A Comprehensive Multiphysics Model for Organic Photovoltaics

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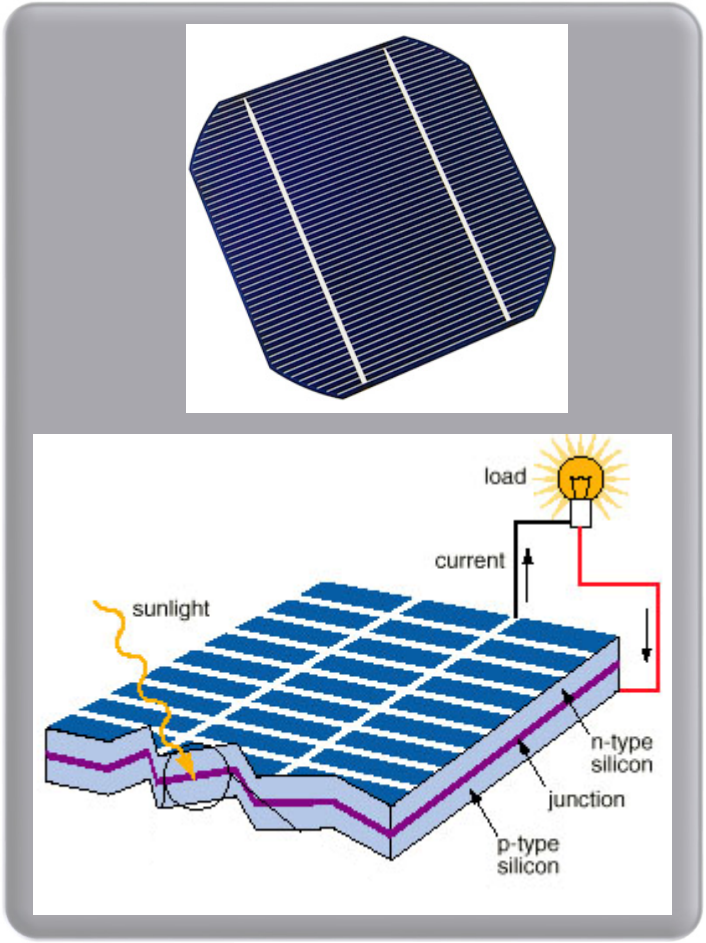
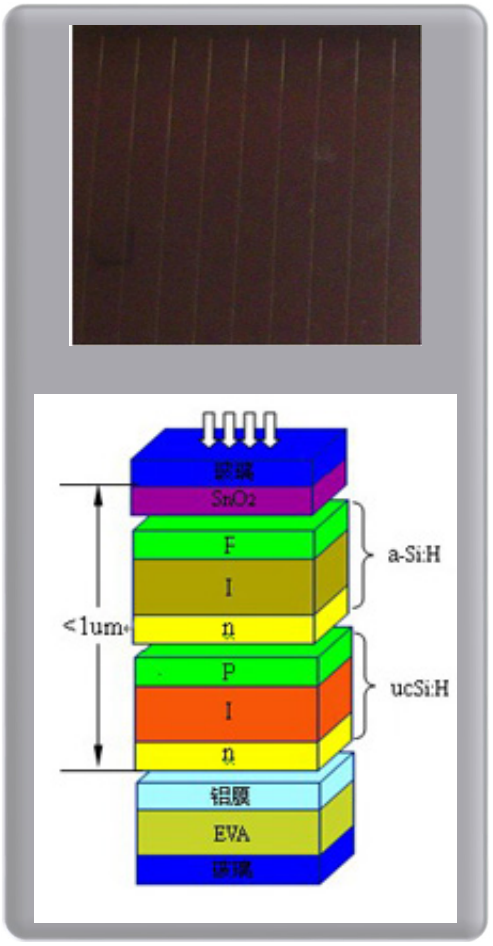
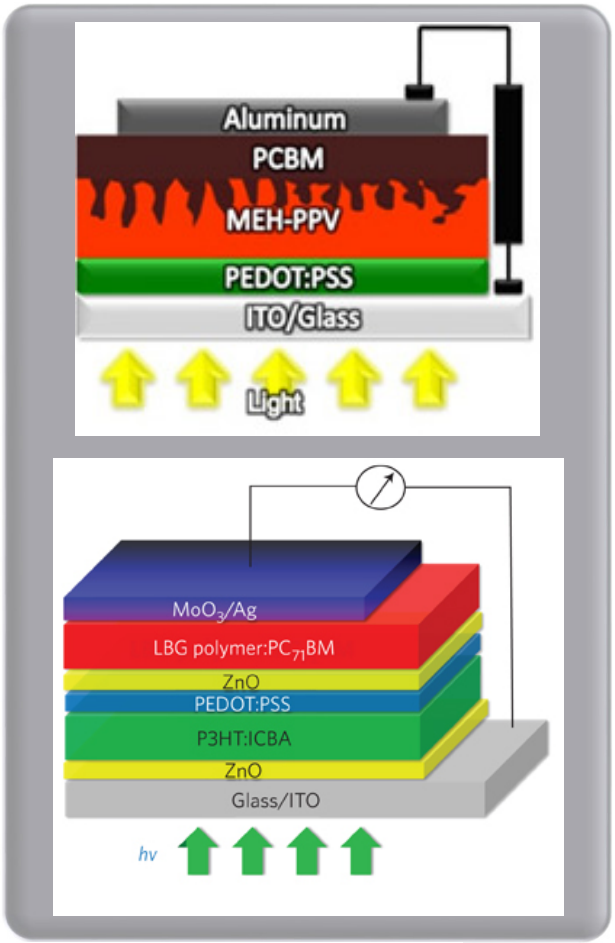
ADVANCES OF SOLAR CELL TECHNOLOGY



