Multiphysics Modeling and Understanding for Plasmonic Organic Solar Cells

Wei E.I. Sha, Wallace C.H. Choy, and Weng Cho Chew

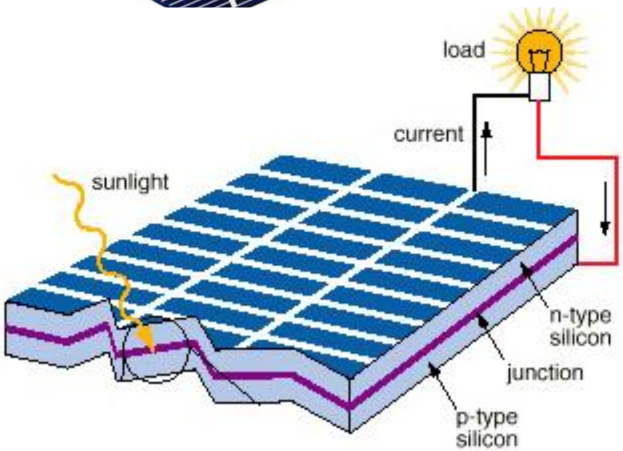
Department of Electrical and Electronic Engineering,

The University of Hong Kong, Hong Kong

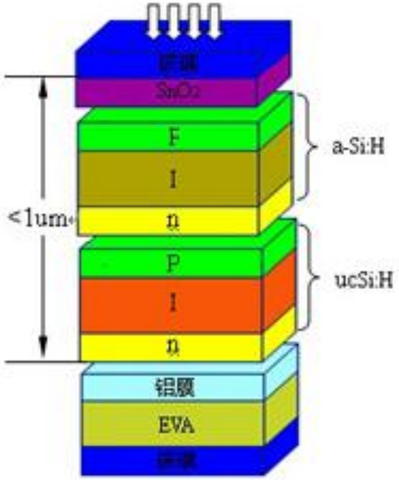
Email: wsha@eee.hku.hk (W.E.I. Sha)

Organic Solar Cell (1)

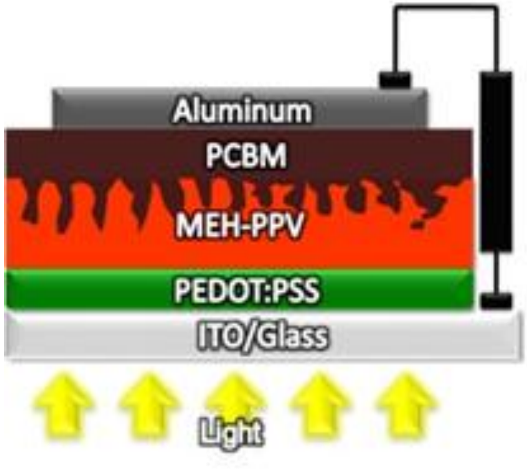
Advances of solar cell technology



monocrystalline silicon solar cell



amorphous/polycrystalline silicon solar cell

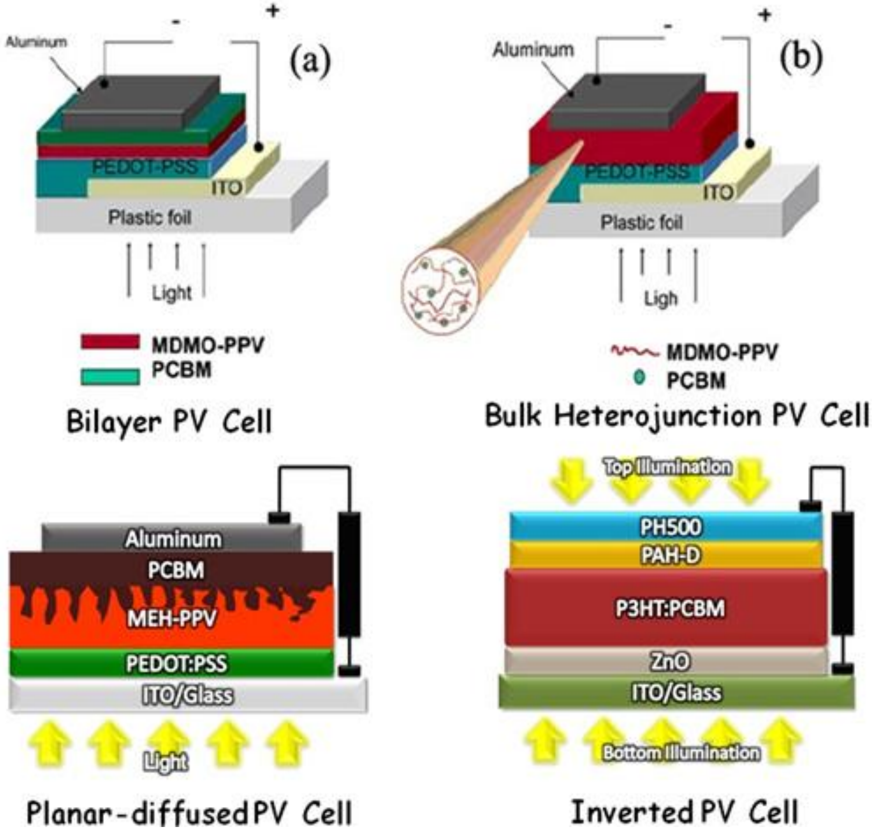


organic solar cell

Organic Solar Cell (2)

