

# Comparative study of of PN, PIN and new Schottky based InGaN thin films solar cells

## NanoMaterials for Energy and Environment 2016

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## What is this all about ?

- 1 InGaN Schottky Solar Cell modeling & optimization
  - Modeling the Solar Cell
  - Multi-variate optimization
  - An optimal design
- 2 Proposal for a new InGaN MIN structure
  - Optimal PN and PIN structure
  - Schottky Based InGaN Solar Cells
  - MIN structure behavior
- 3 From simulation to realization
  - InGaN composition
  - Crystal defects
  - Metal work function
  - Future work

## And now...

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# InGaN for solar cells

Decisive advantages vs. Technological issues

## Continuous solar spectrum covering

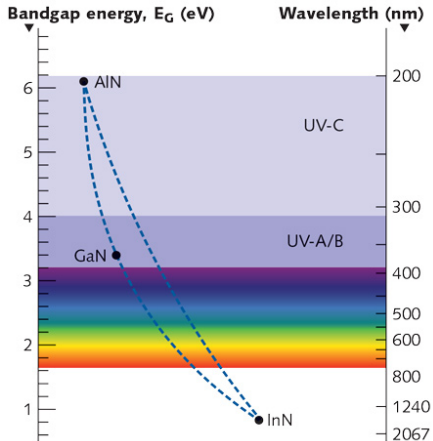
- Indium composition change
- Multi-junction solar cells

## Robust material

- High temperatures
- Radiation resistant

## High light absorption

- Thin layers
- Nanoscale



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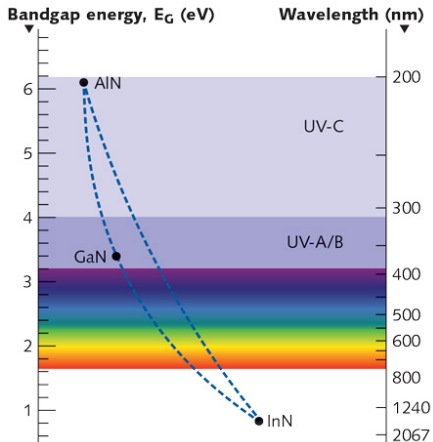
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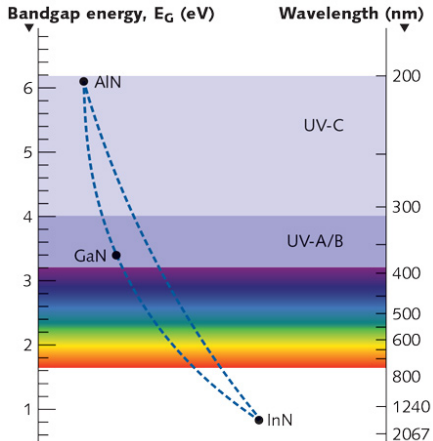
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## Lack of lattice matched substrate

- Difficult elaboration
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## Rough road to the device

- P doping uneasy
  - lack of acceptors
  - natural N doping
- Contact deposition difficult

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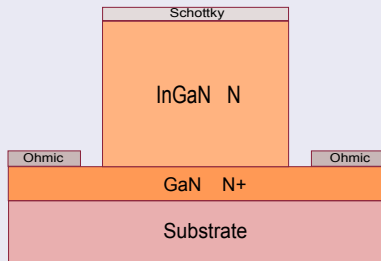
# Optimizing the Schottky design

Removing the need for a p-layer

## One junction only in this talk

- Get the best out of 1 junction
- First step towards multi-junction

## The Schottky design



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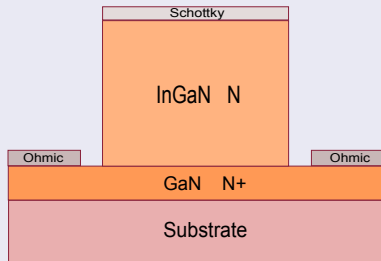
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## This talk objective

- **p-layer free device**
- Predict InGaN solar cell efficiency
- Predict the parameter set for the best efficiency
  - Dopings
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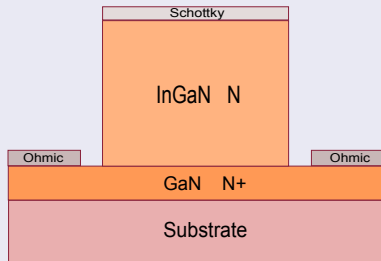
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# Modeling and simulation

