Simulation of organic solar cell with graphene transparent electrode

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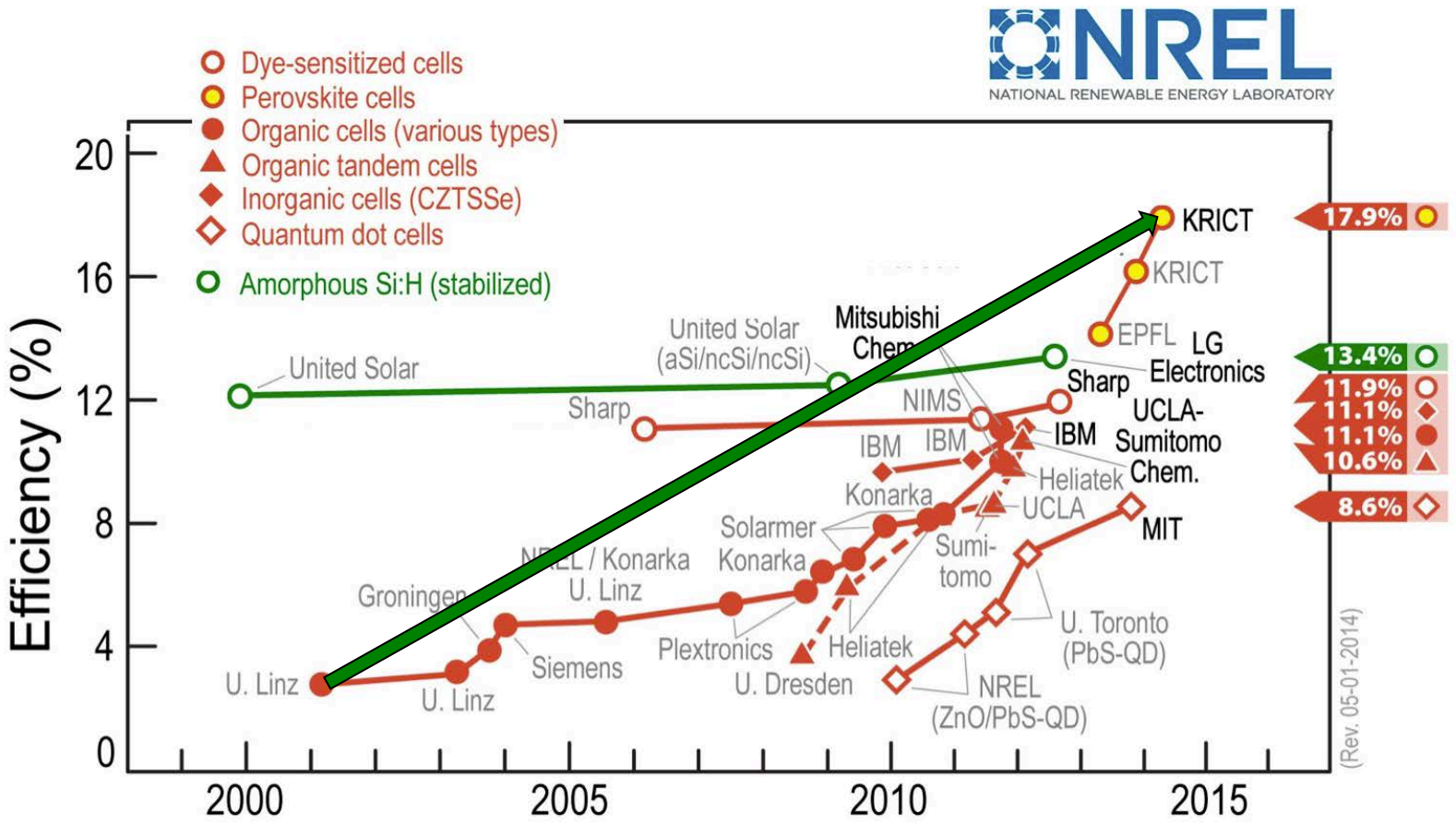
Go-NEXTs project (EC FP7 NMP)

Introduction

- **Organic semiconductor solar cells (OSCs) have recently shown an impressive acceleration in power conversion efficiency (PCE) improvement.**



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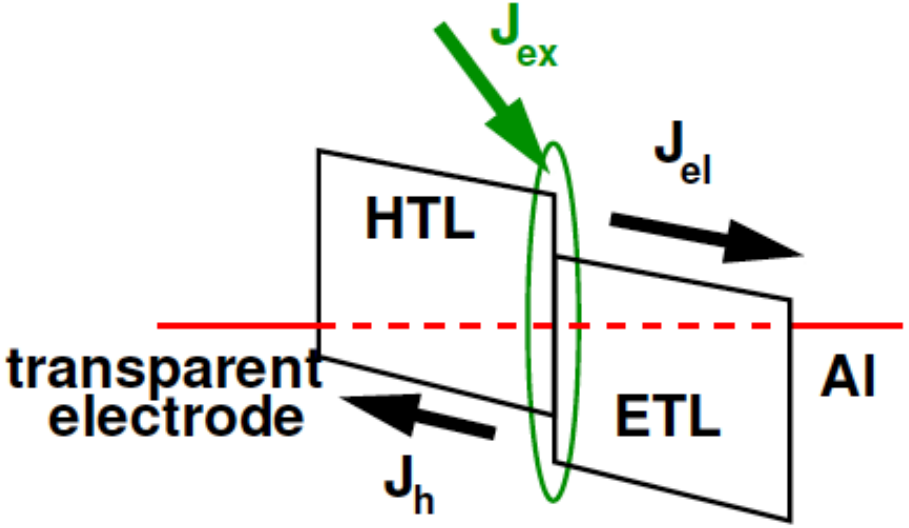
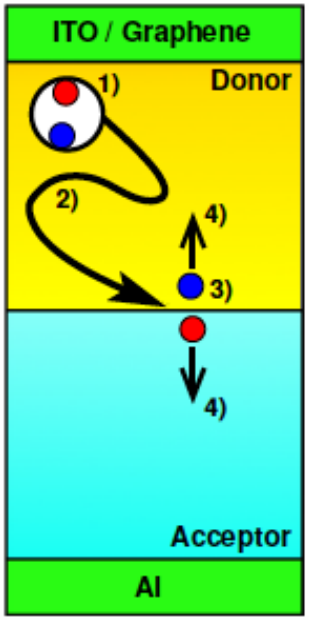
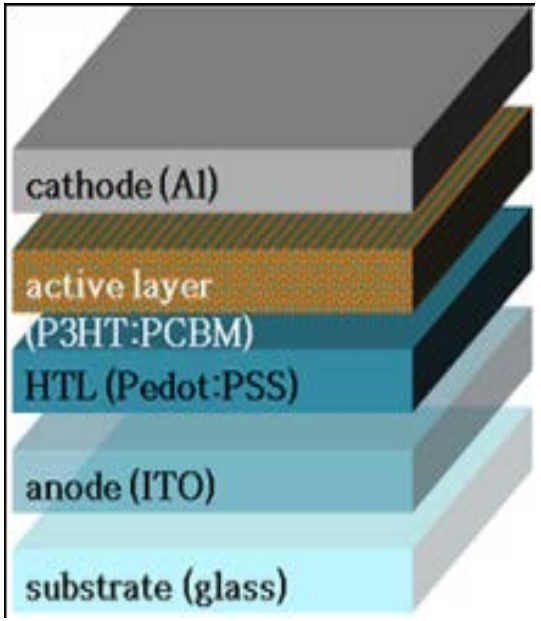
  - **stiffness, which prevents its use in flexible solar cells**

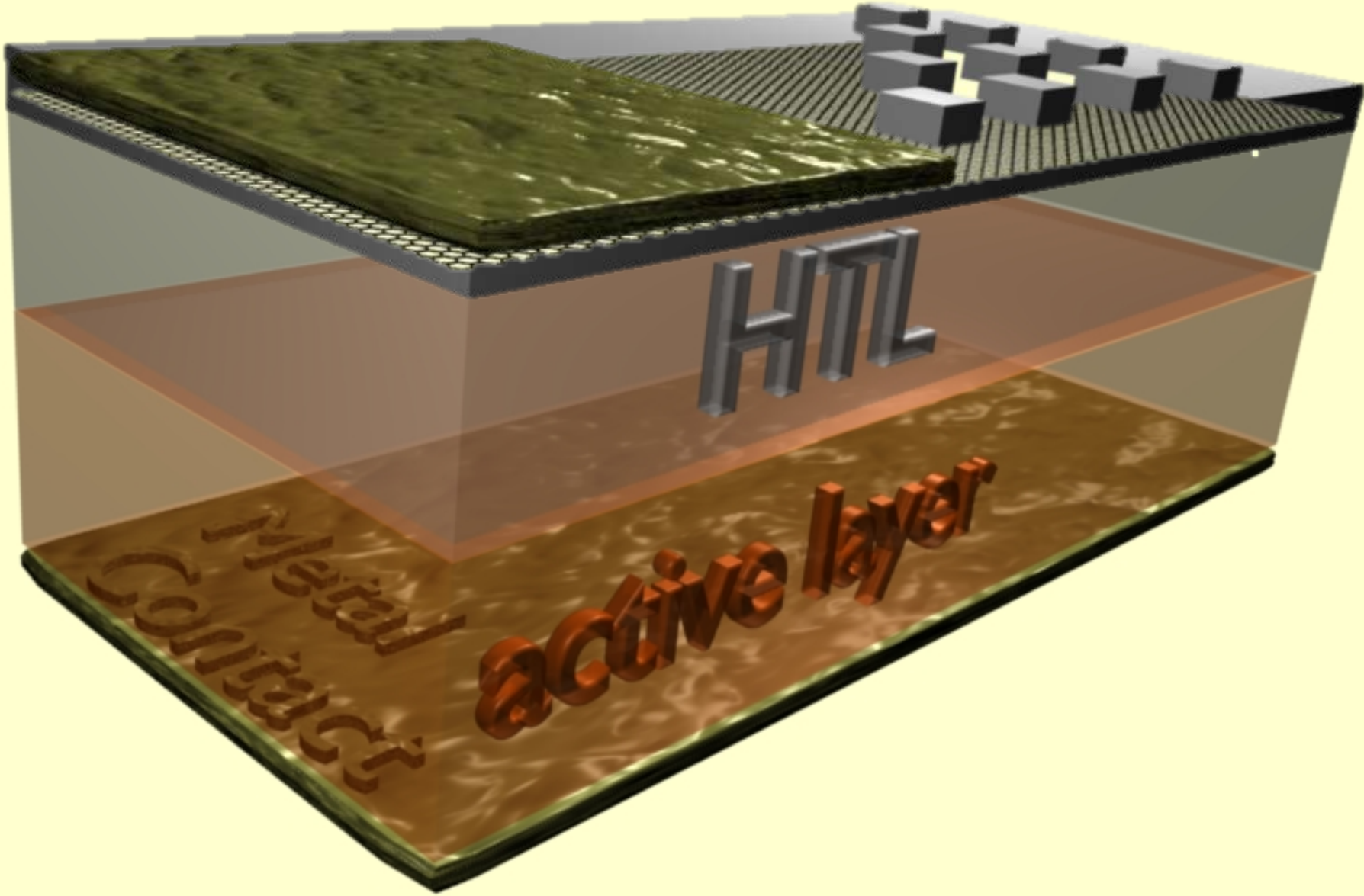
  - **large cost due to the limited supply of indium**