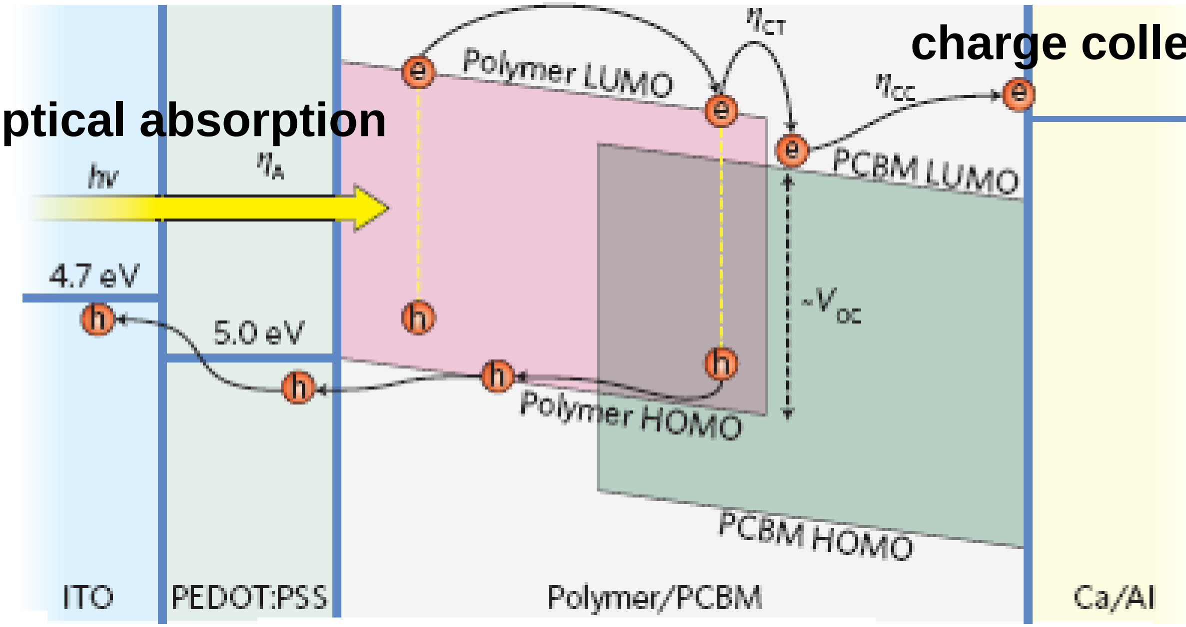
Thin-film organic solar cell

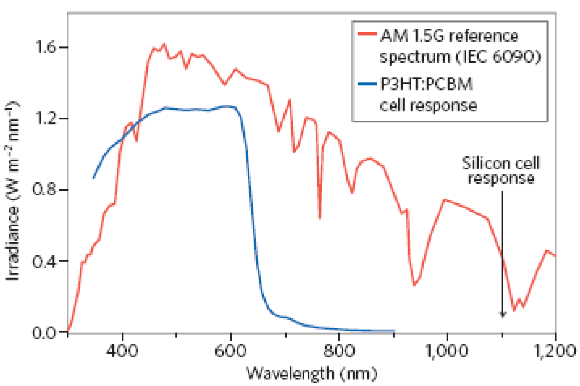
- ✓ *low-cost processing*
- ✓ *mechanically flexible*
- ✓ *large-area application*
- ✓ *environmentally friendly*
- X *low exciton diffusion length*
- X *low carrier mobility*

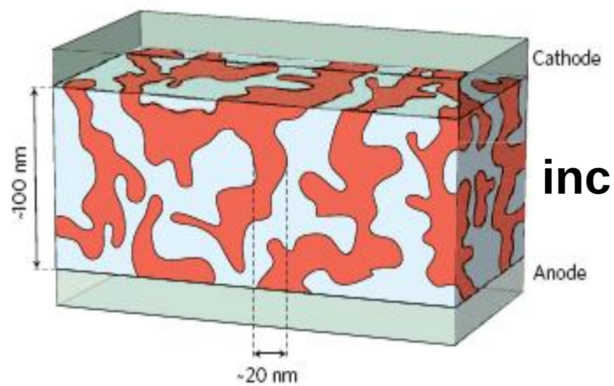


Organic Solar Cell (3)

Working principle





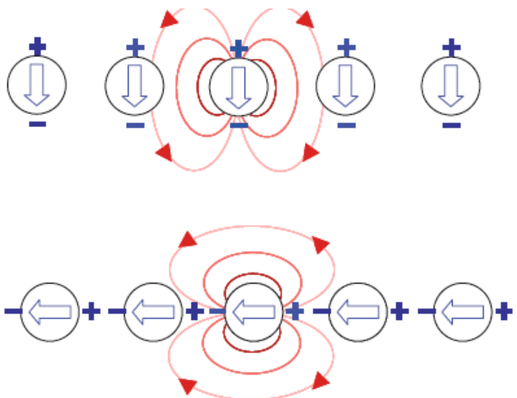


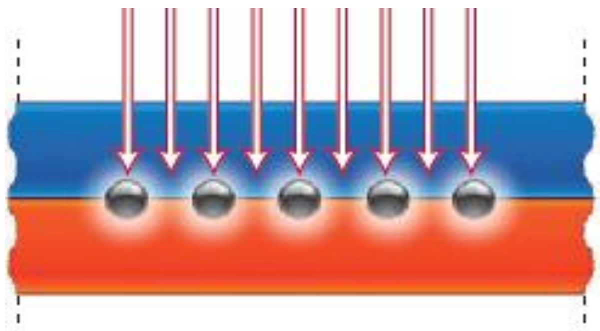
increase interface area

Plasmonic Organic Solar Cell

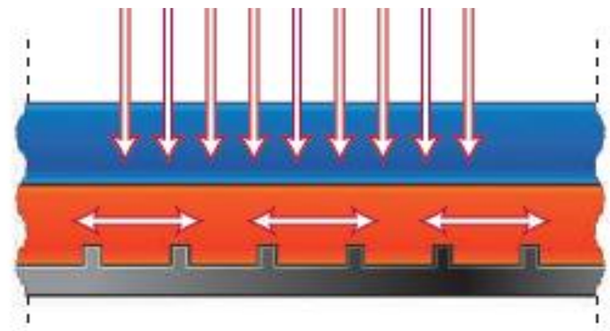
Why optical enhancement?