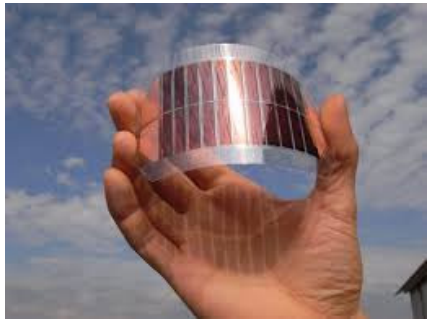


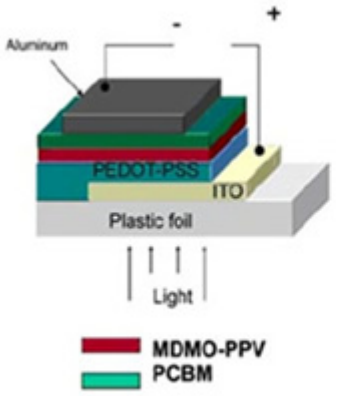


Crystalline silicon → Amorphous silicon → Polymer Small-molecules

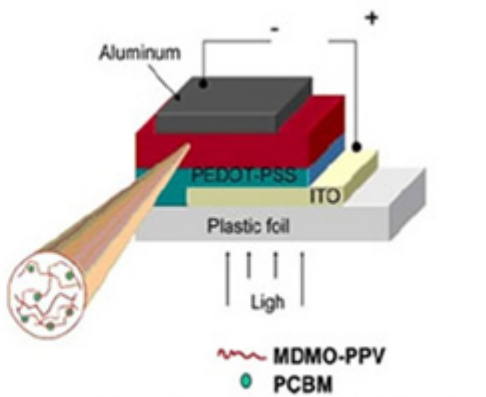
PROPERTIES OF ORGANIC SOLAR CELLS

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

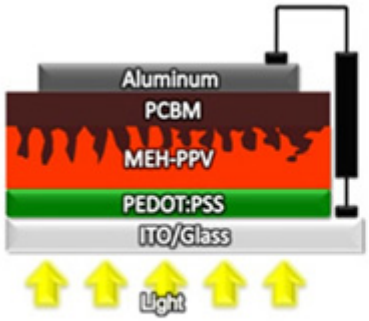




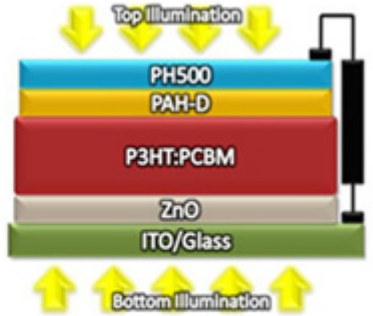
Bilayer PV Cell



Bulk Heterojunction PV Cell

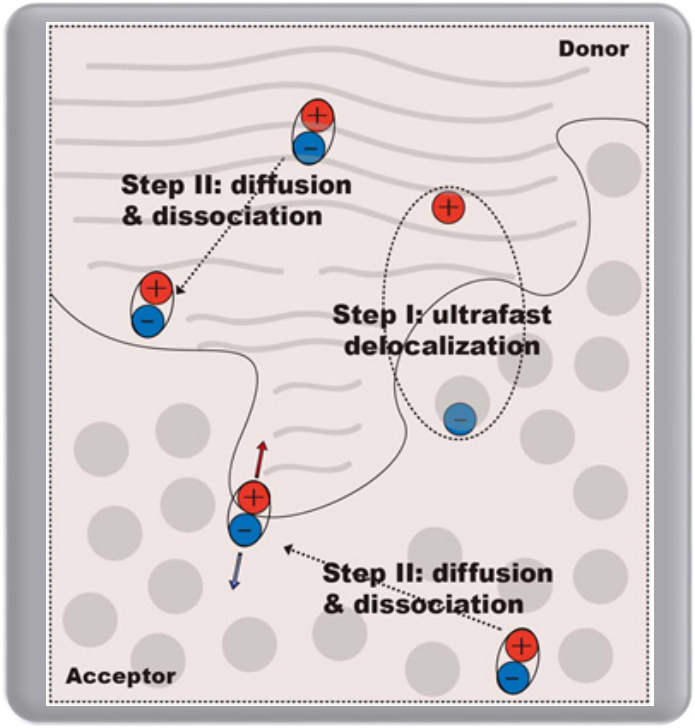


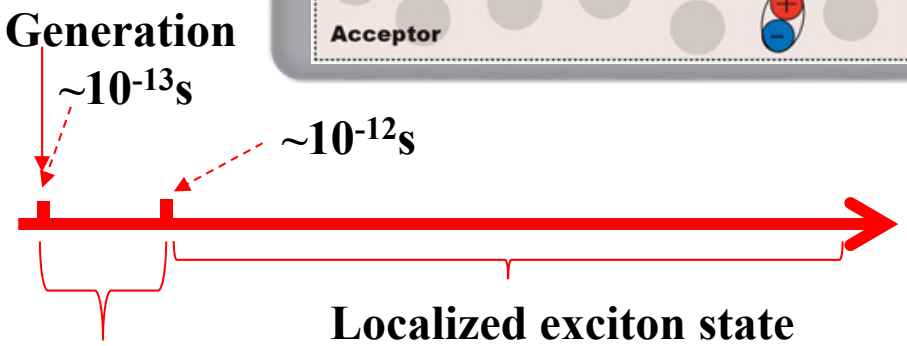
Planar-diffused PV Cell

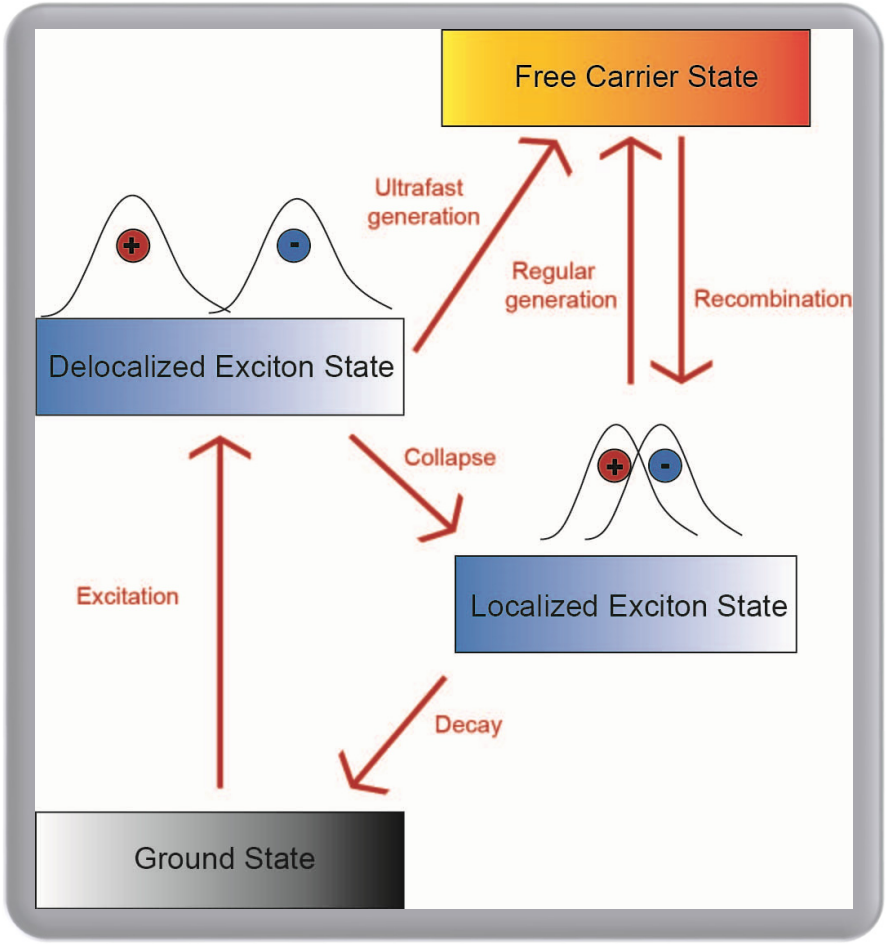


Inverted PV Cell

DEVICE PHYSICS

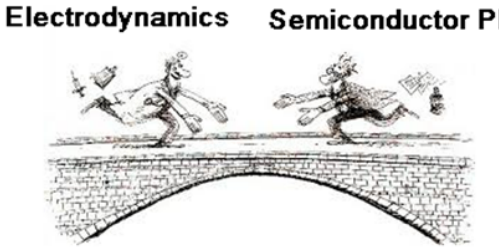






David Beljonne, *Multiscale Modelling of Organic and Hybrid Photovoltaics*, Springer.

DEVICE MODEL



permittivity

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

optical E-field

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

Maxwell's equations

Generation rate

electrostatic potential

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

Poisson equation

electron density

$$\frac{\partial n}{\partial t} = \eta_d G + \frac{1}{q}\nabla\cdot(q\mu_n n E_n + qD_n \nabla n) + k_d X_l - R(n,p)$$

