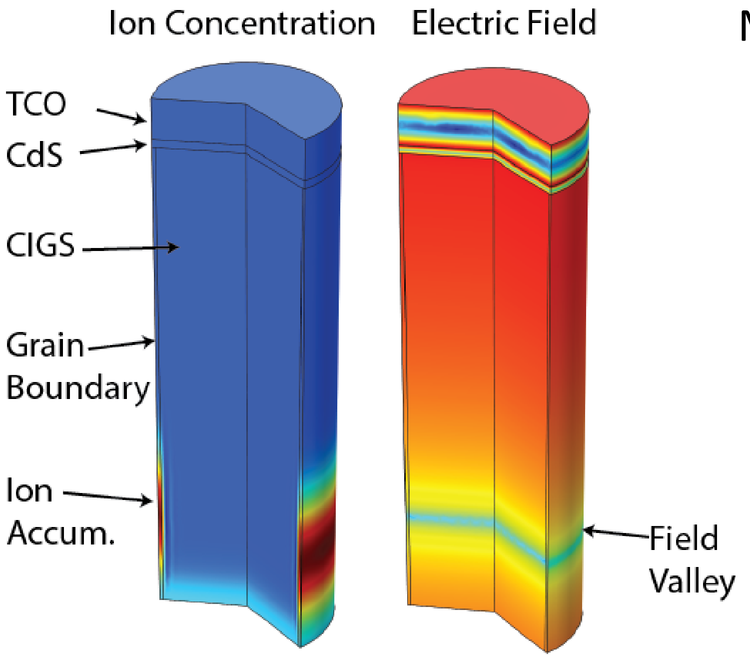
Degradation Physics

- Defect concentrations vary with time:

$$\frac{\partial N_t}{\partial t} = \alpha n(N_t) - \beta N_t$$

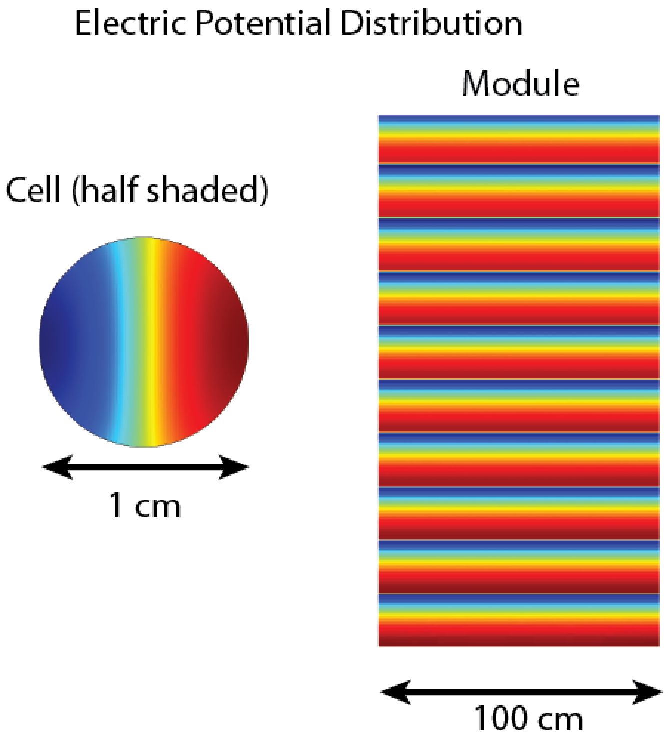
Nardone, M., & Albin, D. S. (2015). Degradation of CdTe Solar Cells: Simulation and Experiment. *Photovoltaics, IEEE Journal of*, *5*(3), 962-967.

Multi-Scale Modeling



Micron Scale

Micron-Scale to Product-Scale Simulation



Centimeter/Meter Scale

Challenges, Tips, and Tricks

- Ramp up dopant and defect concentrations
- Solve equilibrium problem first with segregated solver
- Sometimes helps to use coarse mesh first, then refine
- Ramp up light intensity
- Solar spectrum split into 54 chunks