Experimental data linked to SILVACO™ ATLAS™ 2D state of the art simulator

## Simulation framework

- ATLAS™ back-end from SILVACO™
- 2D drift-diffusion non linear differential problem
- Coupled & decoupled methods

## InGaN parameters from experiment

- From GaN & InN binaries
- Linear Vegard interpolation for InGaN
- Bowing for affinity & bandgap: 0.8eV & 1.43eV

## Carrier Transport

- Caughey-Thomas for mobility
- Recombinations : direct, Auger, SRH and bandgap narrowing
- 1ns carrier lifetime

## Solar Light & Absorption

- Standard AM1.5 Solar Spectrum
- Adachi model
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# Simulation process

Simulation up and running : inputs and outputs

## Input data: photovoltaic cell physical parameters

- N InGaN composition, doping and thickness
- Metal work function
- In short: 4 parameters

## Simulation output data: comprehensive electrical analysis

- I-V curves
- Electric field mapping
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# The need for math

When hand driven parameter variation fails

## A multivariate optimization problem

- Efficiency is a function of 4 parameters
- Varying one parameter at a time **fails**

$$\eta : (\mathbb{R}^+)^4 \mapsto \mathbb{R}^+$$

## Various multivariate optimization methods

- Brute Force
- Gradient descent
- Conjugate gradient
- ...

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# Multivariate optimization method

## SAGE/python interface to SciPy algorithms

- Formalize ATLAS<sup>TM</sup> calculations as a multivariate function
- Use the appropriate optimization method on it

## Choosing the optimization method

- Gradient and Hessian have to be approximated
- Problem bounded by physics and technology
- Bounded approximate gradient methods

## The question of the starting point

- Several random starting points
- To ensure maximum efficiency uniqueness

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# InGaN Schottky Solar Cell optimal design<sup>1</sup>

Using very loose technological constraints

Optimal 18.2% efficiency with 10% tolerance

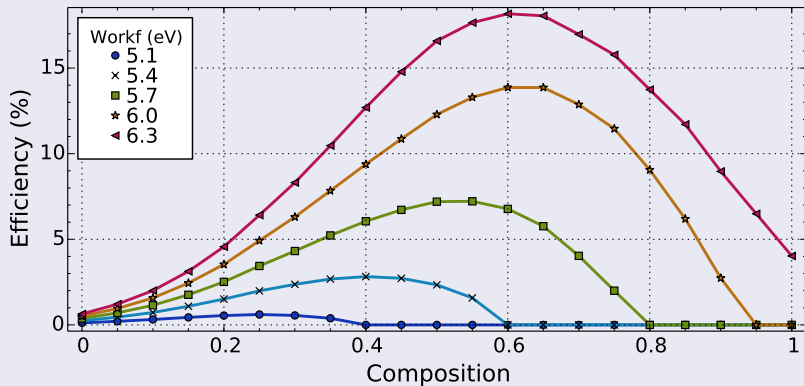
	$L_n(\mu m)$	$N_d(cm^{-3})$	$W_f(eV)$	$x$	$\eta(\%)$ $V_{OC}(V)$ $J_{SC}(mA/cm^2)$ $FF(\%)$
Range	[0.10 – 1.00]	$[1.0 \times 10^{16} - 1.0 \times 10^{19}]$	[5.50 – 6.30]	[0.00 – 1.00]	
Schottky	0.86 [0.53 – 1.00]	$6.5 \times 10^{16}$ [ $1.0 \times 10^{16} - 3.0 \times 10^{17}$ ]	6.30 [6.15 – 6.30]	0.56 [0.50 – 0.72]	18.2 0.863 26.80 78.82

<sup>1</sup> *Materials Science in Semiconductor Processing*, 2016, 41, pp.219-225.