The thickness of the active layer must be smaller than the exciton diffusion length to avoid bulk recombination. As a result, the thin-film organic solar cell has poor photon absorption or harvesting. Plasmonic solar cell is one of emerging solar cell technologies to enhance the optical absorption.

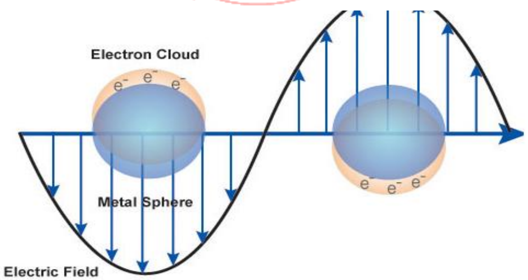


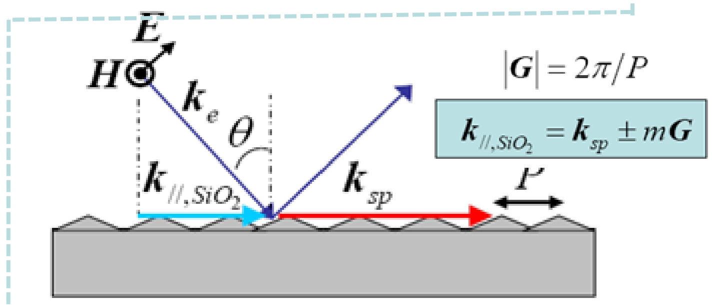


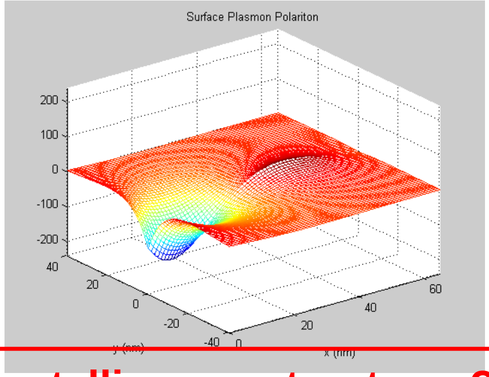
nanoparticles: local plasmon



nanograting: surface plasmon



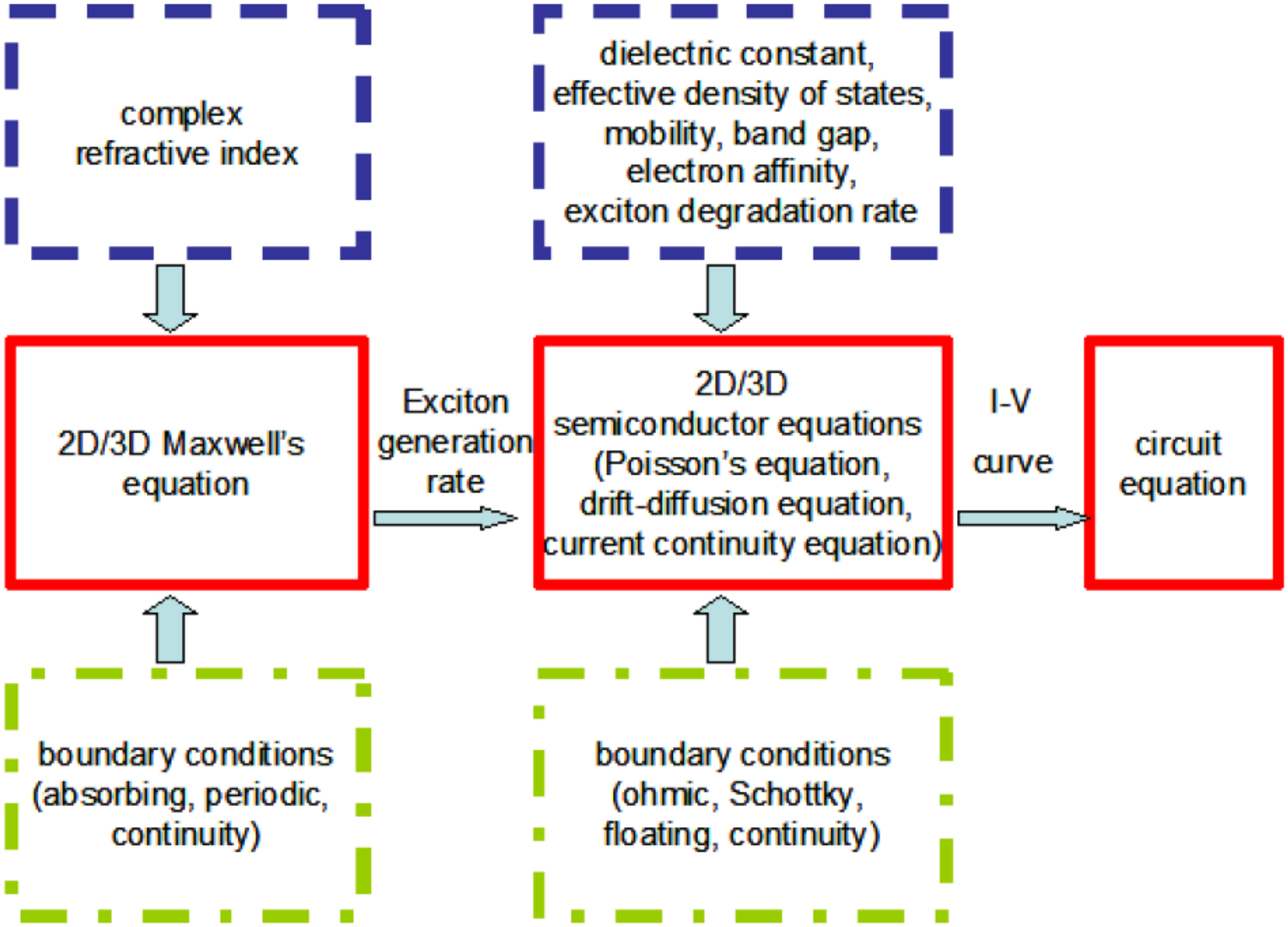




Could electrical properties of OSCs be affected by introducing the metallic nanostructures?

Multiphysics Model (1)

Schematic diagram



Multiphysics Model (2)

Governing equations

frequency dependent permittivity

$$\nabla \times \mathbf{E} = -j\omega\mu_0 \mathbf{H}, \quad \nabla \times \mathbf{H} = j\omega\varepsilon(\omega)\mathbf{E}$$

Maxwell's equation

optical electric field

$$G(\mathbf{r}) = \int_{400}^{800} \frac{\lambda}{hc} A(\mathbf{r},\lambda)\, d\lambda, \quad A(\mathbf{r},\lambda) = \omega\varepsilon_0 n_r k_i \left|\mathbf{E}(\mathbf{r})\right|^2$$

generation rate

Generation rate

electrostatic potential

electron density

$$\nabla \cdot (\varepsilon \nabla \phi) = -q(p-n)$$

bimolecular recombination rate

electrostatic dielectric constant

$$\frac{\partial n}{\partial t} = \frac{1}{q}\nabla \cdot (-q\mu_n n \nabla \phi + qD_n \nabla n) + QG - (1-Q)R$$