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Bonus Slides

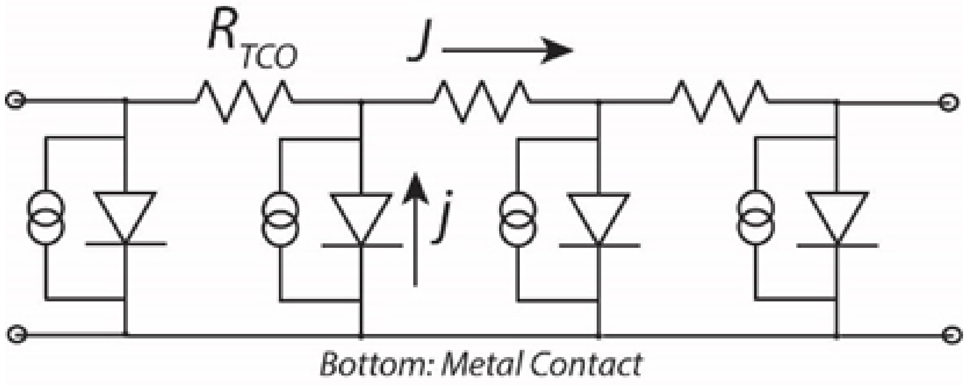
Semiconductor Parameters

Device	SnO2/CdS/CdTe baseline[1]		
	CONTACTS		
	Front		**Back**
ϕ_b [eV]	$\phi_{bn} = 0.1$		$\phi_{bp} = 0.4$
Se [cm/s]	1.00E+07		1.00E+07
Sh [cm/s]	1.00E+07		1.00E+07
Reflectivity Rf	0.1		0.8
	LAYERS		
	SnO2	**CdS**	**CdTe**
W [nm]	500	25	4000
$\varepsilon/\varepsilon 0$	9	10	9.4
μe [cm2/V/s]	100	100	320
μh [cm2/V/s]	25	25	40
NA [cm-3]	0	0	2.00E+14
ND [cm-3]	1.00E+17	1.10E+18	0
Eg [eV]	3.6	2.4	1.5
NC [cm-3]	2.20E+18	2.20E+18	8.00E+17
NV [cm-3]	1.80E+19	1.80E+19	1.80E+19
χ [eV]	4.0	4.0	3.9
ΔEc [eV]	0.00	-0.10	
ΔEv [eV]			
	DEFECTS (Gaussian)		
N_{DG} [cm-3]	1.00E+15	0.00E+00	2.00E+14
N_{AG} [cm-3]	0	1.00E+18	0
EA		mid-gap	
ED	mid-gap		mid-gap
WG [eV]	0.1	0.1	0.1
σ_e [cm2]	1.00E-12	1.00E-17	1.00E-12
σ_h [cm2]	1.00E-15	1.00E-12	1.00E-15

Cell and Module Modeling

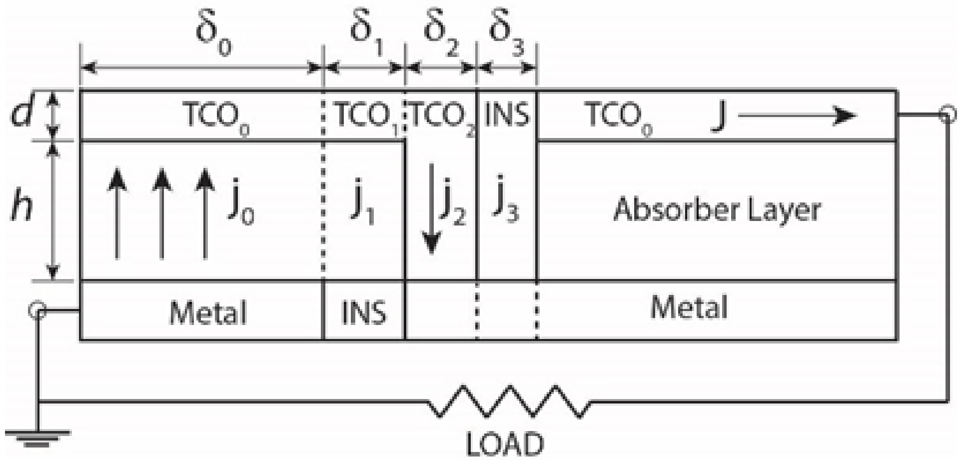
$$-\nabla \cdot (\sigma \nabla \phi) = j/d$$

Cell Equivalent Circuit



- j is the current from micro-diode model

Monolithic Module Model



- j_0 is the current from micro-diode model
- $j_2 = -V_2/(h\ d\ R_{TCO})$, ohmic current
- $j_1 = j_3 = 0$