# Varying metal work function and composition

around the optimal values

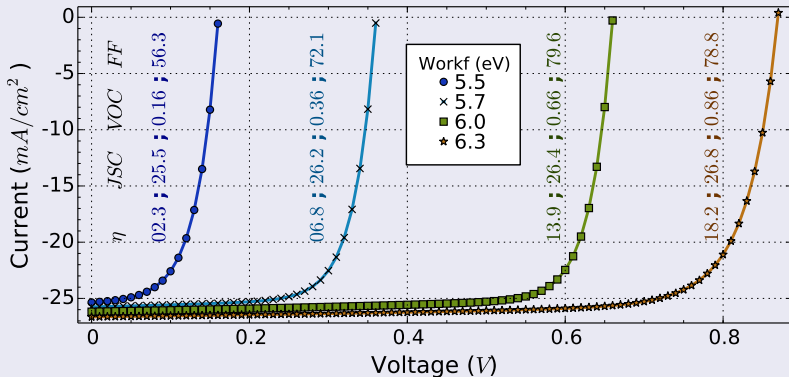
## Changing work function and composition modulates SCR



# I - V for various work functions

around the optimal values

The efficiency increase is mainly due to  $V_{OC}$  increase



## And now...

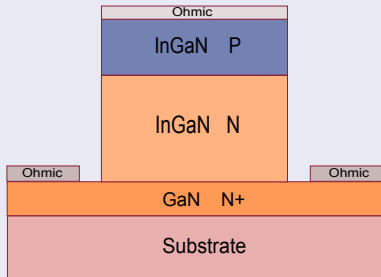
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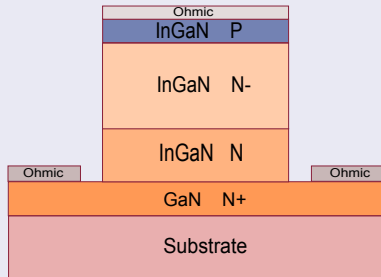
## InGaN PN & PIN structure optimal designs<sup>2</sup>

PN & PIN are standard structures worth optimizing

### PN InGaN PV Cell



### PIN InGaN PV Cell

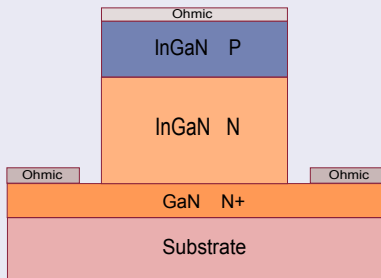


<sup>2</sup> *Superlattices and Microstructures*, 2016, 96, pp.121-133.

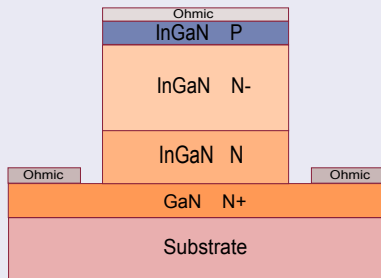
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InGaN is naturally n-doped

InGaN I layer is actually slightly N doped

# Optimal InGaN PN & PIN : 17.8% & 19% efficiency

Notice the huge 90% tolerances and the ultra-small P layer

	$L_p(\mu m)$	$L_n(\mu m)$	$N_a(cm^{-3})$	$N_d(cm^{-3})$	$x$	$\eta(\%)$ $V_{OC}(V)$ $J_{SC}(mA/cm^2)$ $FF(\%)$
Range	[0.01 – 1.00]	[0.10 – 1.00]	$[10^{16} - 10^{19}]$	$[10^{16} - 10^{19}]$	[0.00 – 1.00]	
PN	0.01 [0.01 – 0.04]	1.00 [0.48 – 1.00]	$10^{19}$ [ $4.4 \times 10^{16} - 10^{19}$ ]	$3.9 \times 10^{16}$ [ $10^{16} - 3.5 \times 10^{17}$ ]	0.56 [0.50 – 0.72]	17.8 0.855 26.75 77.85
PIN	0.01 [0.01 – 0.04]	0.50 [0.10 – 1.00]	$10^{19}$ [ $5.9 \times 10^{16} - 10^{19}$ ]	$5.0 \times 10^{17}$ [ $1.9 \times 10^{16} - 10^{19}$ ]	0.59 [0.47 – 0.71]	19.0 0.875 27.36 79.39

- I layer optimal thickness :  $0.54\mu m$
- I layer thickness 90% tolerance :  $[0.18 - 1]\mu m$
- I layer optimal n-doping :  $5.8 \times 10^{16}cm^{-3}$
- I layer n-doping 90% tolerance :  $[10^{14} - 10^{17}]cm^{-3}$