semiconductor equations

hole density

mobility

Diffusion coefficients

exciton dissociation probability

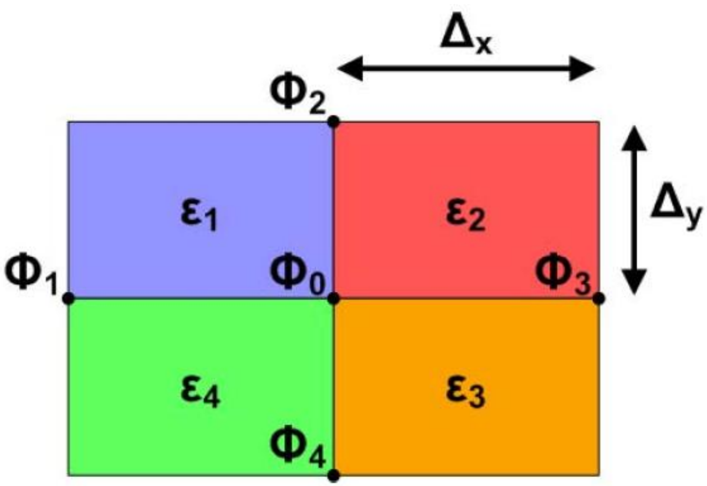
$$\frac{\partial p}{\partial t} = -\frac{1}{q}\nabla \cdot (-q\mu_p p \nabla \phi - qD_p \nabla p) + QG - (1-Q)R$$

Multiphysics Model (3)

Unified finite difference method

optical properties

spatial step depends on the dielectric wavelength and skin depth of surface plasmons



2D wave equations: TE & TM

$$2\left(\frac{1}{\Delta_x^2}+\frac{1}{\Delta_y^2}\right)\frac{\Phi_0}{\bar{\epsilon}}-k_0^2\Phi_0-\frac{\Phi_1+\Phi_3}{\bar{\epsilon}\Delta_x^2}-\frac{\Phi_2+\Phi_4}{\bar{\epsilon}\Delta_y^2}=0, \quad \Phi=E_z$$

$$2\left(\frac{1}{\Delta_x^2}+\frac{1}{\Delta_y^2}\right)\frac{\Phi_0}{\bar{\epsilon}}-k_0^2\Phi_0-\frac{\epsilon_1^{-1}+\epsilon_4^{-1}}{2\Delta_x^2}\Phi_1-\frac{\epsilon_2^{-1}+\epsilon_3^{-1}}{2\Delta_x^2}\Phi_3 -\frac{\epsilon_1^{-1}+\epsilon_2^{-1}}{2\Delta_y^2}\Phi_2-\frac{\epsilon_3^{-1}+\epsilon_4^{-1}}{2\Delta_y^2}\Phi_4=0, \quad \Phi=H_z$$

periodic boundary conditions

stretched-coordinate perfectly matched layer

$$\bar{\epsilon}=\begin{cases}\dfrac{\epsilon_1+\epsilon_2+\epsilon_3+\epsilon_4}{4}, & \Phi=E_z\\ 4(\epsilon_1^{-1}+\epsilon_2^{-1}+\epsilon_3^{-1}+\epsilon_4^{-1})^{-1}, & \Phi=H_z\end{cases}$$

Multiphysics Model (4)