Heterojunction organic solar cell

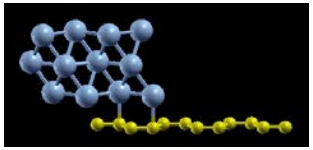




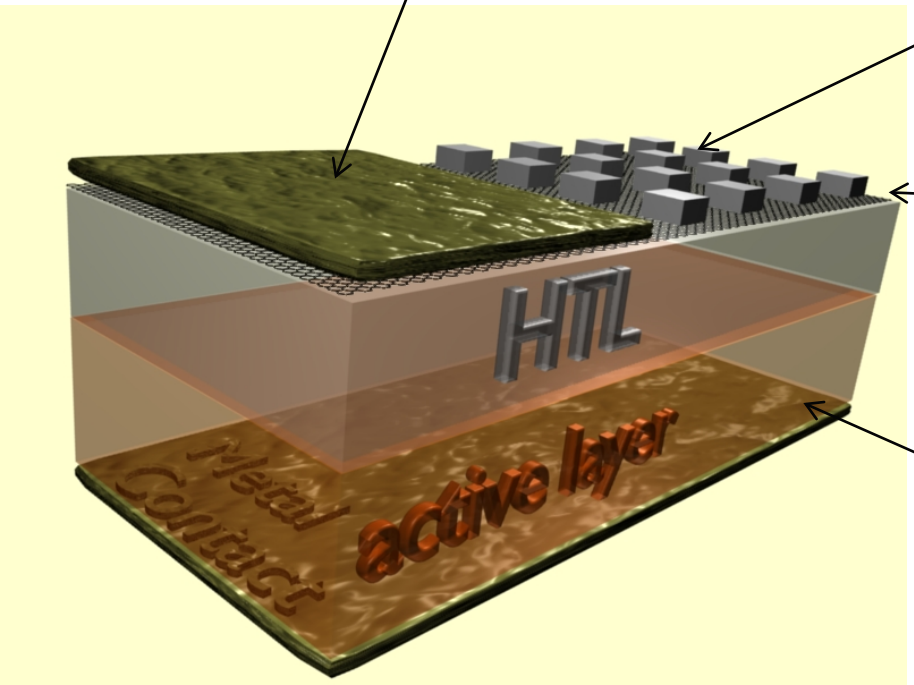



HTL
active layer
Metal Contact

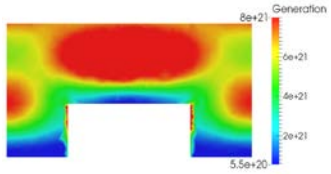
Investigated issues



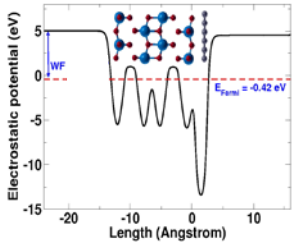
Understanding the role of graphene/metal contact



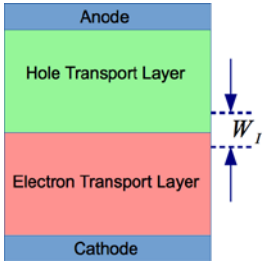
Light management



Work-function tuning of graphene



Sensitivity of solar cell to design parameters



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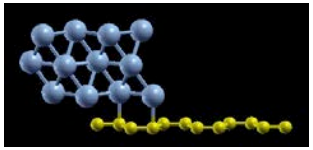

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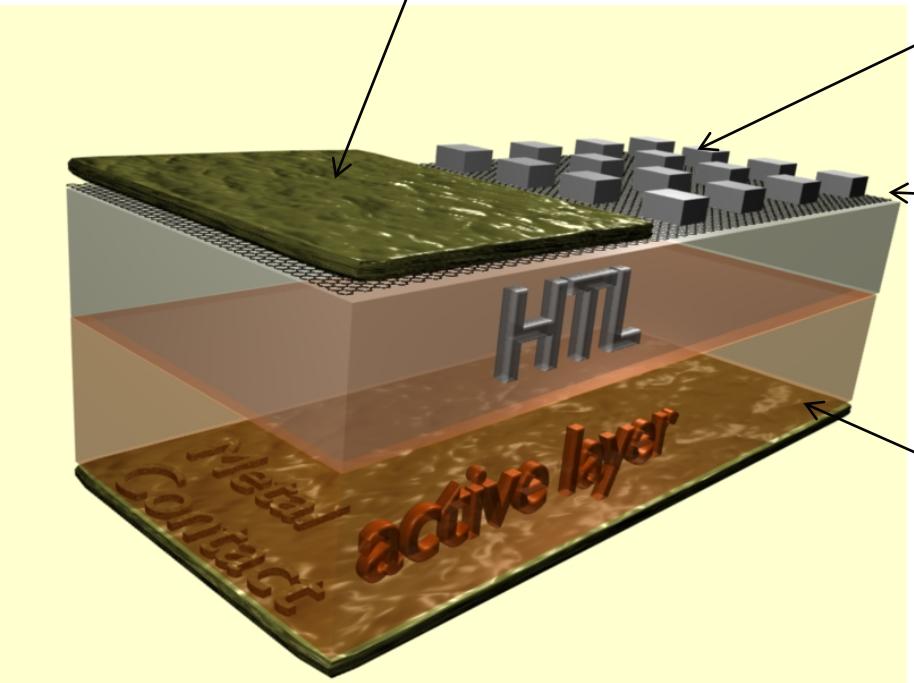

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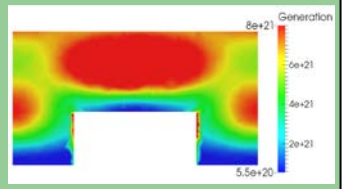

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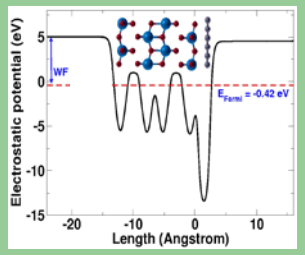

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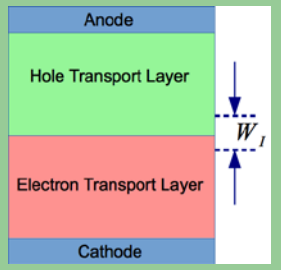

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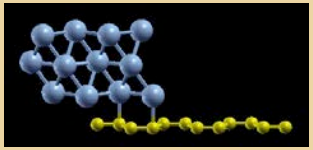

G. Iannaccone this morning

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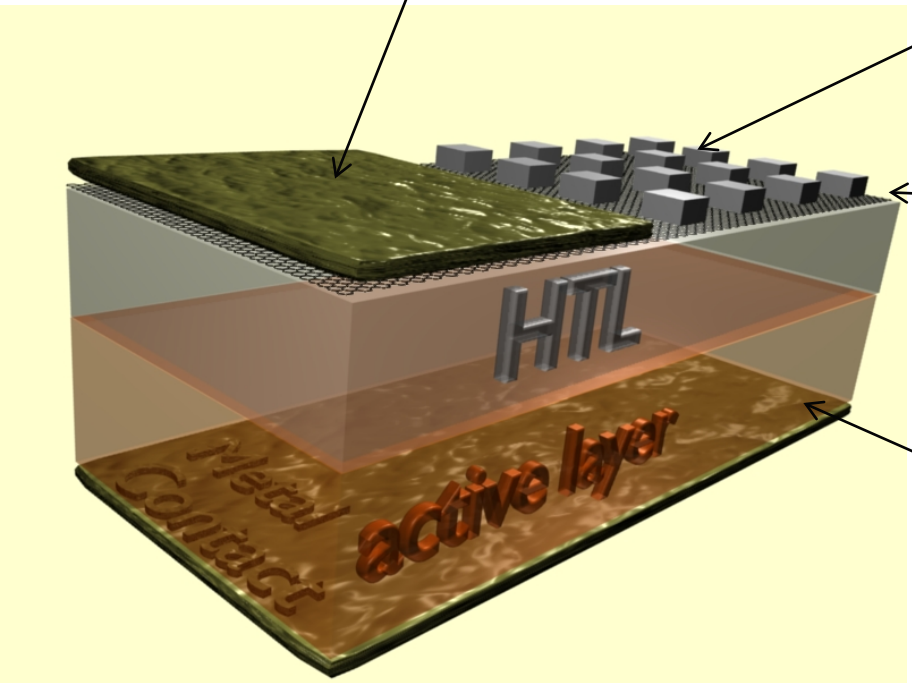

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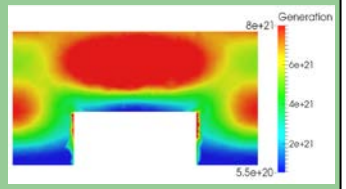

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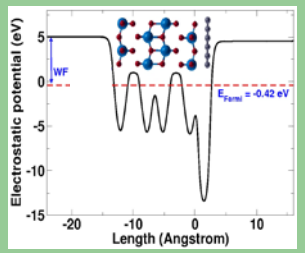

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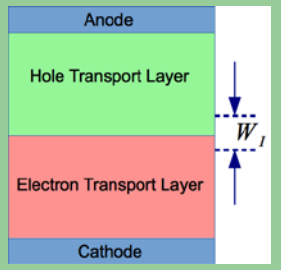

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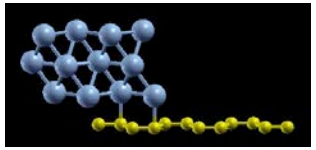

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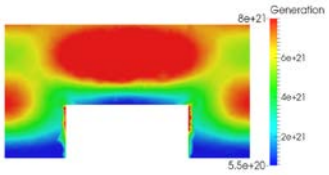

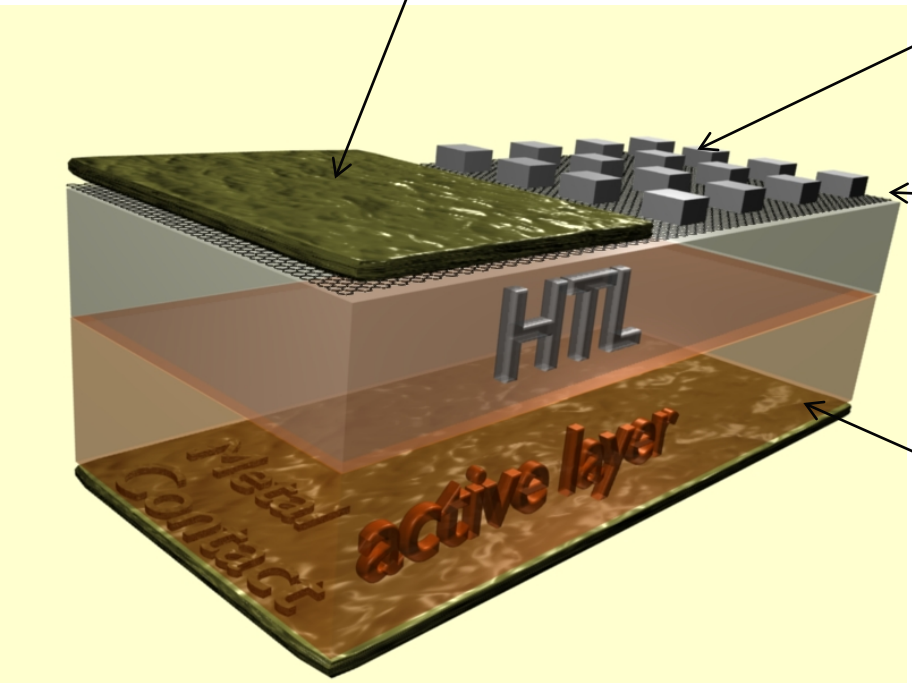

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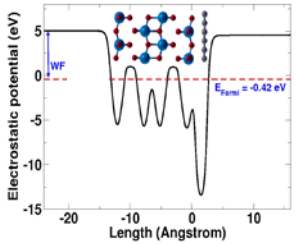

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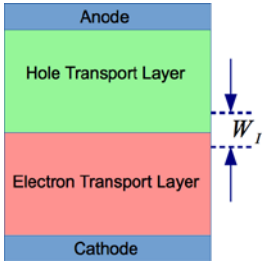
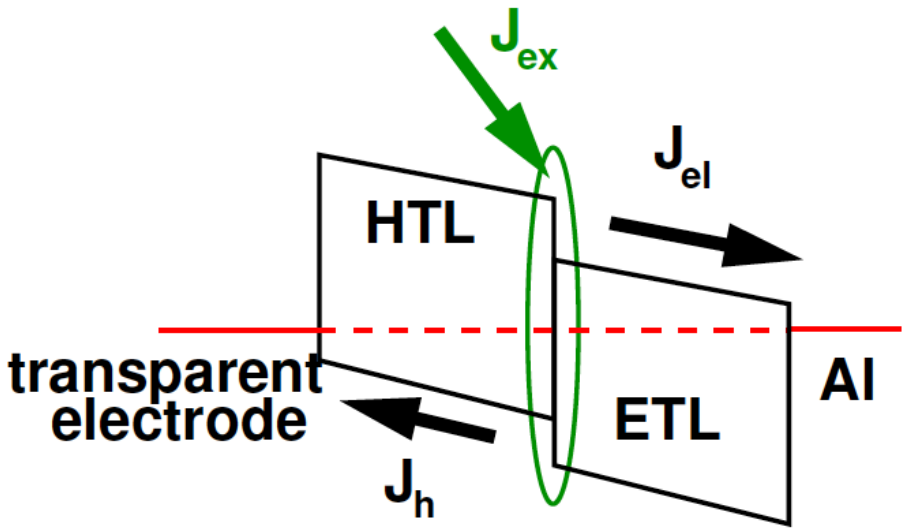