Huge tolerances : **robust device**

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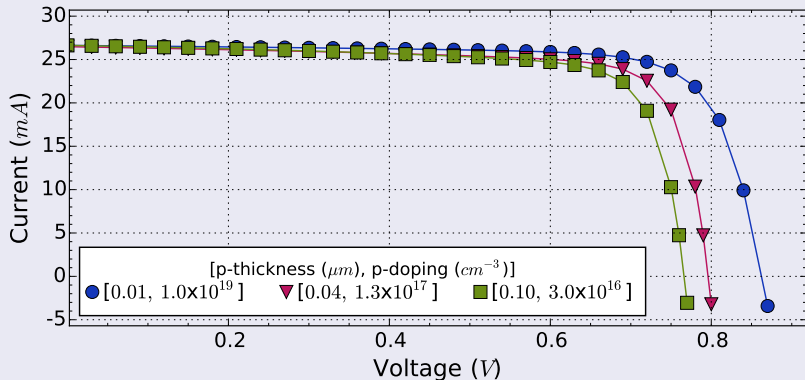
Nanoscale P layer : suggests P layer removal

# Optimal InGaN PN Current-Voltage characteristics

Fixing the p-thickness and finding the optimal p-doping associated to it

For several optimal (p-thickness, p-doping) couples

PN

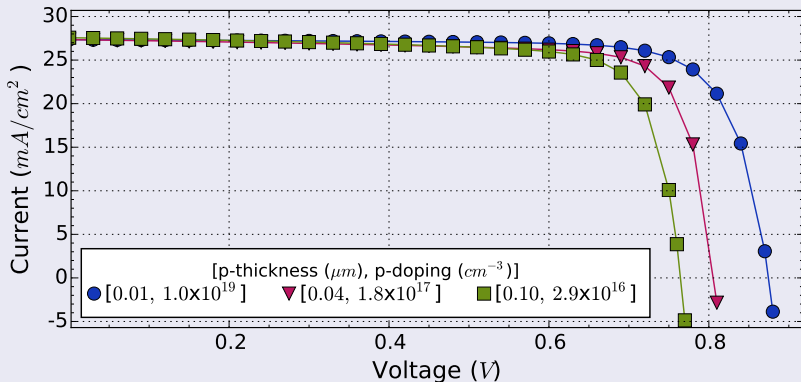


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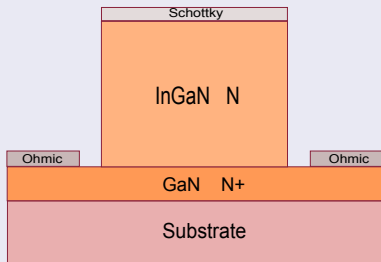
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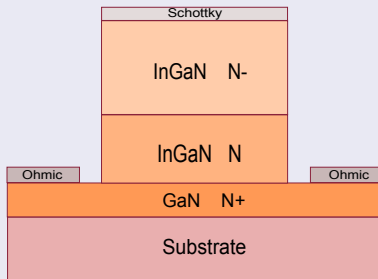
(SBSC)

P layer removed and replaced by a Schottky contact

## Schottky InGaN PV Cell



## New Metal-IN InGaN PV Cell



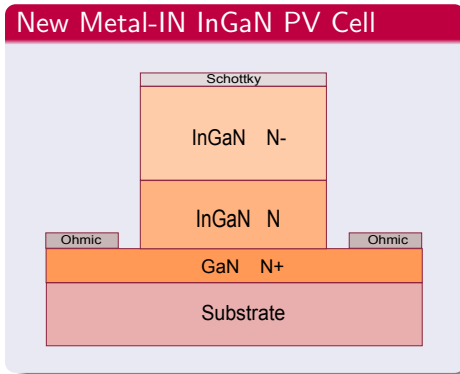
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Up to 18.2% & 19.8% efficiency