Poisson equation (Gummel's method)

electrical properties

spatial step depends on the Debye length

$$\frac{1}{\Delta_x^2}\epsilon^d_{i+1/2,j}\phi^{t+1}_{i+1,j} + \frac{1}{\Delta_x^2}\epsilon^d_{i-1/2,j}\phi^{t+1}_{i-1,j} + \frac{1}{\Delta_y^2}\epsilon^d_{i,j+1/2}\phi^{t+1}_{i,j+1} + \frac{1}{\Delta_y^2}\epsilon^d_{i,j-1/2}\phi^{t+1}_{i,j-1}$$

$$-\left(\epsilon^d_{i+1/2,j} + \epsilon^d_{i-1/2,j} + \epsilon^d_{i,j+1/2} + \epsilon^d_{i,j-1/2}\right)\left(\frac{1}{2\Delta_x^2} + \frac{1}{2\Delta_y^2}\right)\phi^{t+1}_{i,j} - \frac{n^t_{i,j} + p^t_{i,j}}{U_t}\phi^{t+1}_{i,j}$$

$$= q(n^t_{i,j} - p^t_{i,j}) - \frac{n^t_{i,j} + p^t_{i,j}}{U_t}\phi^t_{i,j}$$

scaling unit

cm	$\max\{\mathrm{DOS}\}^{1/3}$
s	10^{12}
V	1
C	$\frac{1}{1.602\times 10^{-19}}$
K	$\frac{1}{300}$

drift-diffusion and continuity equations of electron (Scharfetter-Gummel scheme in spatial domain semi-implicit strategy in time domain)

$$\frac{n^{t+1}_{i,j} - n^t_{i,j}}{\Delta_t} = Q^t_{i,j}G_{i,j} - (1 - Q^t_{i,j})R^t_{i,j} + \frac{D^n_{i+1/2,j}}{\Delta_x^2}B\left(\frac{\phi^{t+1}_{i+1,j} - \phi^{t+1}_{i,j}}{U_t}\right)n^{t+1}_{i+1,j}$$

$$+\frac{D^n_{i-1/2,j}}{\Delta_x^2}B\left(\frac{\phi^{t+1}_{i-1,j} - \phi^{t+1}_{i,j}}{U_t}\right)n^{t+1}_{i-1,j} + \frac{D^n_{i,j+1/2}}{\Delta_y^2}B\left(\frac{\phi^{t+1}_{i,j+1} - \phi^{t+1}_{i,j}}{U_t}\right)n^{t+1}_{i,j+1}$$

$$+\frac{D^n_{i,j-1/2}}{\Delta_y^2}B\left(\frac{\phi^{t+1}_{i,j-1} - \phi^{t+1}_{i,j}}{U_t}\right)n^{t+1}_{i,j-1} - \left[\frac{D^n_{i+1/2,j}}{\Delta_x^2}B\left(\frac{\phi^{t+1}_{i,j} - \phi^{t+1}_{i+1,j}}{U_t}\right)\right.$$

$$+\frac{D^n_{i-1/2,j}}{\Delta_x^2}B\left(\frac{\phi^{t+1}_{i,j} - \phi^{t+1}_{i-1,j}}{U_t}\right) + \frac{D^n_{i,j+1/2}}{\Delta_y^2}B\left(\frac{\phi^{t+1}_{i,j} - \phi^{t+1}_{i,j+1}}{U_t}\right)$$

$$\left.+\frac{D^n_{i,j-1/2}}{\Delta_y^2}B\left(\frac{\phi^{t+1}_{i,j} - \phi^{t+1}_{i,j-1}}{U_t}\right)\right]n^{t+1}_{i,j}$$