hole density — mobility — diffusion coef. — recombination

$$\frac{\partial p}{\partial t} = \eta_d G - \frac{1}{q}\nabla\cdot(q\mu_p p E_p - qD_p \nabla p) + k_d X_l - R(n,p)$$

Drift-diffusion equation & Current-continuity equation

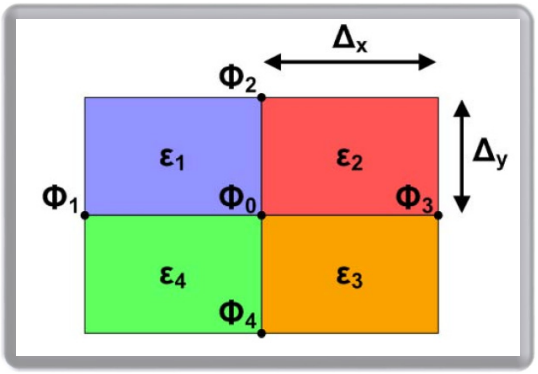
singlet Ex density — Ex diffusion coef. — Ex dissociation & decay

$$\frac{\partial X}{\partial t} = (1-\eta_d)G + \nabla\cdot(D_X \nabla X_l) - k_d X_l - k_f X_l + \eta_s R(n,p)$$

Exciton diffusion-dissociation equation

SOLUTION: SOME REMARKS

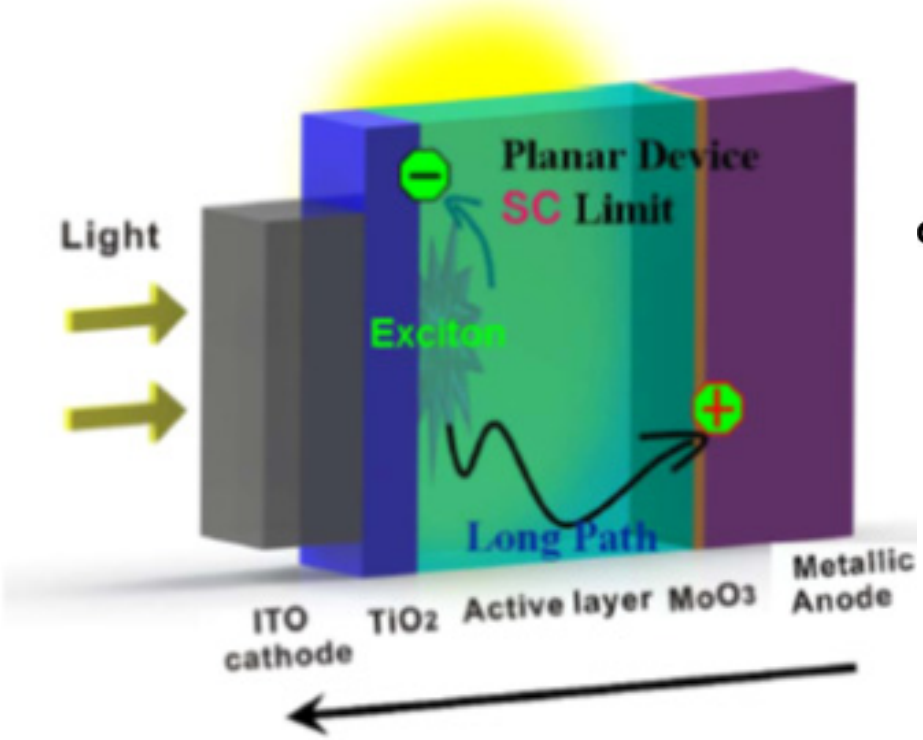
- Unified finite-difference method with identical spatial grids is used. Debye length of organic materials is comparable to decay length of plasmonic waves.
- For Maxwell's equations, frequency-domain or explicit time-domain methods can be employed; For organic semiconductor equations, semi-implicit time-domain method (steady and transient solution) or Newton's method (steady solution) can be adopted.
- For stable multiphysics model, five international units should be redefined.
- Commercial software do not describe exciton behaviors properly.