Workfunction tuning of graphene with MoO_3

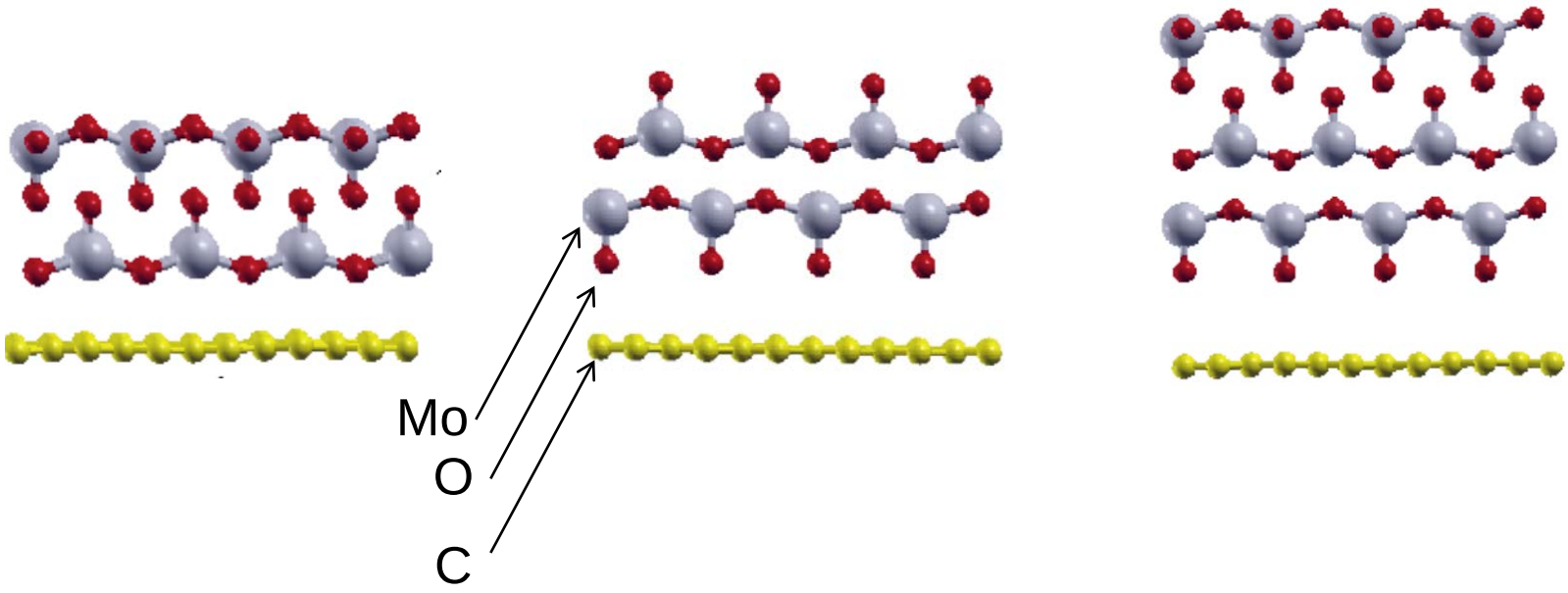
Deposition of MoO_3 on graphene can increase graphene WF [Tong et al., Adv. Materials 23, 1514, 2011]



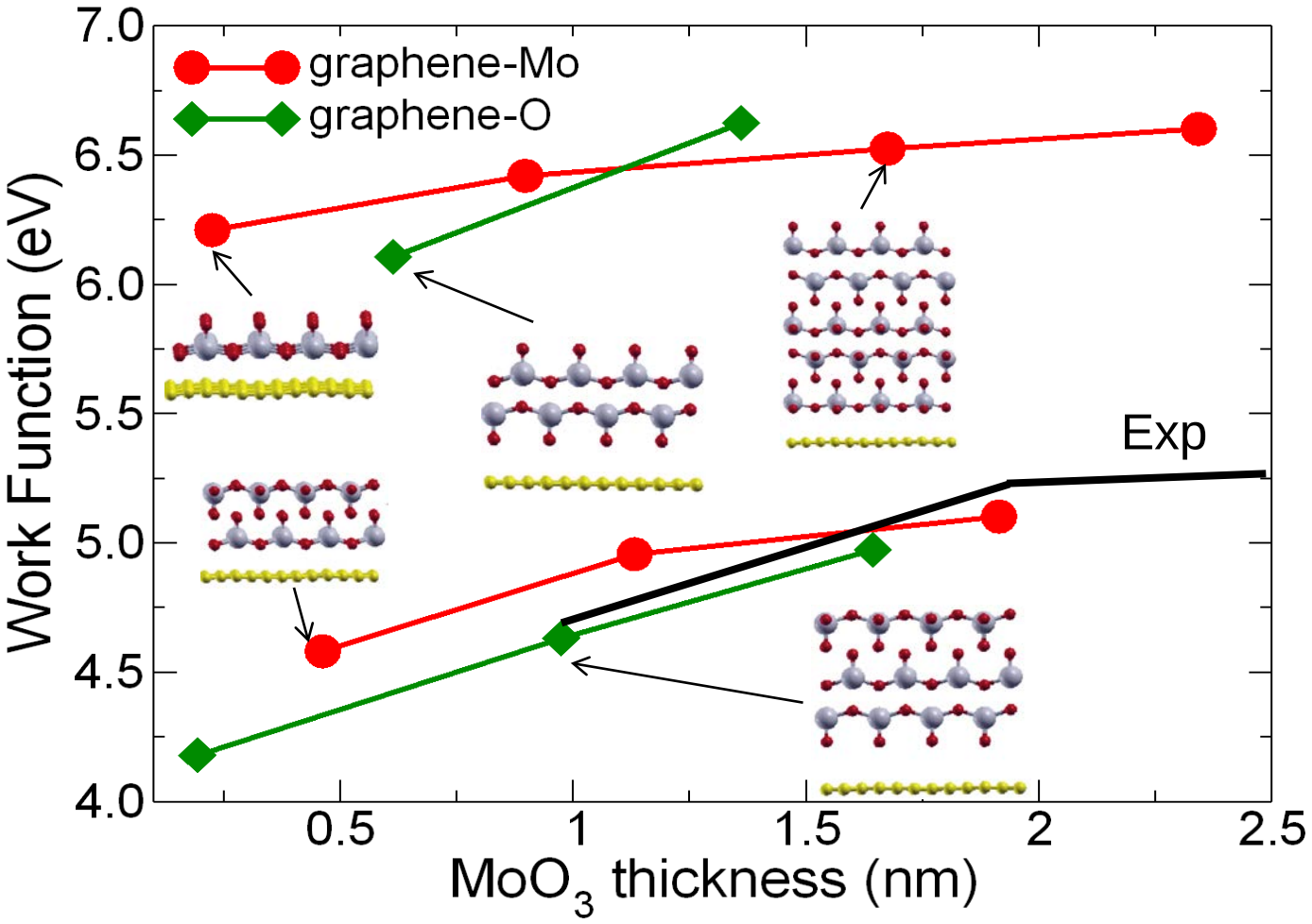
Fermi level closer to the valence band edge of the HTL can improve efficiency

DFT modeling of the MoO_3–graphene interface

- **Optimized geometries (both Mo- or O-terminated top interfaces)**
- **Van der Waals interactions are considered**
- **DFT with Quantum Espresso**



Work Function tuning



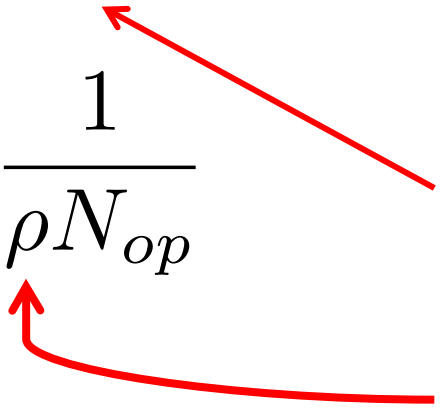
UV Photoelectron spectroscopy exp. are consistent with Mo-term. layers (electronegativity of Mo: 2.15 eV – electronegativity of O: 3.44 eV)

Graphene mobility

- **Phonon-limited mobility: acoustic + optical phonons**
  [Perebeinos et al., PRB, 81, 1, 2010], [Shishir et al., Jour. Of Physics-Cond. Matter, 21, 344201, 2009]

$$\mu_{ac} = \frac{q\rho_m \hbar^2 v_F^2 v_{ph}^2}{4\pi D_{ac}^2} \frac{1}{\rho K_B T}$$

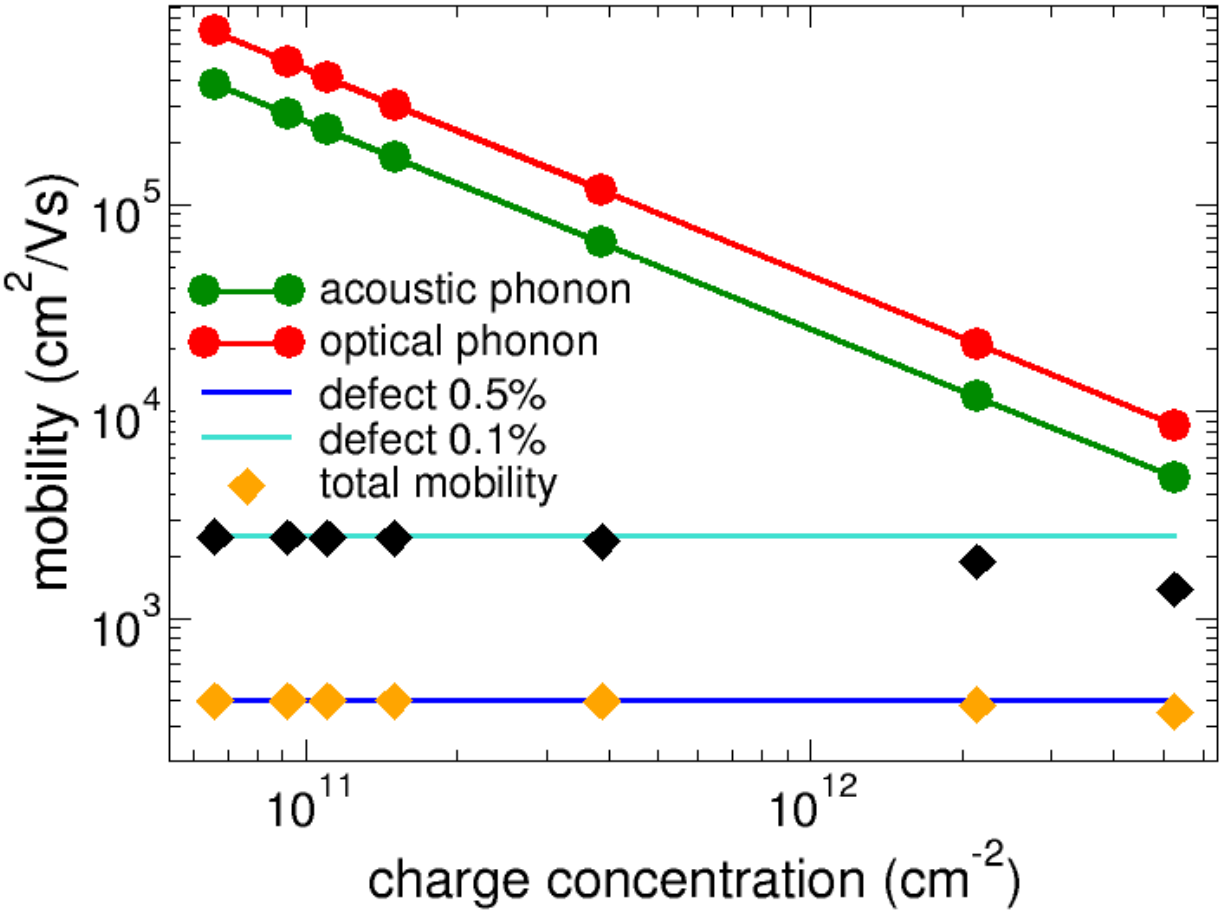
$$\mu_{op} = \frac{q\rho_m v_F^2 \omega_{op}}{2\pi D_{op}^2} \frac{1}{\rho N_{op}}$$



- **Defect limited mobility through atomistic simulations**

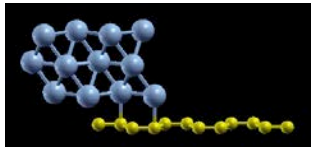
[A. Betti et al., IEEE TED, Vol. 58, p. 2824, 2011]