Dirichlet and Neumann boundary conditions

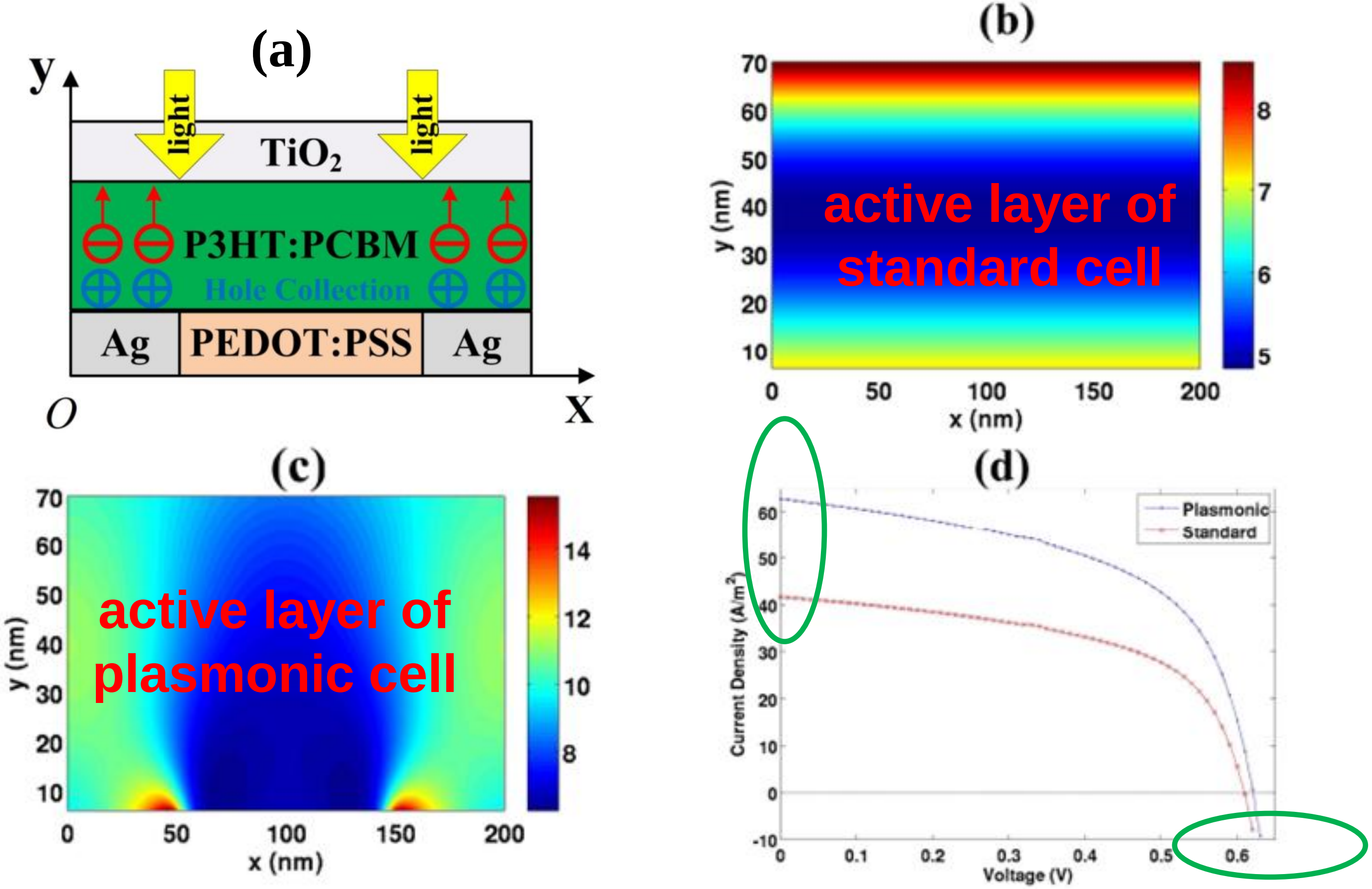
time step for stable algorithm

$$\Delta_t < \min\left(\frac{C\varepsilon}{\mu_n \cdot n + \mu_p \cdot p}\right)$$

Multiphysics Model (5)

Beyond optical absorption enhancement: facilitating hole collection!

schematic pattern of nanostrip plasmonic cell



Model settings

active layer thickness
70 nm
periodicity
200 nm
PEDOT:PSS width
100 nm
anode
ohmic
cathode barrier height
0.2 eV
hole mobility
0.1*electron mobility
effective band gap
1.1 eV

W.E.I. Sha, W.C.H. Choy, Y.M. Wu, and W.C. Chew, Opt. Express, 20(3), 2572-2580, 2012.*

Multiphysics Model (6)

Characteristic parameters

	J_{sc} (A/m^2)	V_{oc} (V)	MP (W)	FF	PCE (%)
Plasmonic	62.84	0.62	21.47	0.55	2.15
Standard	41.67	0.61	14.03	0.55	1.40

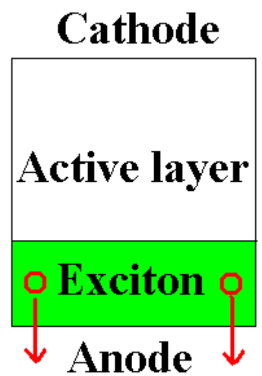
Plasmonic	V (V)	J (A/m^2)	$\langle$Diss$\rangle$ (%)	$\langle$Rec loss$\rangle$ (%)
SC	0	62.84	66.96	2.62
MP	0.48	44.73	58.97	14.55
OC	0.62	0	55.47	80.88
Standard	**V (V)**	**J (A/m^2)**	**$\langle$Diss$\rangle$ (%)**	**$\langle$Rec loss$\rangle$ (%)**
SC	0	41.67	66.96	3.18
MP	0.47	30.42	59.19	14.93
OC	0.61	0	55.75	81.91

- ➢**reduce recombination loss**
- ➢**increase short-circuit current**
- ➢**improve open-circuit voltage**
- ➢**boost power conversion efficiency**

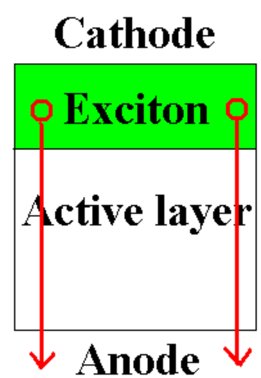
Multiphysics Model (7)

Dummy case for further illustrating physics (hole transport and collection)

$$G_{grating} = \begin{cases} G_c, & d_3 \le y \le d_3 + L_g \\ 0, & \text{else} \end{cases}$$

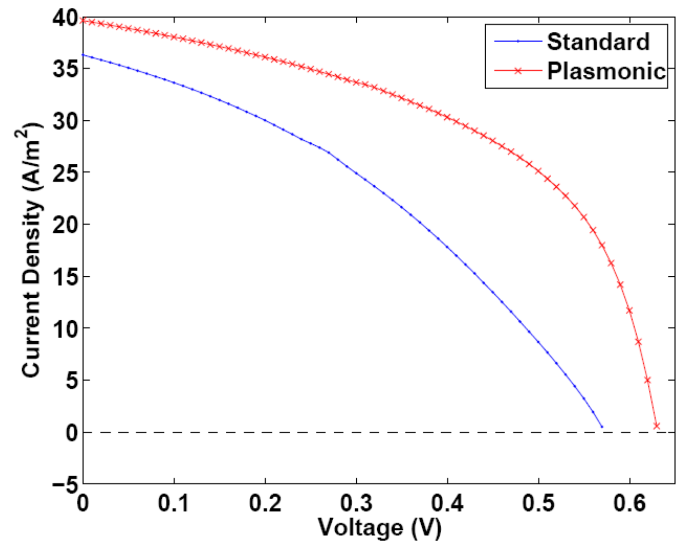


$$G_{planar} = \begin{cases} G_c, & d_3 + d_2 - L_g \le y \le d_3 + d_2 \\ 0, & \text{else} \end{cases}$$