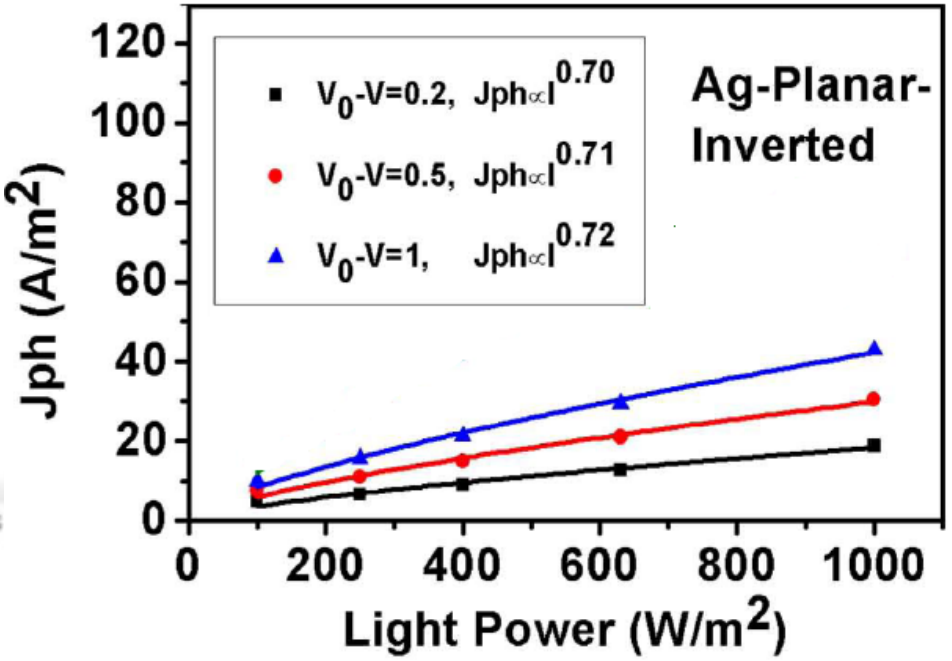


cm	$\max\{\mathrm{DOS}\}^{1/3}$
s	10^{12}
V	1
C	$\frac{1}{1.602\times10^{-19}}$
K	$\frac{1}{300}$

SCL FOR PLANAR INVERTED OPVS

Wei E.I. Sha, Xuanhua Li, and Wallace C.H. Choy, *Scientific Reports*, vol. 4, pp. 6236, Aug. 2014.