Mobility vs charge density



Mobility is mainly limited by defects (vacancies, grain boundaries)

Investigated issues



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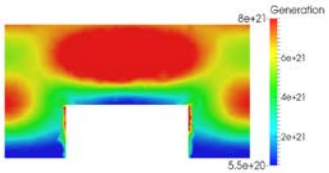

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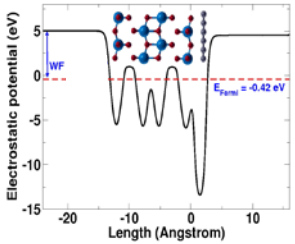
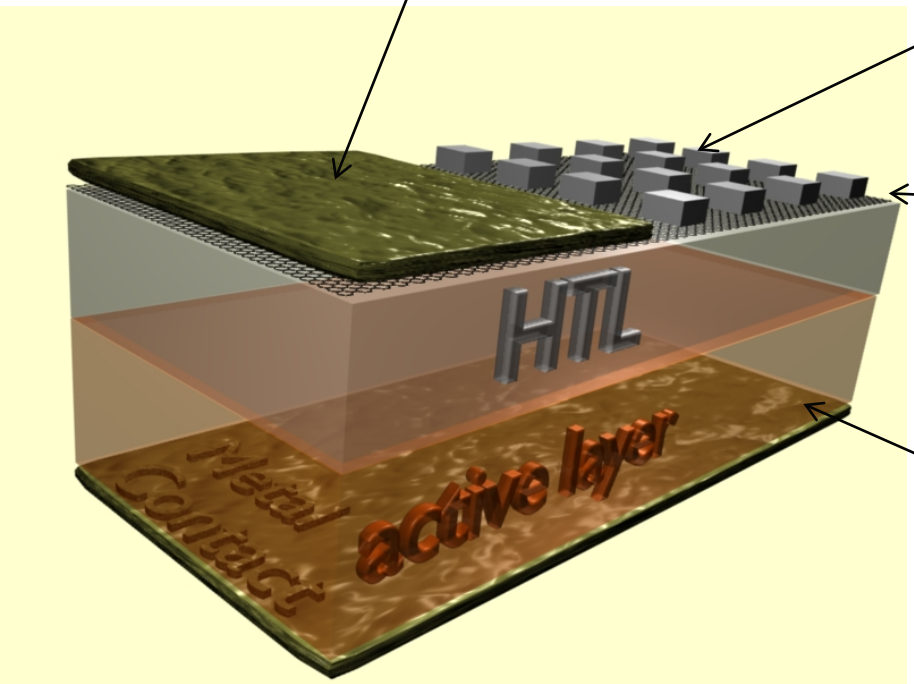
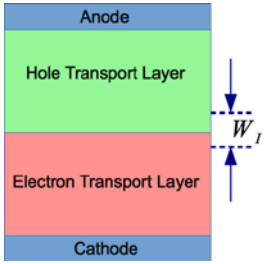




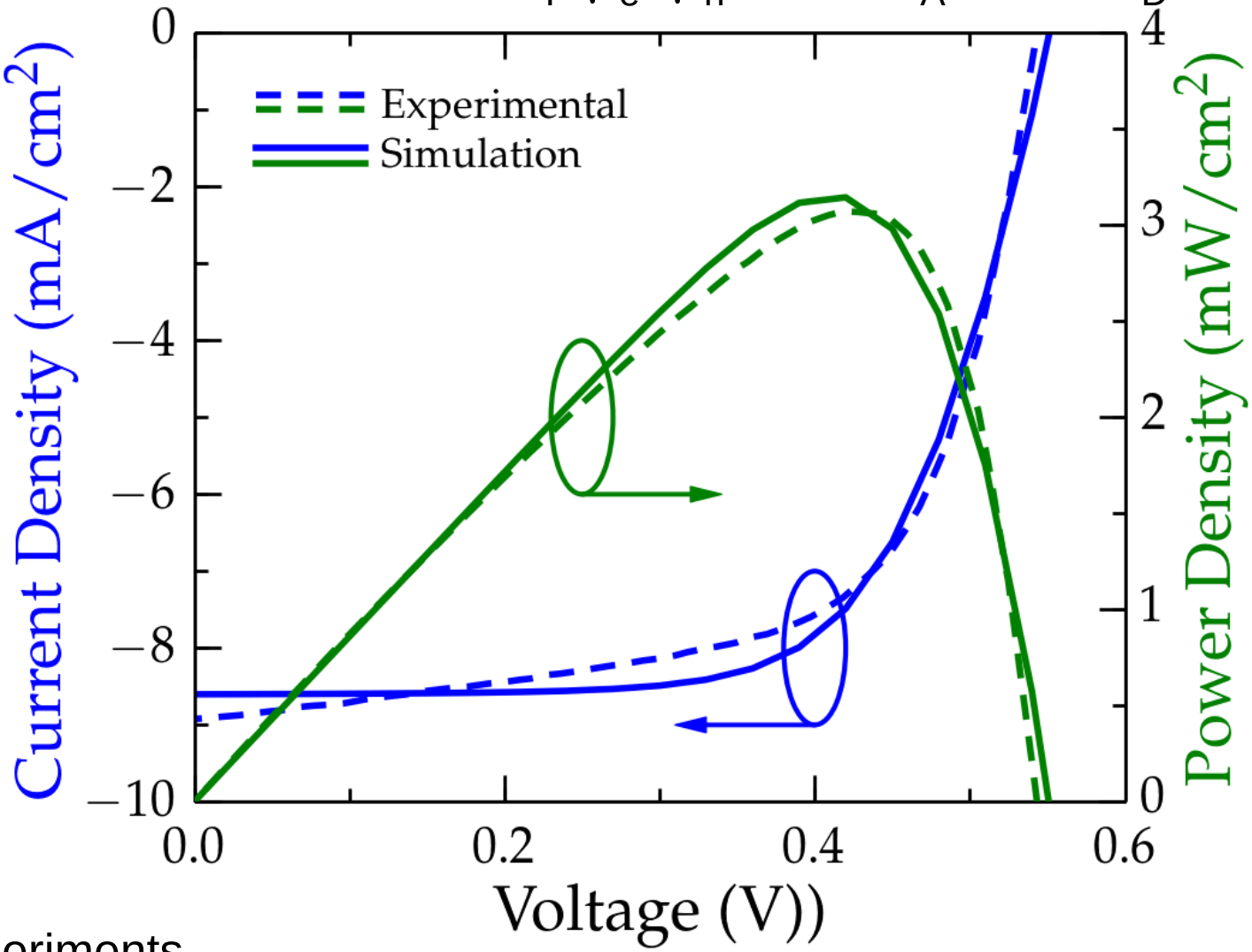
Sensitivity of solar cell to design parameters