hole mobility is set to be two order of magnitude lower than electron mobility

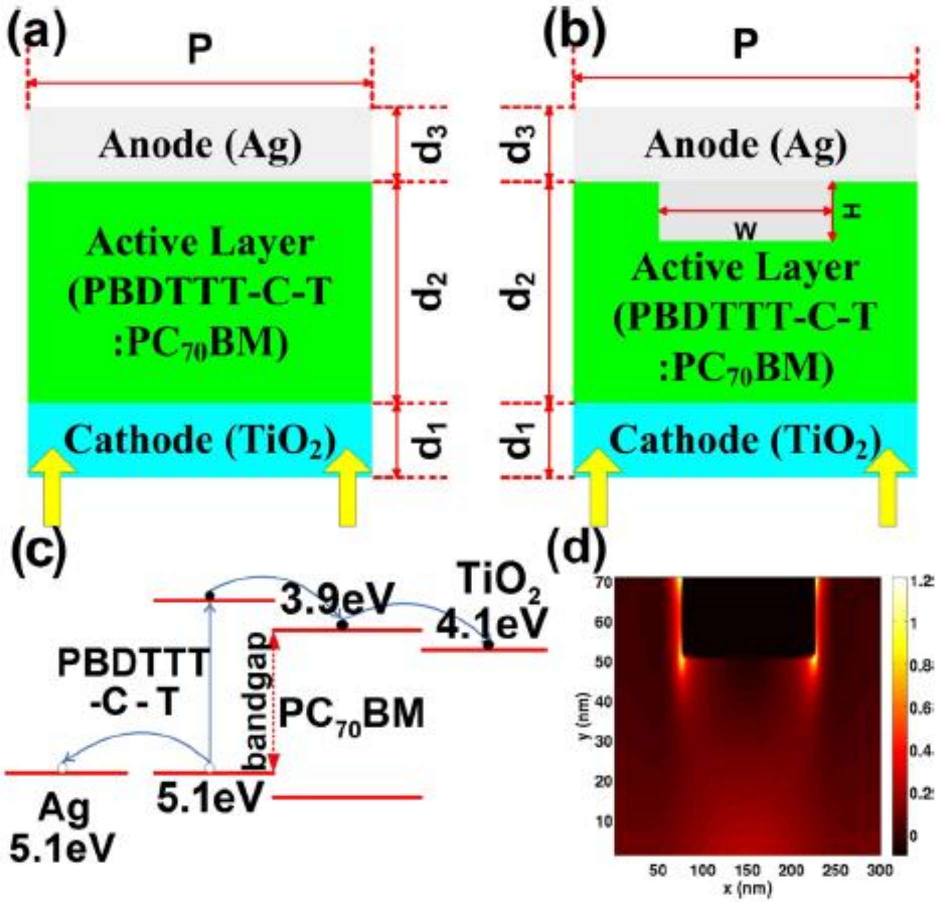
J-V curve



inhomogeneous exciton generation significantly affects fill factor and open-circuit voltage

Multiphysics Model (8)