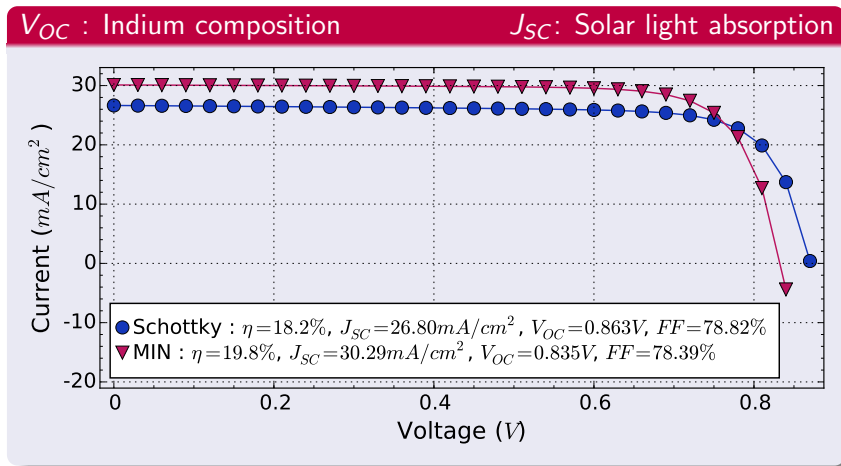
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<b>MIN</b>	0.83 [0.10 – 1.00]	$3.6 \times 10^{17}$ [ $1.8 \times 10^{16} - 1.0 \times 10^{19}$ ]	6.30 [6.11 – 6.30]	0.60 [0.48 – 0.72]	19.8 0.835 30.29 78.39

- I layer optimal thickness :  $0.61\mu m$
- I layer thickness 90% tolerance :  $[0.1 - 1]\mu m$
- I layer optimal n-doping :  $6.1 \times 10^{16}cm^{-3}$
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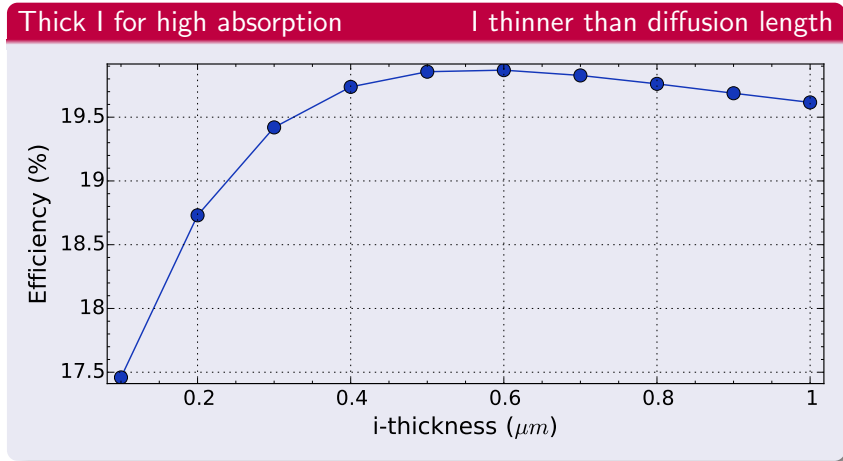
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# InGaN Schottky and MIN Current-Voltage characteristics



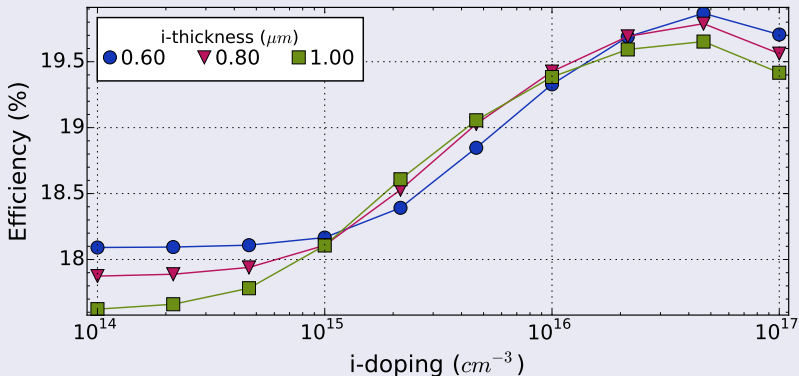
# MIN PV efficiency as a function of the i-layer thickness



# MIN PV efficiency as a function of i-doping

for various i-thicknesses

## Optimal I-doping for optimal Space Charge Region



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# Optimal InGaN 0.60 composition is still difficult to achieve