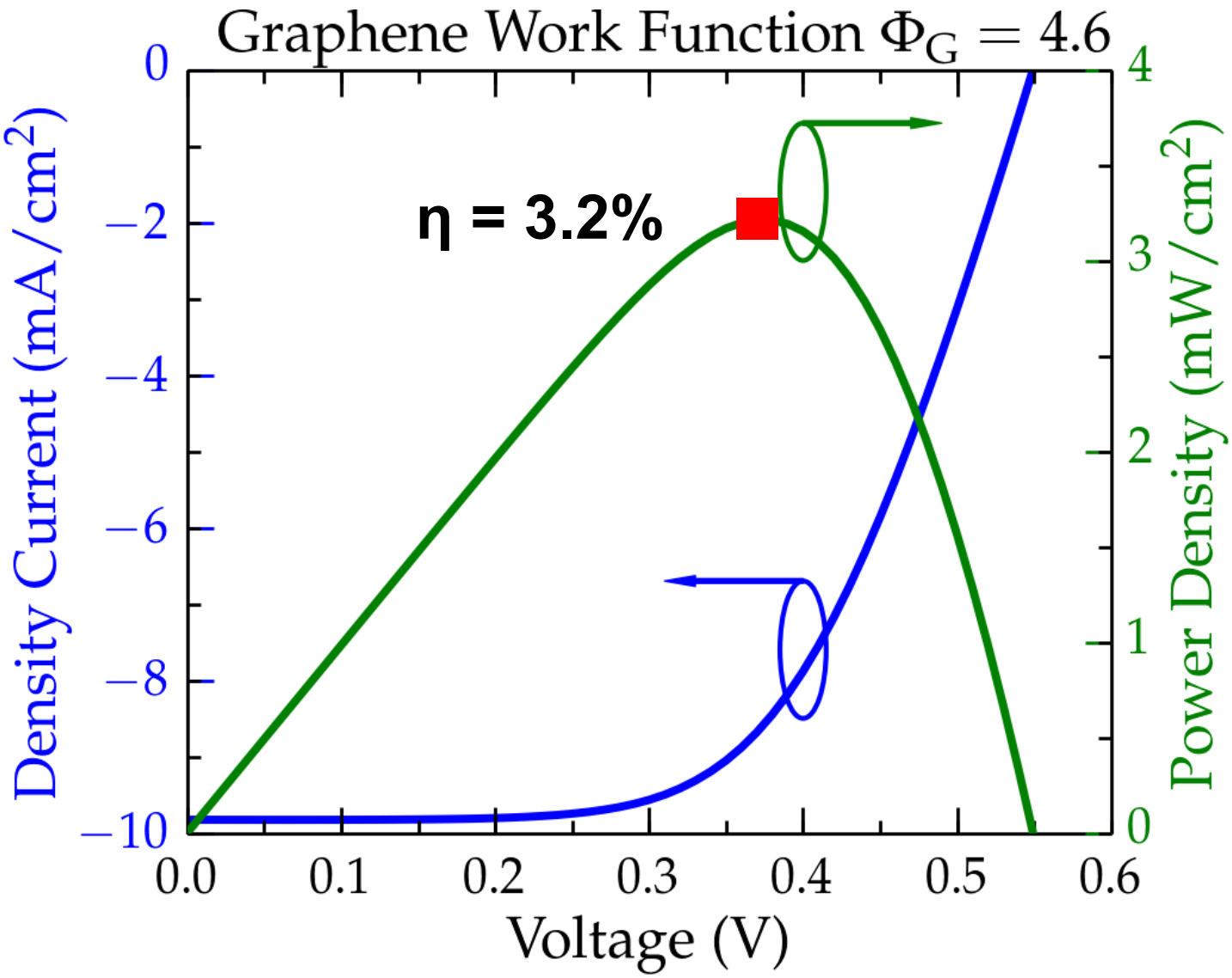
P3HT

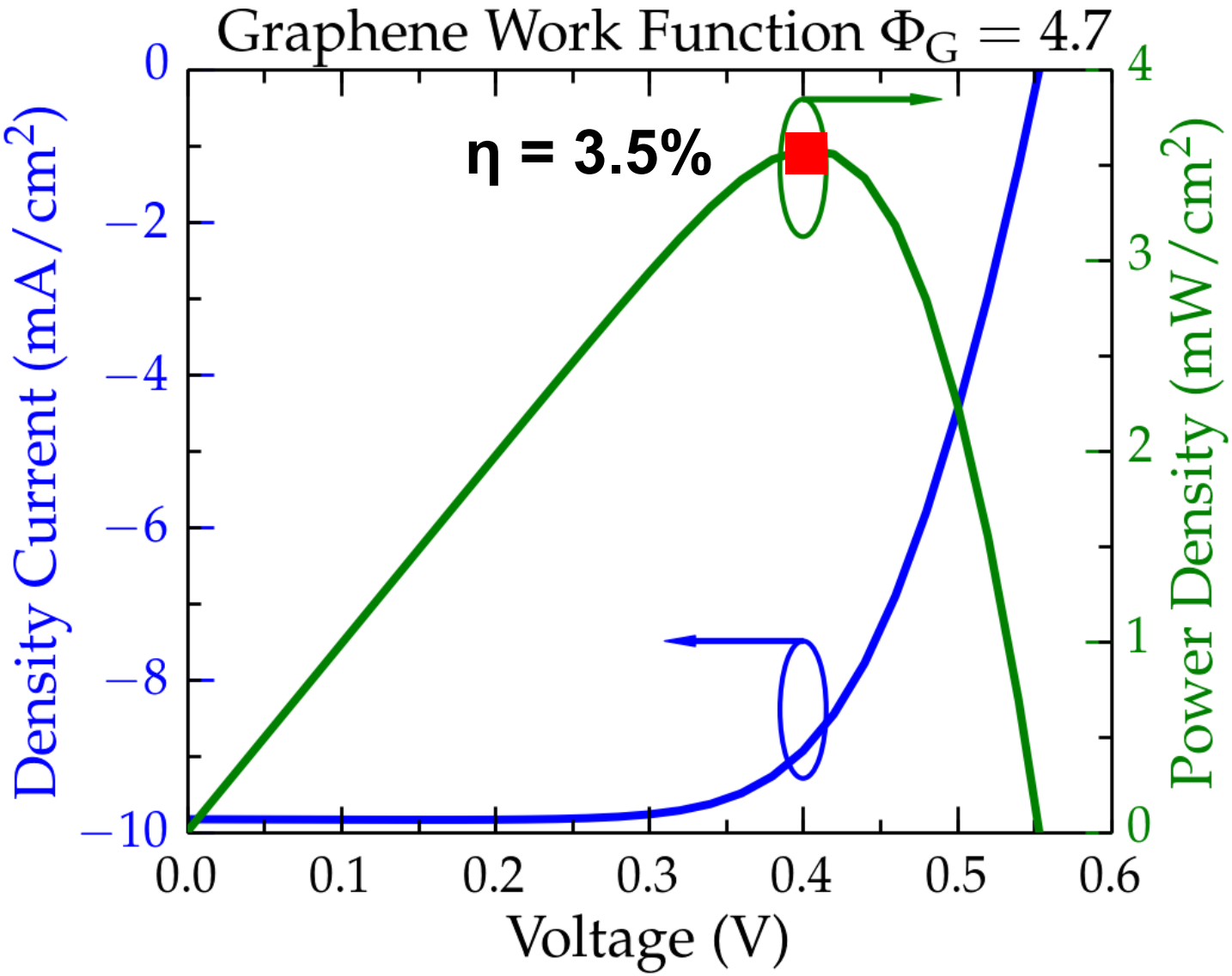
Parameter calibration with experiments

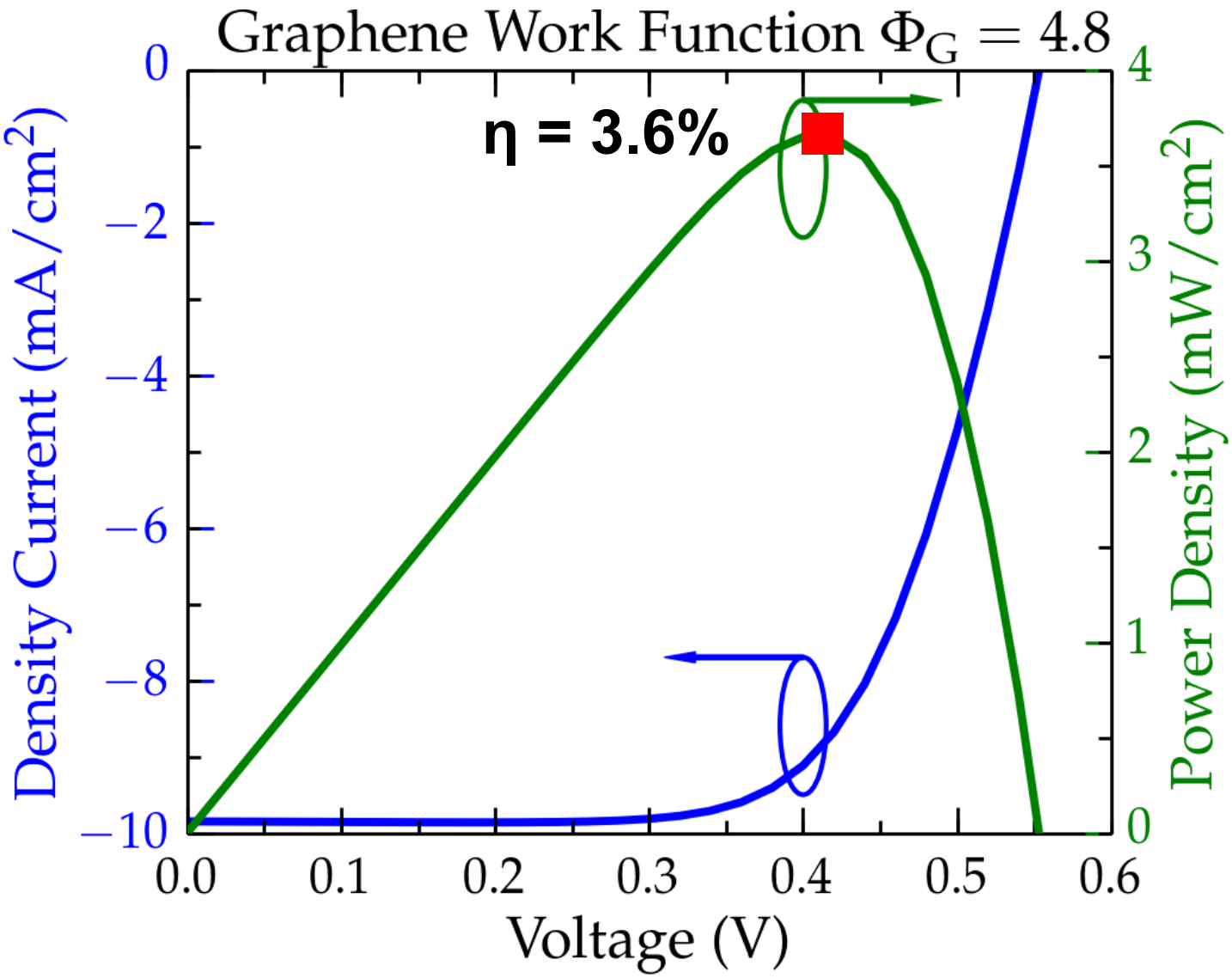
Parameters: W_I, μ_e, μ_h, $LUMO_A$-$HOMO_D$

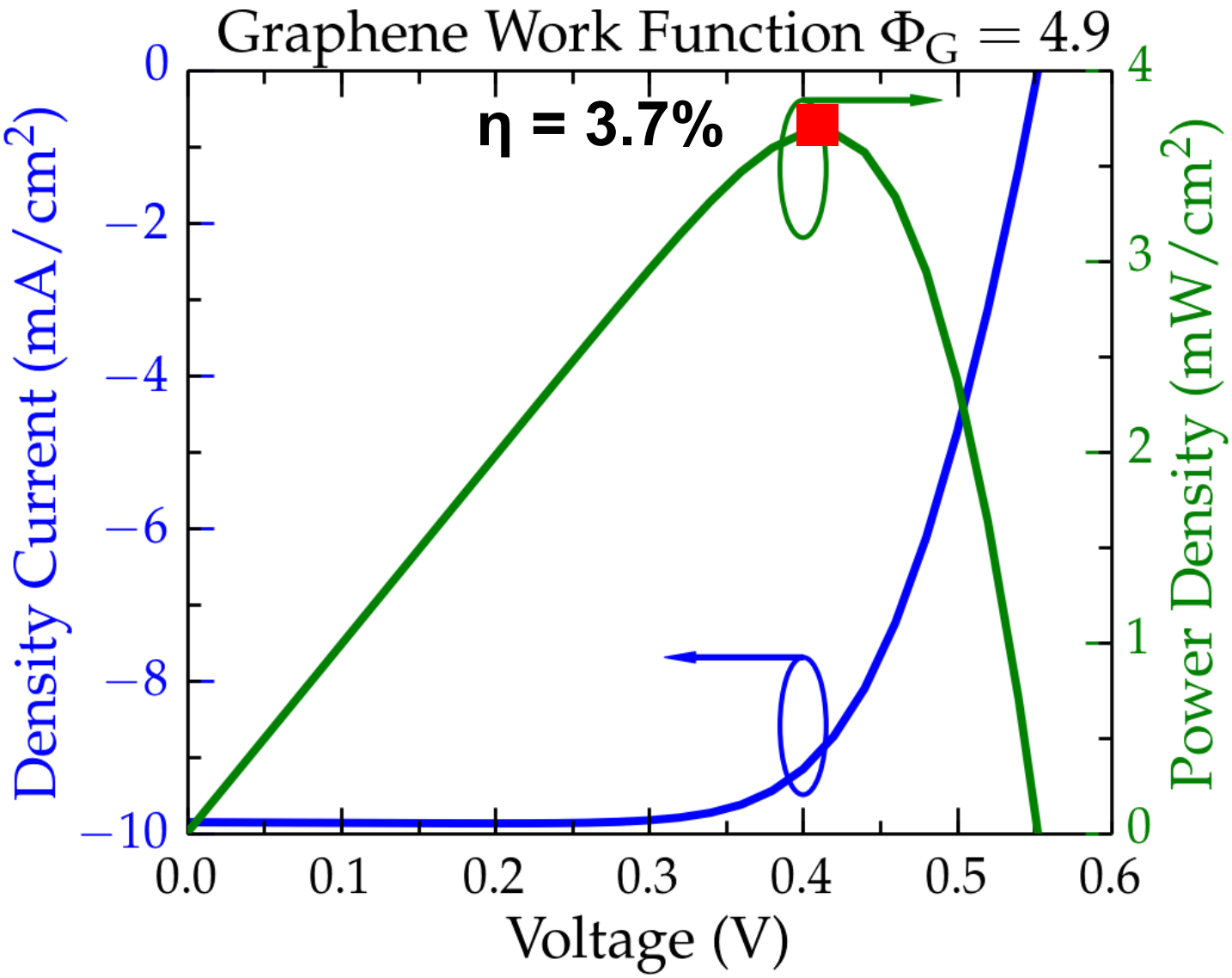


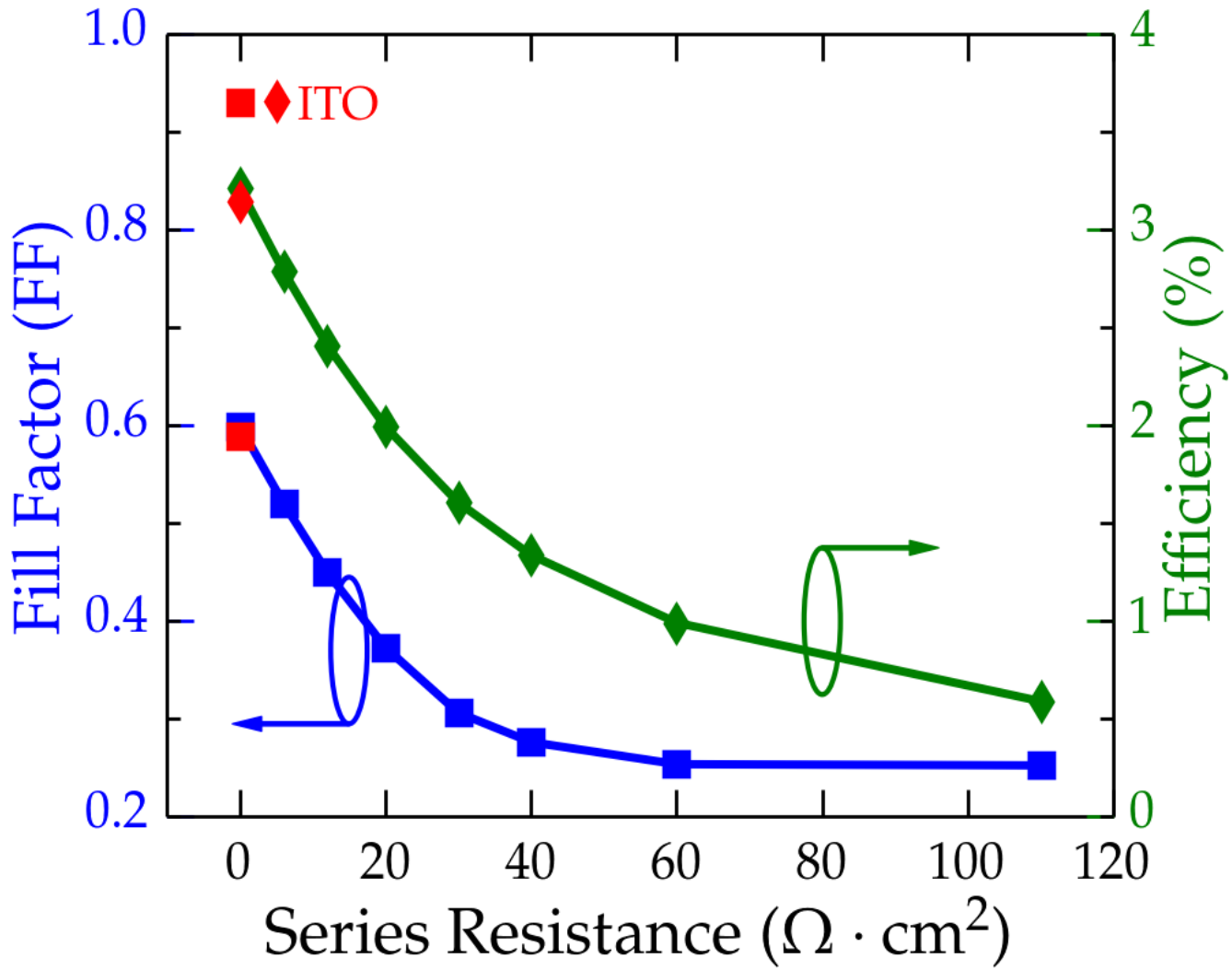
Our experiments


Graphene Work Function $\Phi_G = 4.6$
η = 3.2%
Density Current (mA/cm^2)
Power Density (mW/cm^2)
Voltage (V)
0
−2
−4
−6
−8
−10
4
3
2
1
0
0.0
0.1
0.2
0.3
0.4
0.5
0.6