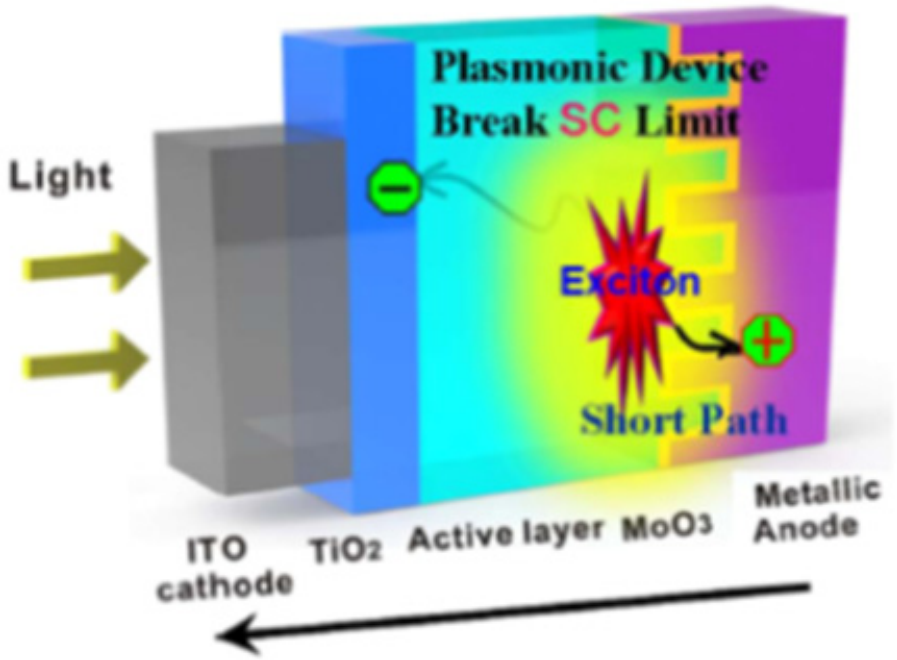


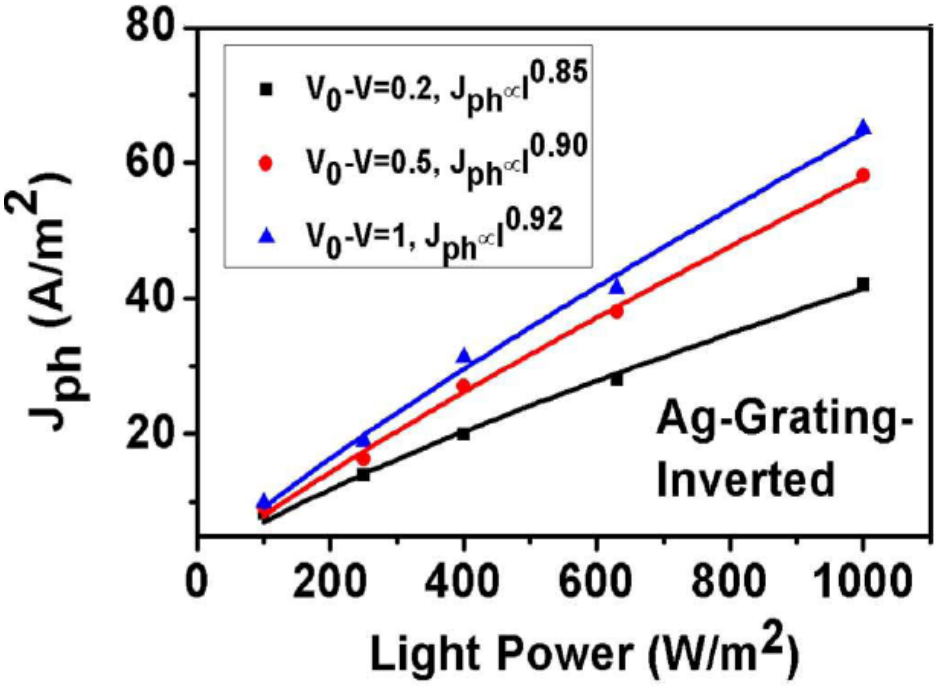


Light distribution mainly concentrates around cathode.
Low-mobility holes travel a long distance.
High-mobility electrons travel a short distance.
Space charge limit (SCL) effect occurs.

$$J_{SCL} = q\left(\frac{9\varepsilon\mu_h}{8q}\right)^{1/4} G^{3/4}V^{1/2}$$

SCL BREAKING FOR GRATING INVERTED OPVS



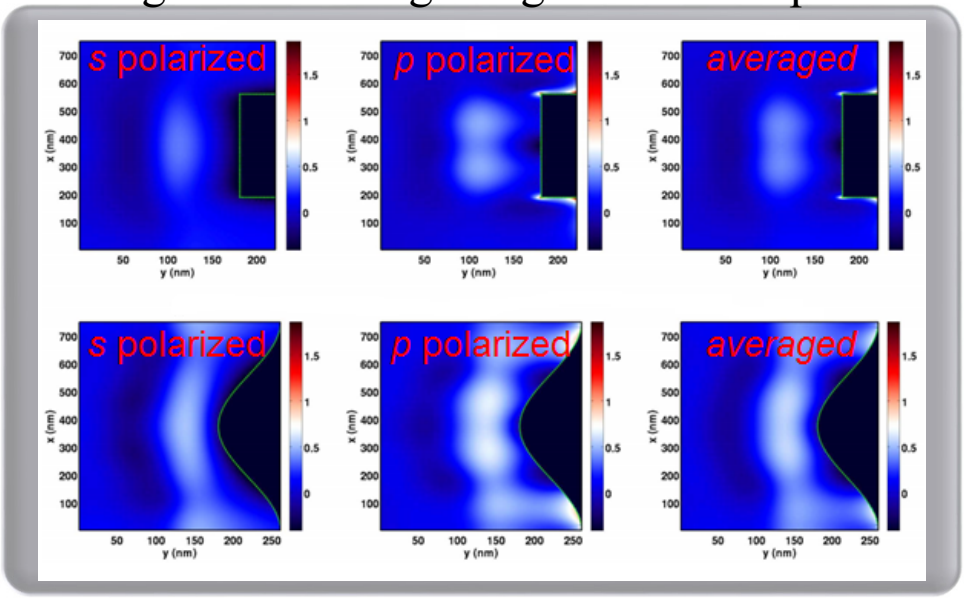


Light distribution concentrates around anode.
Low-mobility holes travel a short distance.
high-mobility electrons travel a long distance.
SCL effect is broken by the plasmonic-electrical effect!

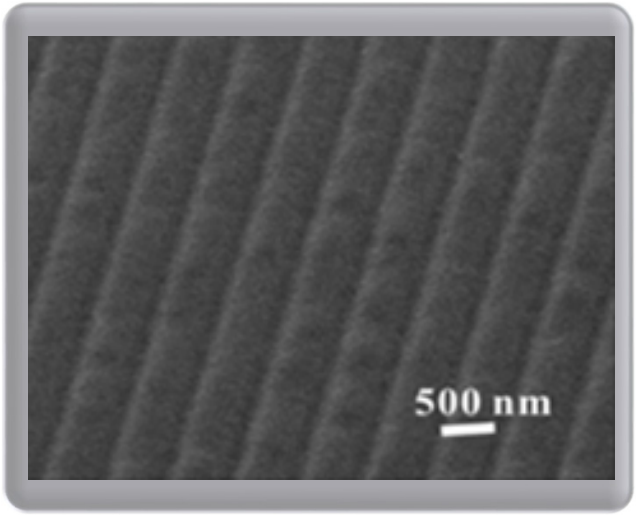
$$J_{normal} = qGL$$

THEORETICAL RESULTS

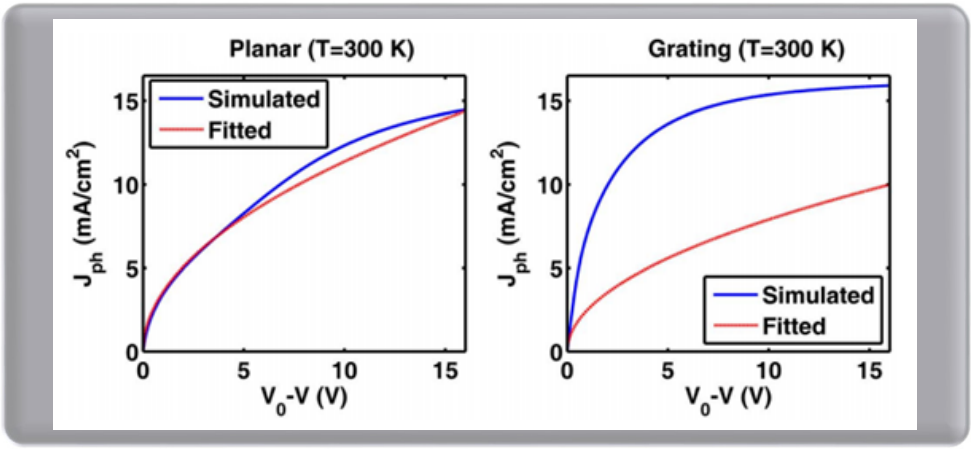
exciton generation of grating over that of planar devices