Even more if several hundreds of nanometers are required

## Recent (2015) experimental work reports 0.22 composition

- Limit In composition to 0.22
- Limit thickness to 400nm

Huge tolerances

7.25% efficiency

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Range	[0.10 – 0.40]	[0.10 – 0.40]	$[1.0 \times 10^{14} - 1.0 \times 10^{17}]$	$[1.0 \times 10^{16} - 1.0 \times 10^{19}]$	[5.50 – 6.30]	[0 – 0.22]	
MIN	0.40	0.40	$6.27 \times 10^{15}$	$7.46 \times 10^{16}$	6.30	0.22	7.25 1.438
	[0.18 – 0.40]	[0.29 – 0.40]	$[4.6 \times 10^{14} - 2.2 \times 10^{16}]$	$[2.0 \times 10^{16} - 1.0 \times 10^{18}]$	[6.20 – 6.30]	[0.19 – 0.22]	5.92 85.2



# Optimal InGaN 0.60 composition is still difficult to achieve

Even more if several hundreds of nanometers are required

## Recent (2015) experimental work reports 0.22 composition

- Limit In composition to 0.22
- Limit thickness to 400nm

## Huge tolerances

## 7.25% efficiency

	$L_i(\mu m)$	$L_n(\mu m)$	$N_i(cm^{-3})$	$N_d(cm^{-3})$	$W_f(eV)$	$x$	$\eta(\%)$ $V_{OC}(V)$ $J_{SC}(mA/cm^2)$ $FF(\%)$
Range	[0.10 – 0.40]	[0.10 – 0.40]	$[1.0 \times 10^{14} - 1.0 \times 10^{17}]$	$[1.0 \times 10^{16} - 1.0 \times 10^{19}]$	[5.50 – 6.30]	[0 – 0.22]	
MIN	0.40 [0.18 – 0.40]	0.40 [0.29 – 0.40]	$6.27 \times 10^{15}$ $[4.6 \times 10^{14} - 2.2 \times 10^{16}]$	$7.46 \times 10^{16}$ $[2.0 \times 10^{16} - 1.0 \times 10^{18}]$	6.30 [6.20 – 6.30]	0.22 [0.19 – 0.22]	7.25 1.438 5.92 85.2

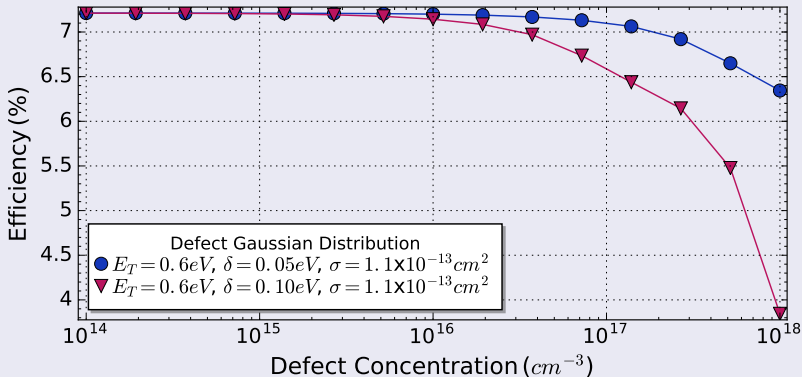
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- 1 InGaN Schottky Solar Cell modeling & optimization
  - Modeling the Solar Cell
  - Multi-variate optimization
  - An optimal design
- 2 Proposal for a new InGaN MIN structure
  - Optimal PN and PIN structure
  - Schottky Based InGaN Solar Cells
  - MIN structure behavior
- 3 From simulation to realization
  - InGaN composition
  - **Crystal defects**
  - Metal work function
  - Future work

# Efficiency degraded by crystalline defects

Urbach tails & Gaussian distribution of defects in the band gap

Defect density must be kept lower than i-layer doping



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## Efficiency lowering with metal work function lowering

Possible defects not included

Both optimal and experimental compositions

### Zero defect efficiency with varying work function

$W_f$ (eV)	$\eta$ for $x = 0.60$ (%)	$\eta$ for $x = 0.22$ (%)
6.30	19.80	7.25
6.10	17.84	6.15
5.93	13.58	5.22
5.65	6.34	3.70

Today state of the art device realization : 3.70% efficiency

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## Future work

### Connect to experiments

### Contact me

- Collaborate with **experimental groups**
- Study their own technological constraints
- Include them in the optimization
- **Realize and test the actual device**
- Original approach to be adapted to other materials for PV

### Details in two recently published paper

(2016)

- Numerical simulation of InGaN Schottky solar cell
- Simulation study of a new InGaN p-layer free Schottky based solar cell
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