Graphene Work Function $\Phi_G = 4.7$
η = 3.5%
Density Current (mA/cm^2)
Power Density (mW/cm^2)
Voltage (V)
0
−2
−4
−6
−8
−10
4
3
2
1
0
0.0
0.1
0.2
0.3
0.4
0.5
0.6

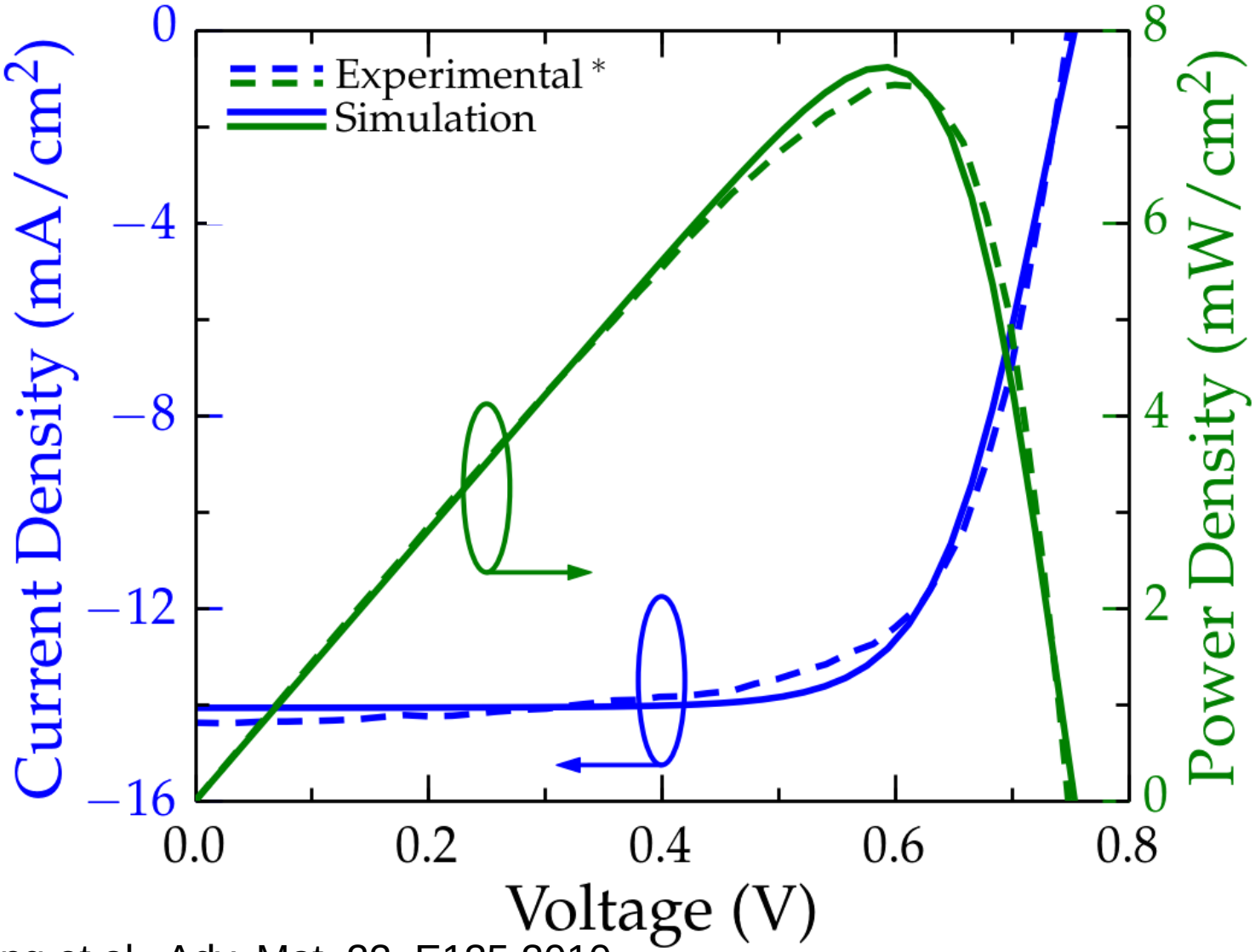

Graphene Work Function $\Phi_G = 4.8$
η = 3.6%
Density Current (mA/cm²)
Power Density (mW/cm²)
Voltage (V)
0
−2
−4
−6
−8
−10
4
3
2
1
0
0.0
0.1
0.2
0.3
0.4
0.5
0.6


Graphene Work Function $\Phi_G = 4.9$
η = 3.7%
Density Current (mA/cm²)
Power Density (mW/cm²)
Voltage (V)
0
−2
−4
−6
−8
−10
4
3
2
1
0
0.0
0.1
0.2
0.3
0.4
0.5
0.6

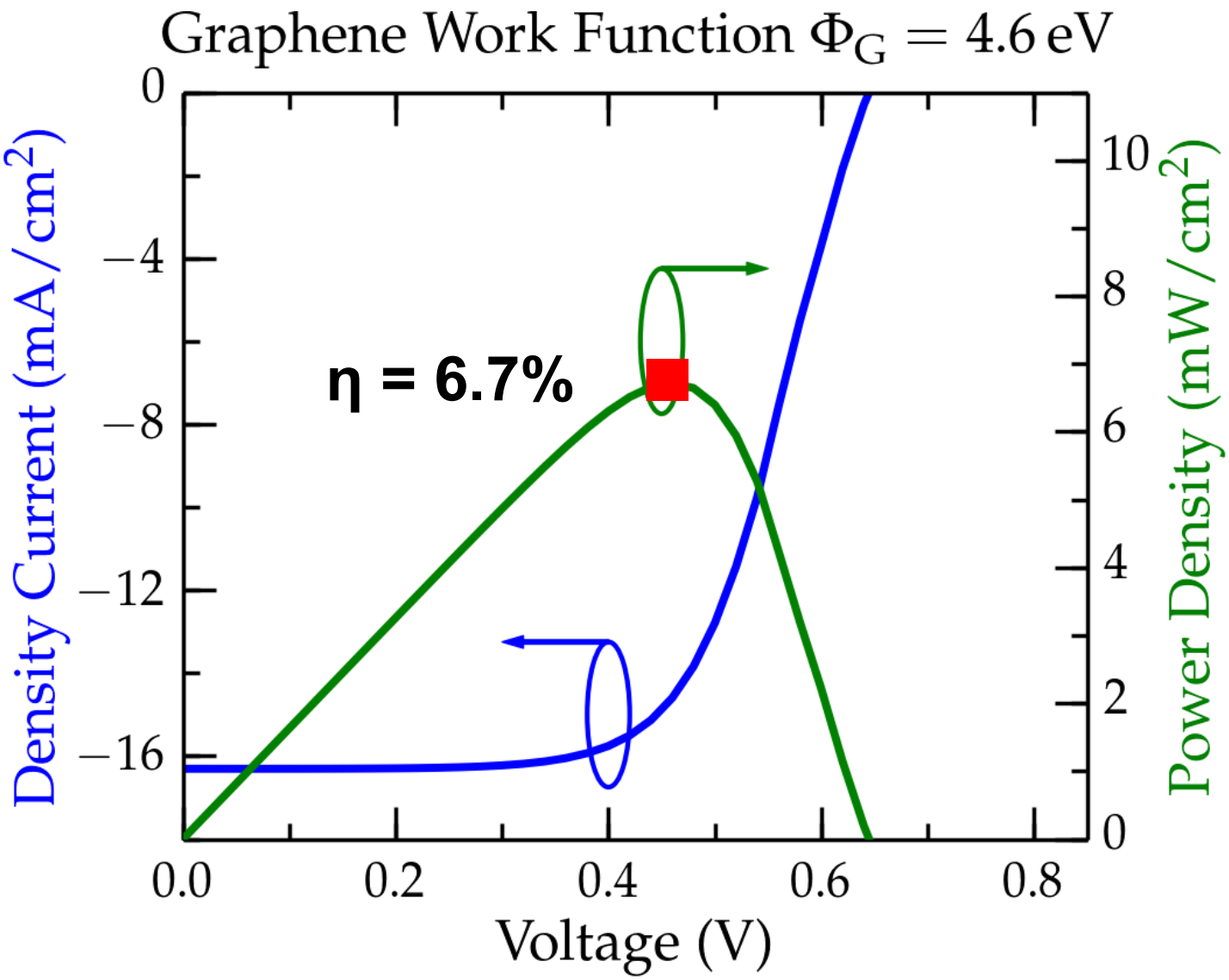

ITO
Fill Factor (FF)
Efficiency (%)
Series Resistance (Ω · cm²)
1.0
0.8
0.6
0.4
0.2
4
3
2
1
0
0
20
40
60
80
100
120