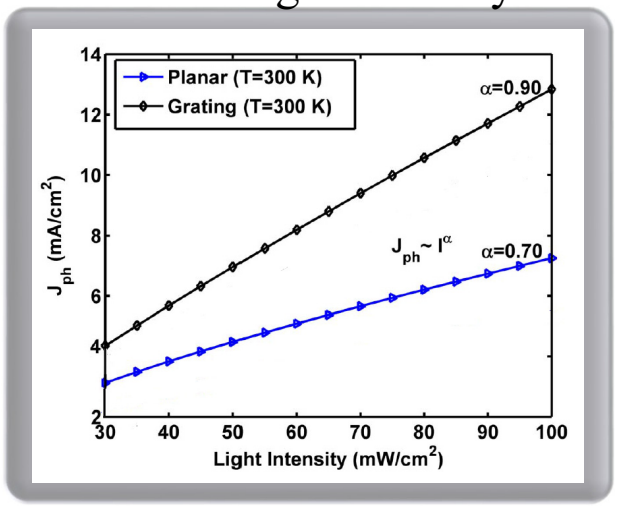
SEM of nanopattered organic thin-film



current density—voltage curves

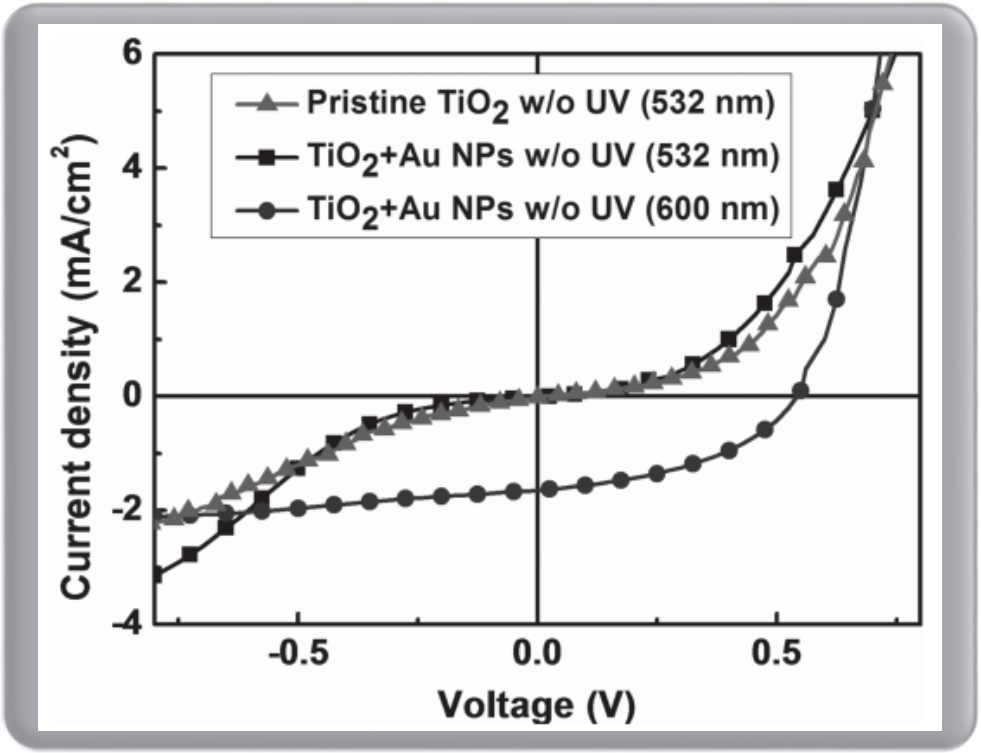


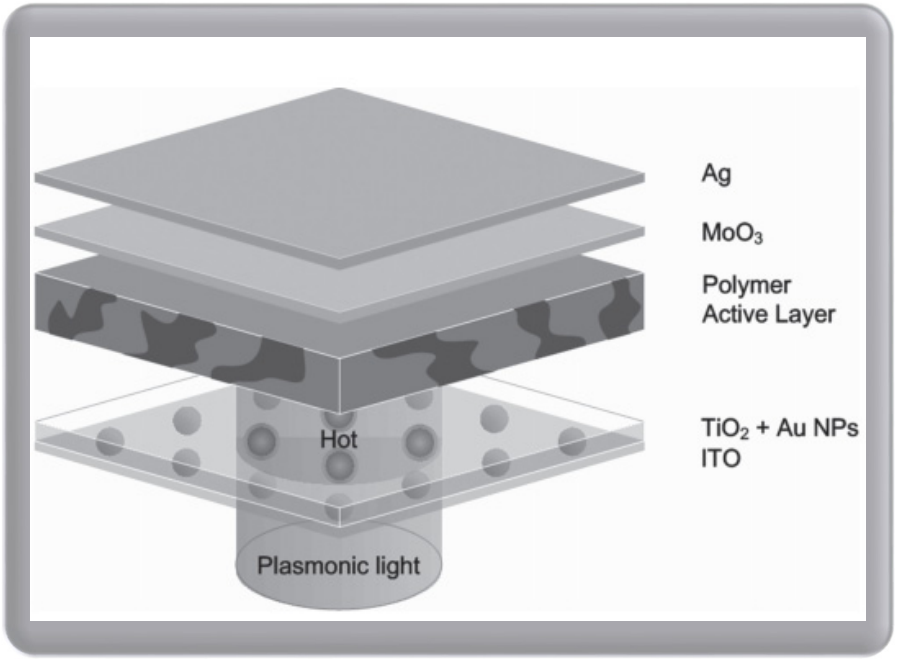
photocurrent—light intensity curves



S-SHAPED *J-V* CHARACTERISTICS