The nanograting structure v.s. flat standard structure

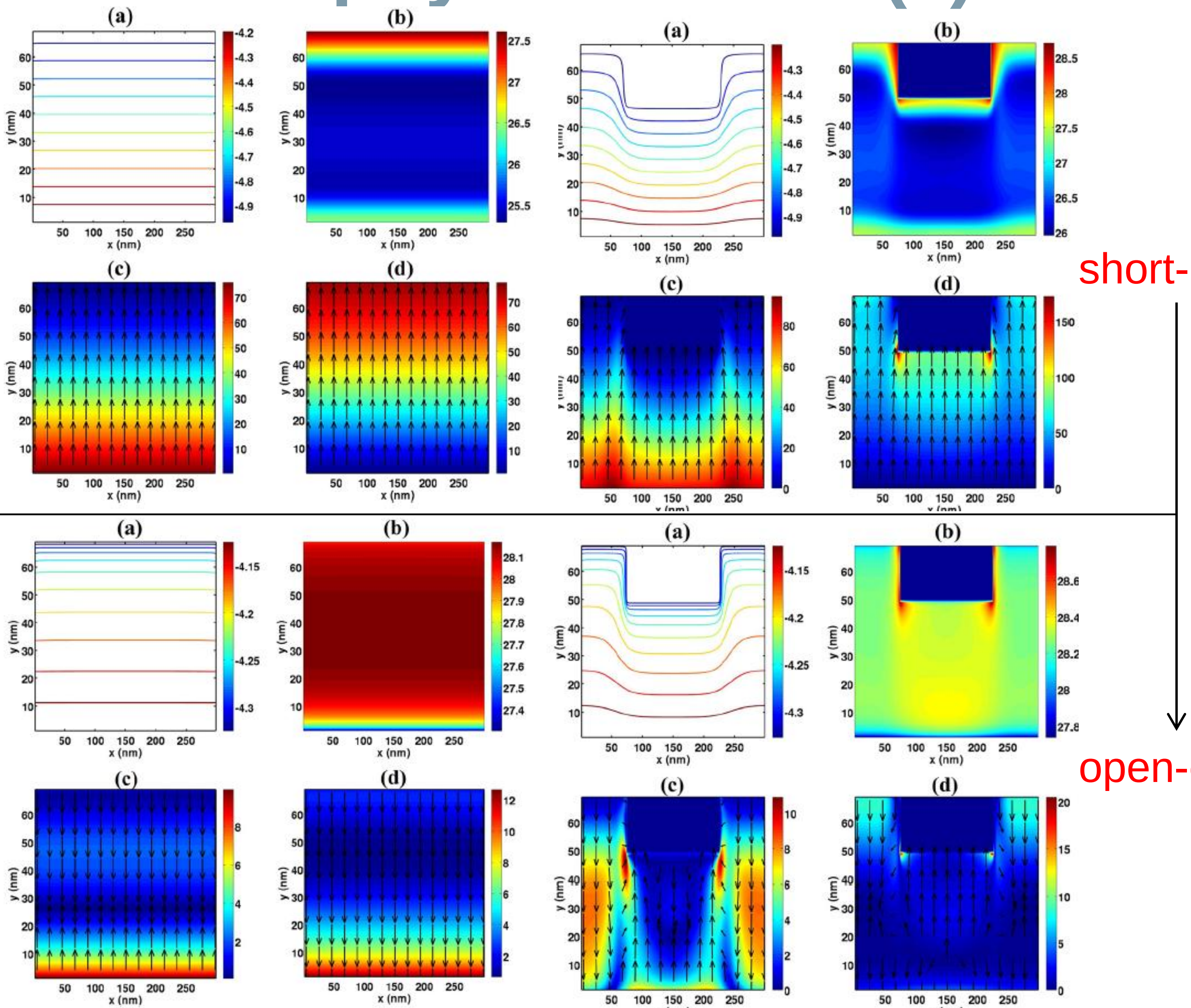


Simulation parameters

E_g	$1.2\ eV$
μ_n	$7.4 \times 10^{-7}\ m^2/(V \cdot S)$
μ_p	$7.4 \times 10^{-8}\ m^2/(V \cdot S)$
N_c	$2.5 \times 10^{19}\ cm^{-3}$
N_v	$2.5 \times 10^{19}\ cm^{-3}$
ϵ^d	$3.4\epsilon_0\ F/m$
a	$1.12\ nm$
k_r	$3 \times 10^5\ s^{-1}$
ψ_b^n	$0.2\ eV$
ψ_b^p	$0\ eV$

W.E.I. Sha, W.C.H. Choy, and W.C. Chew, Appl. Phys. Lett., 101, 223302, 2012.*

Multiphysics Model (9)



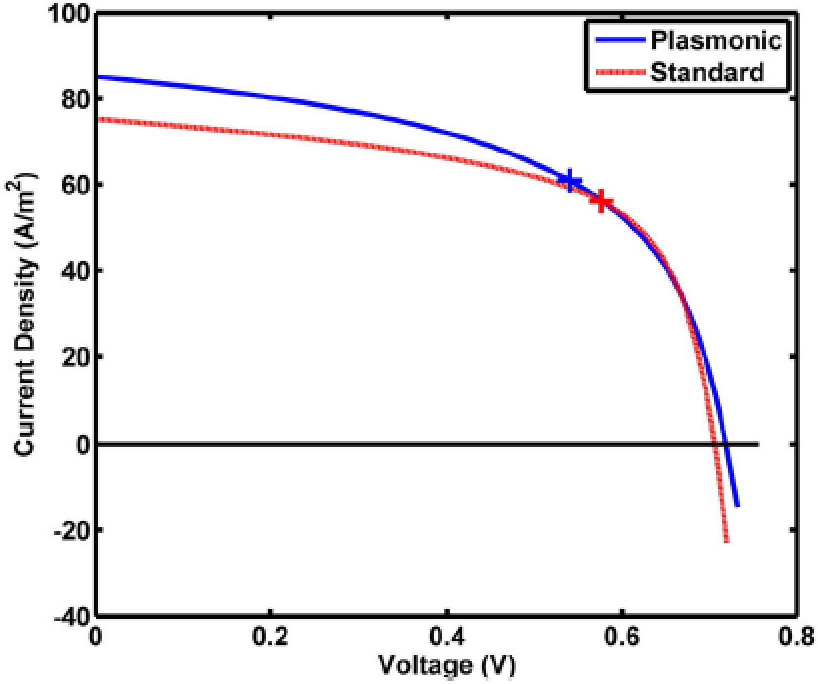
short-circuit

open-circuit

(a) equipotential lines; (b) recombination rate; (c,d) electron and hole current densities.

Multiphysics Model (10)

$$FF = \frac{P_{MAX}}{P_T} = \frac{I_{MP} \cdot V_{MP}}{I_{SC} \cdot V_{OC}}$$



The grating anode induces nonuniform optical absorption and inhomogeneous internal E-field distribution. Thus uneven photocarrier generation and transport are formed in the plasmonic OSC leading to the dropped FF.

TABLE II. The characteristic parameters of the standard and plasmonic OSCs involving short-circuit J_{sc}, open-circuit voltage V_{oc}, MP, FF, and PCE.

	J_{sc} (A/m^2)	V_{oc} (V)	MP (W)	FF (%)	PCE (%)
Standard	75.18	0.706	32.34	60.91	3.23
Plasmonic	85.12	0.719	32.91	53.77	3.29

	SC ⟨Diss⟩	SC ⟨Rec⟩	MP ⟨Diss⟩	MP ⟨Rec⟩	OC ⟨Diss⟩	OC ⟨Rec⟩
Standard (%)	69.83	0.88	62.34	9.19	59.69	82.56
Plasmonic (%)	70.52	2.5	63.38	16.63	59.63	92.75

recombination and exciton dissociation

Acknowledgement

Thanks for your attention!