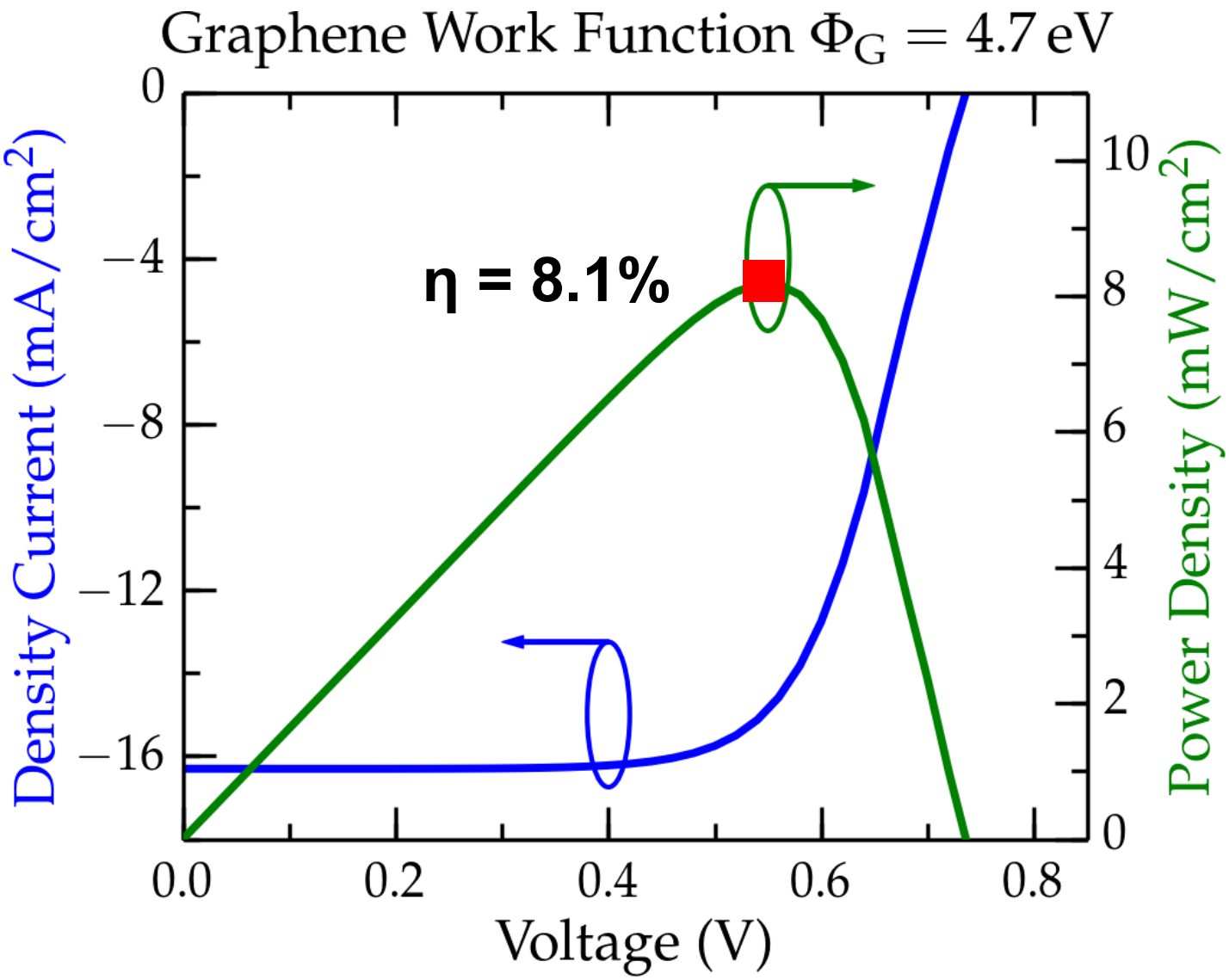
PTB7

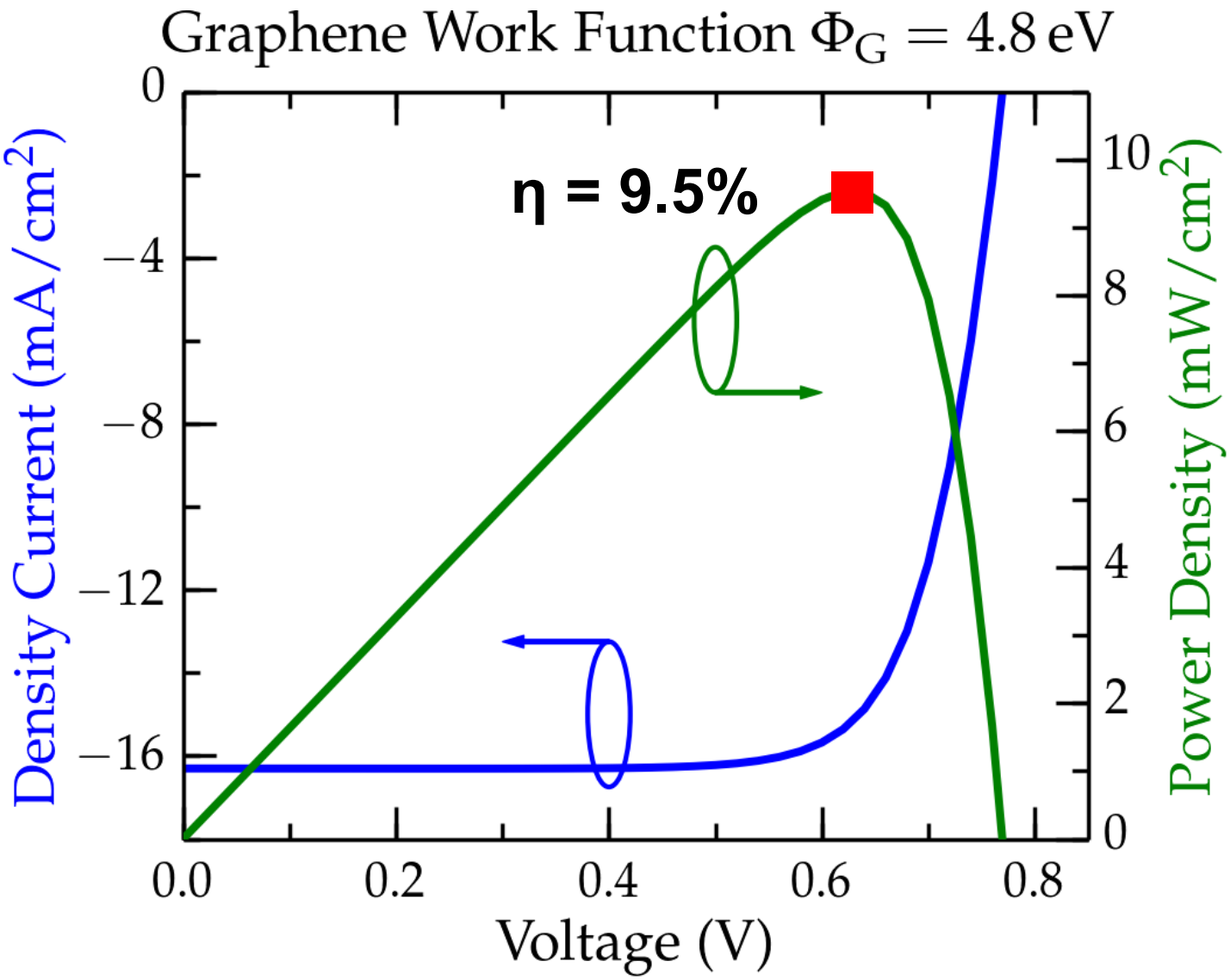
PTB7: Calibration with experiments

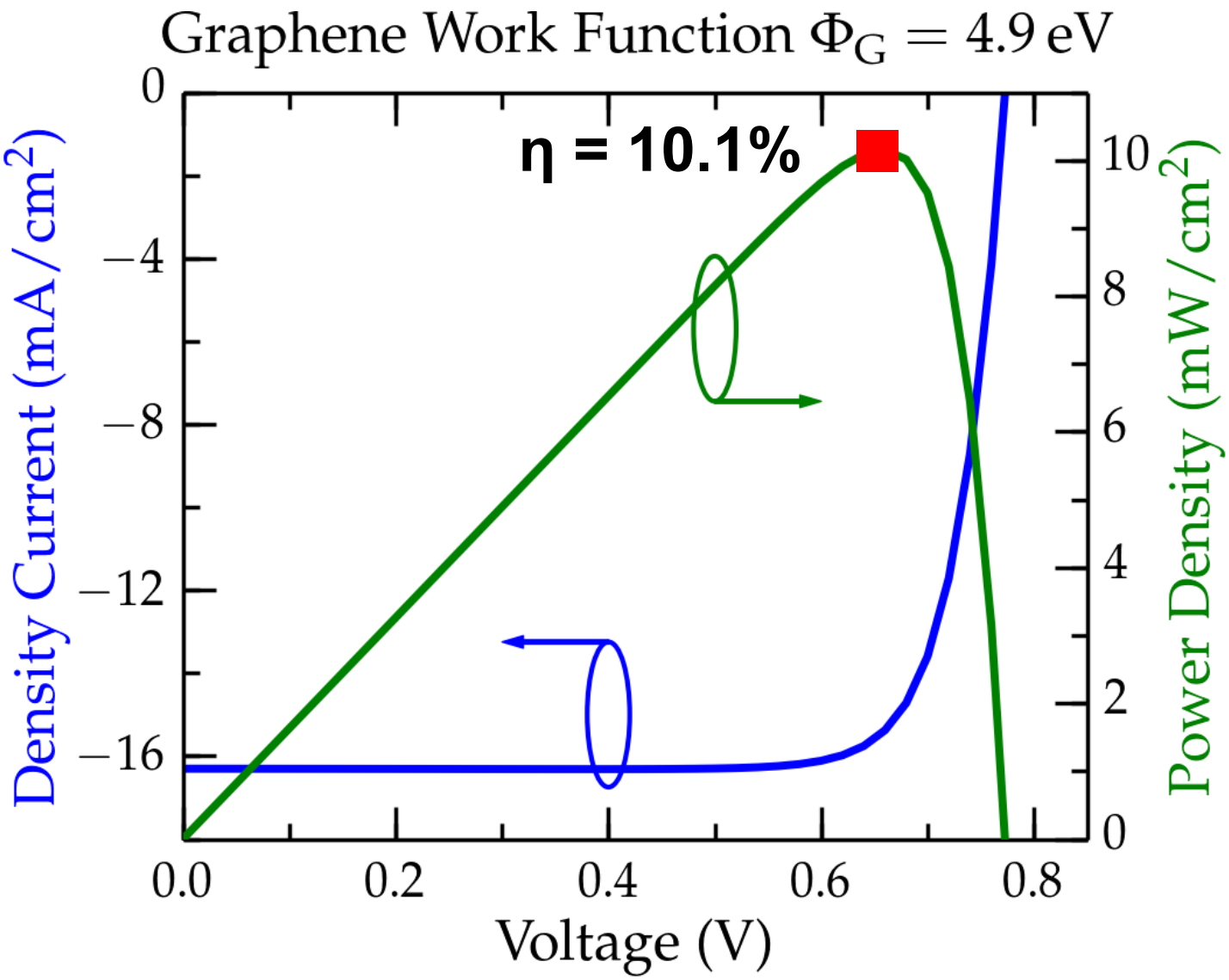


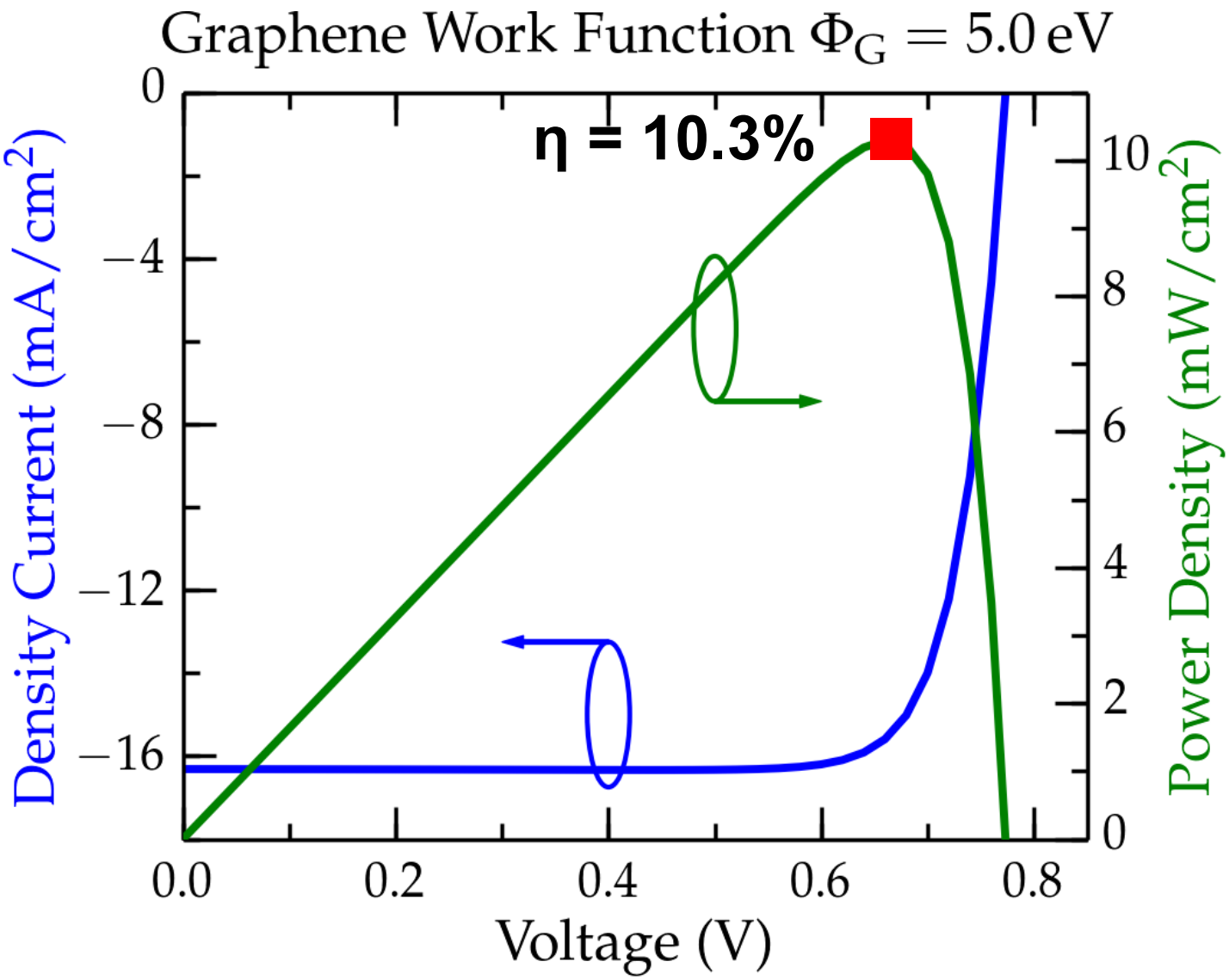
Exp: Liang et al., Adv. Mat. 22, E135 2010