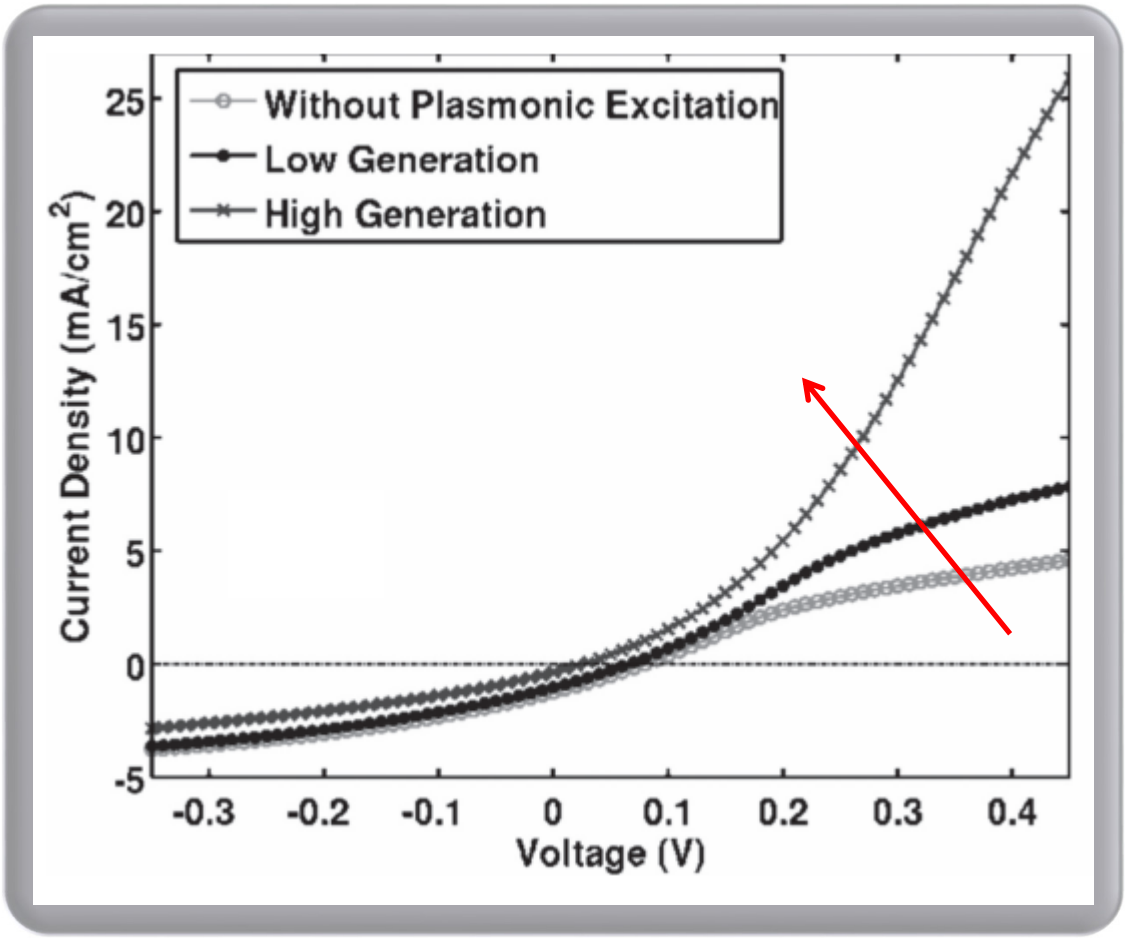
Di Zhang, Wallace C.H. Choy, Fengxian Xie, Wei E.I. Sha, Xinchen Li, Baofu Ding, Kai Zhang, Fei Huang, and Yong Cao, Wiley, *Advanced Functional Materials*, vol. 23, no. 34, pp. 4255-4261, Sep. 2013.

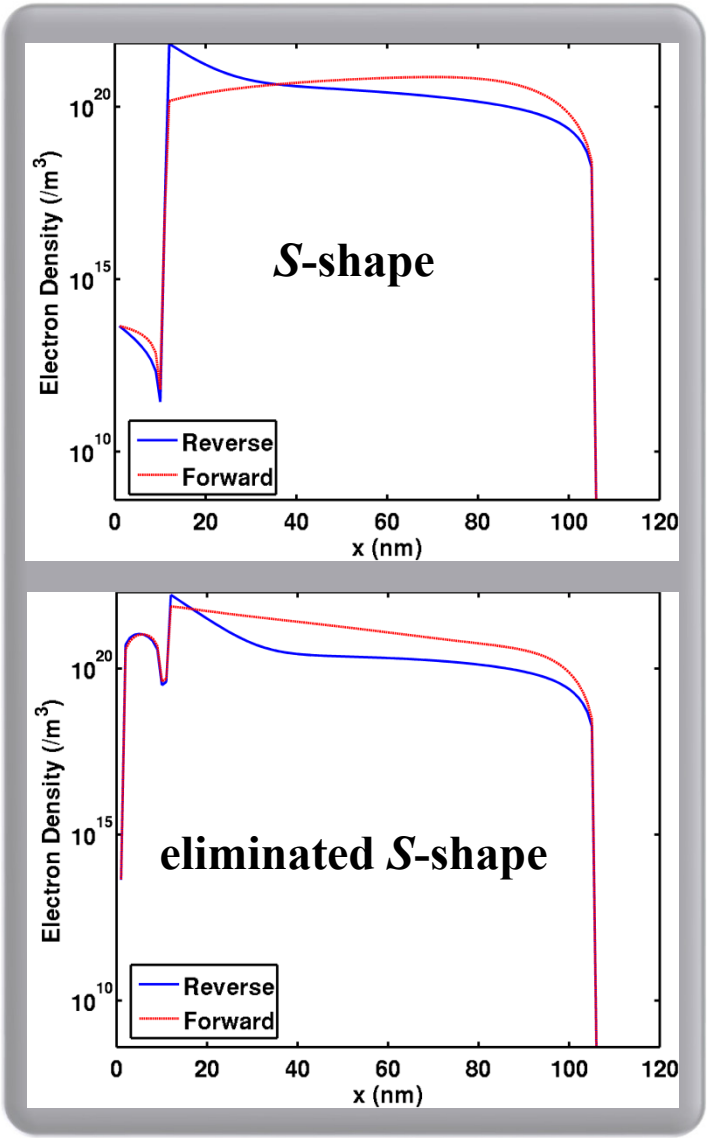




Pristine TiO_2 buffer layer with many trap states induces effective extraction (reverse bias) and injection (forward bias) barriers and thus *S*-shaped current density-voltage (*J-V*) curve. On plasmonic resonance, plasmonically excited hot electrons are injected into TiO_2 layer. The injected electrons eliminate the *S*-shaped *J-V* curve by trap filling and improve charge collection.

THEORETICAL RESULTS

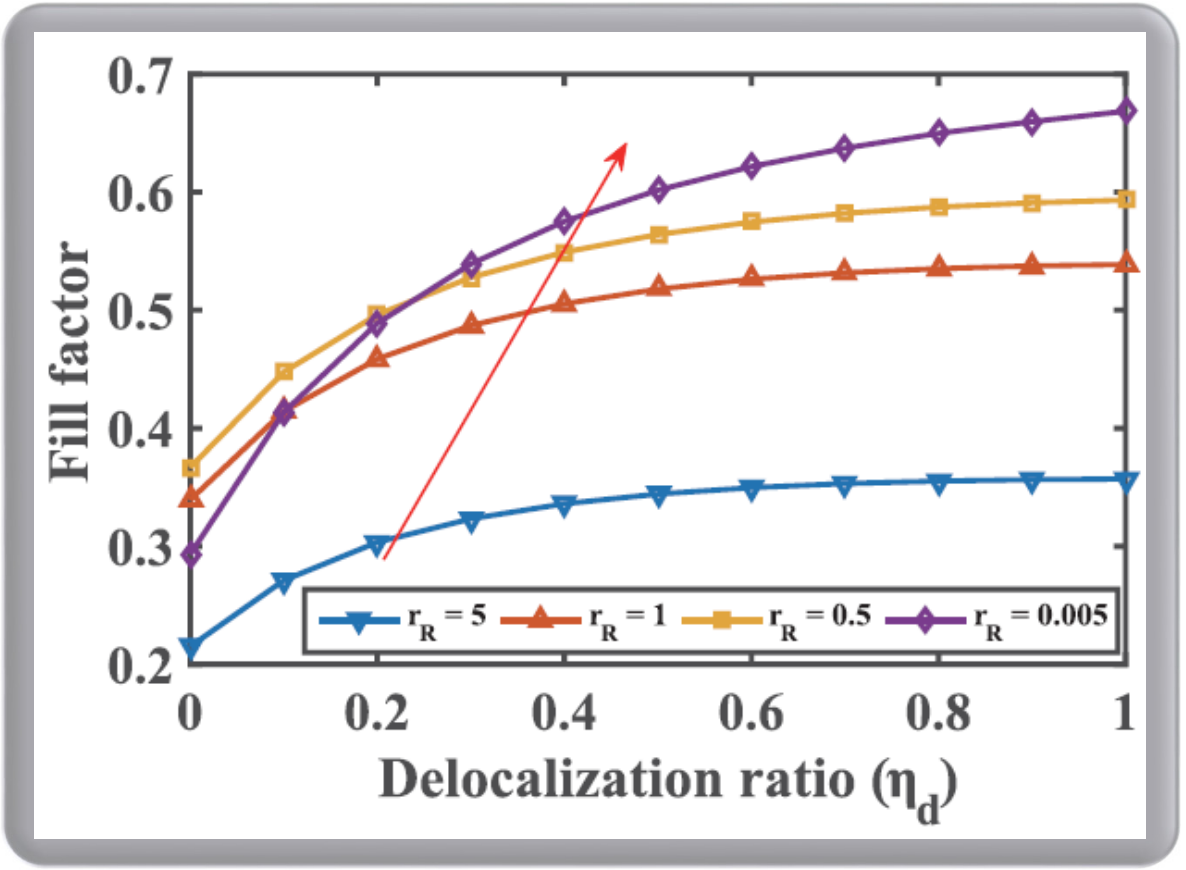




Increasing injected hot electrons will eliminate *S*-shaped *J-V* curve and charge accumulation at the interface will be improved.

INFLUENCE OF EXCITON DELOCALIZATION

Zi Shuai Wang, Wei E.I. Sha, and Wallace C.H. Choy, "Exciton Delocalization Incorporated Drift-Diffusion Model for Bulk-Heterojunction Organic Solar Cells," Journal of Applied Physics, vol. 120, no. 21, pp. 213101, Dec. 2016



The saturation point of fill factor increases when the recombination rate decreases.

CONCLUSION

1. Device model is fundamentally important to high-performance organic photovoltaics.

2. Optical absorption is governed by Maxwell's equations. Carrier transport is governed by semiconductor equations. Exciton delocalization, diffusion, and dissociation are unique physical processes for organic semiconductor devices, which still need to be carefully studied.

3. Space charge limited current, *S*-shaped *J*-*V* characteristics, and exciton delocalization induced fill factor saturation in organic solar cells have been theoretically modeled.

4. More multi-physical effects (optical-electrical-thermal-quantum) in photon-carrier interaction will be explored in future works.

ACKNOWLEDGEMENT

Any Questions and Discussions?