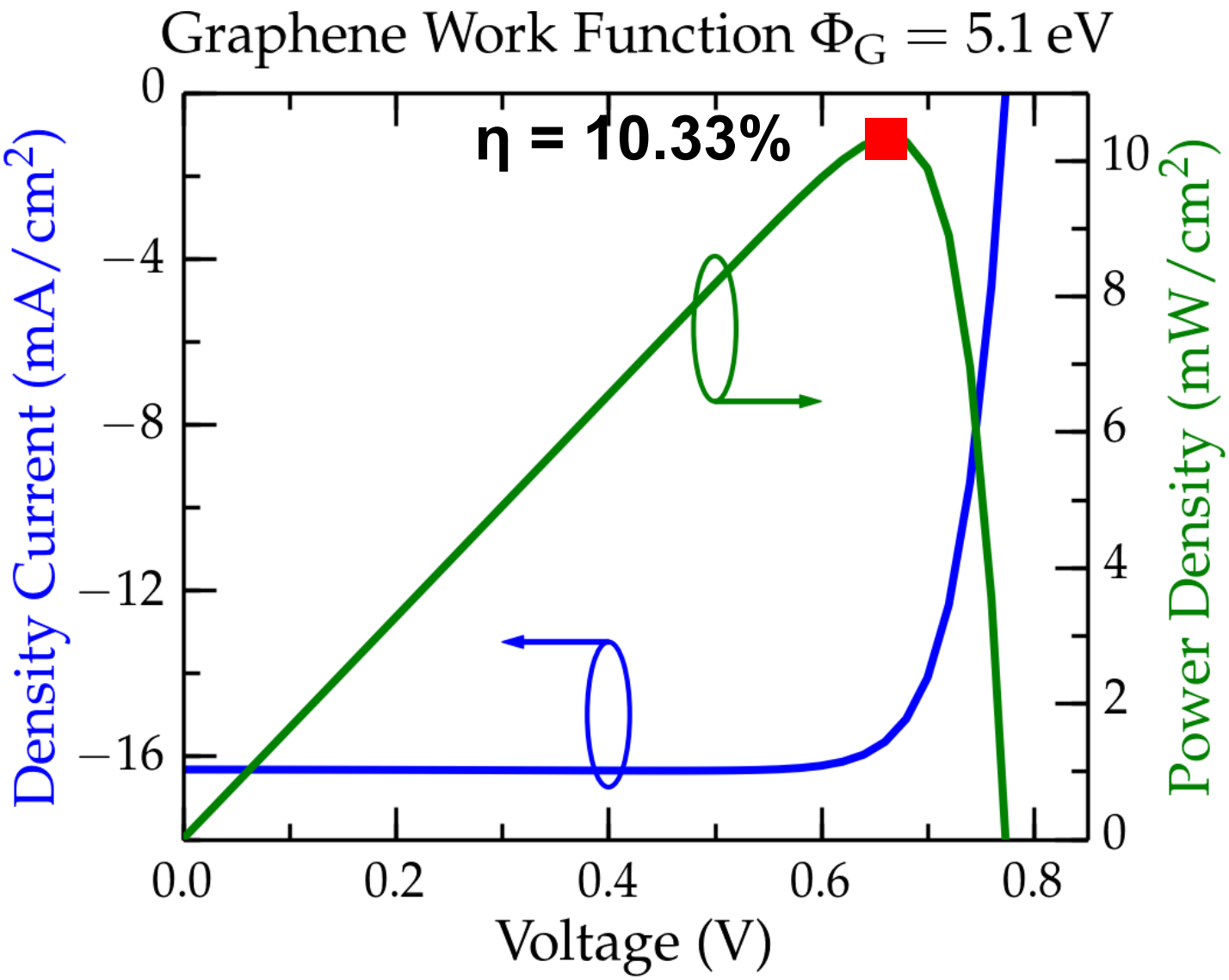

Graphene Work Function $\Phi_G = 4.6$ eV
η = 6.7%
Density Current (mA/cm^2)
Power Density (mW/cm^2)
Voltage (V)
0
−4
−8
−12
−16
10
8
6
4
2
0
0.0
0.2
0.4
0.6
0.8

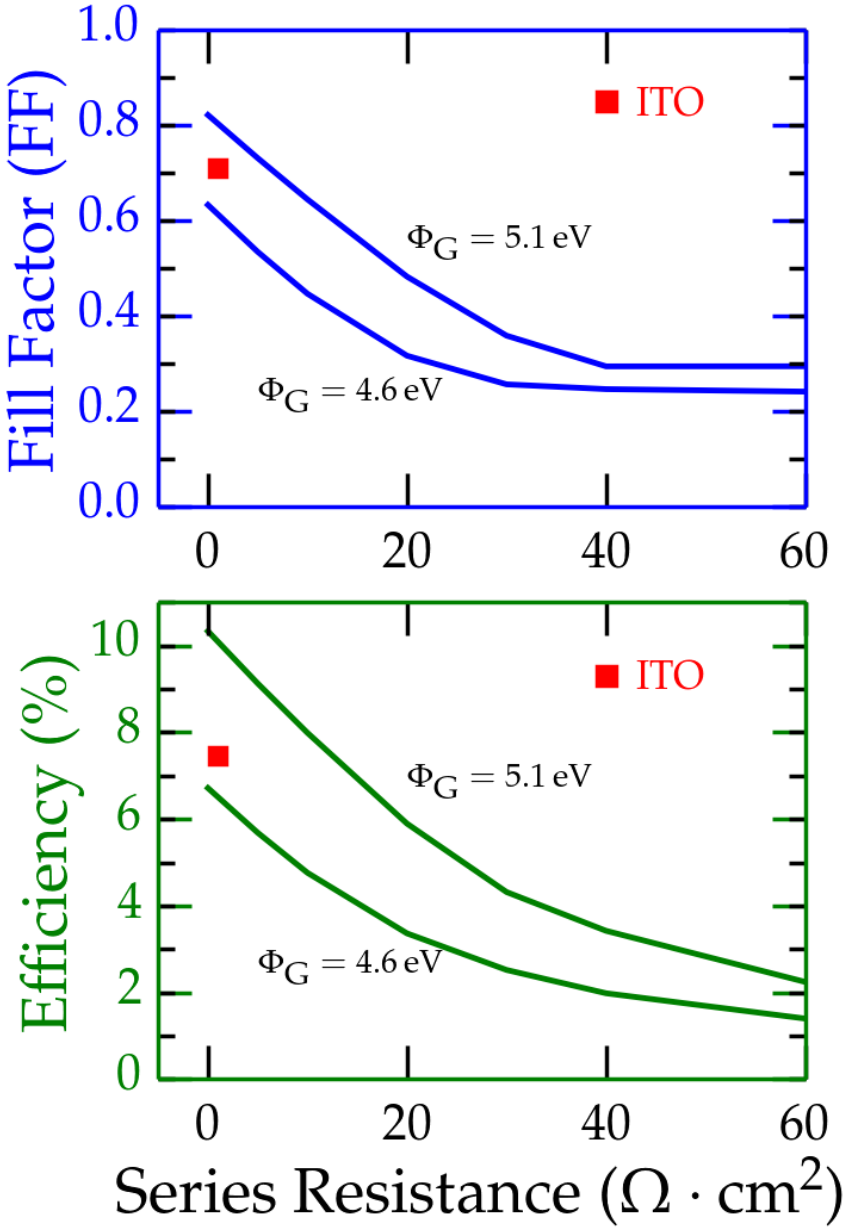

Graphene Work Function $\Phi_G = 4.7$ eV
η = 8.1%
Density Current (mA/cm^2)
Power Density (mW/cm^2)
Voltage (V)
0
−4
−8
−12
−16
10
8
6
4
2
0
0.0
0.2
0.4
0.6
0.8


Graphene Work Function $\Phi_G = 4.8$ eV
η = 9.5%
Density Current (mA/cm^2)
Power Density (mW/cm^2)
Voltage (V)
0
−4
−8
−12
−16
10
8
6
4
2
0
0.0
0.2
0.4
0.6
0.8


Graphene Work Function $\Phi_G = 4.9$ eV
η = 10.1%
Density Current (mA/cm^2)
Power Density (mW/cm^2)
Voltage (V)
0
−4
−8
−12
−16
10
8
6
4
2
0
0.0
0.2
0.4
0.6
0.8

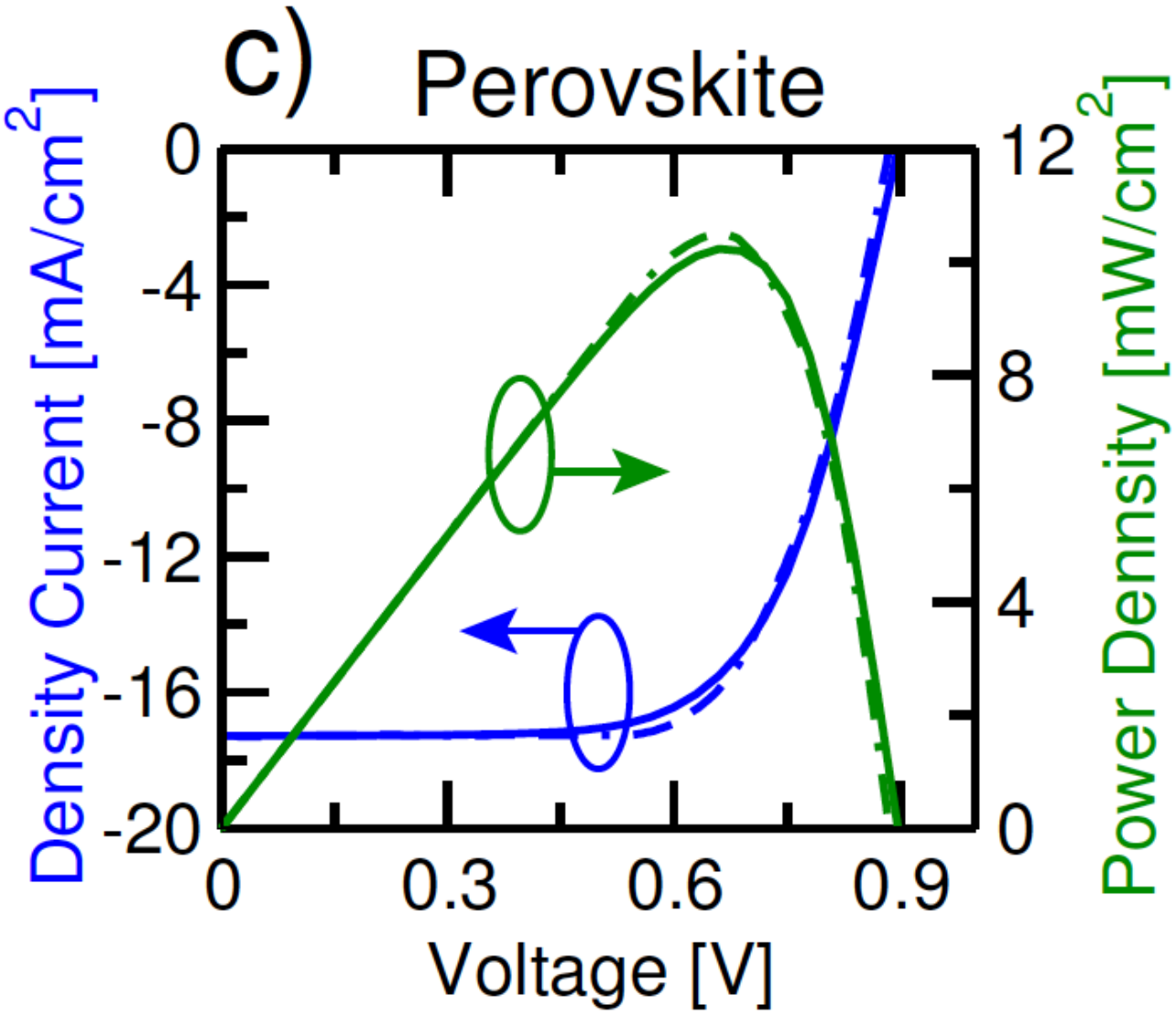

Graphene Work Function $\Phi_G = 5.0$ eV
η = 10.3%
Density Current (mA/cm^2)
Power Density (mW/cm^2)
Voltage (V)
0
−4
−8
−12
−16
10
8
6
4
2
0
0.0
0.2
0.4
0.6
0.8


Graphene Work Function $\Phi_G = 5.1$ eV
η = 10.33%
Density Current (mA/cm^2)
Power Density (mW/cm^2)
Voltage (V)
0
−4
−8
−12
−16
10
8
6
4
2
0
0.0
0.2
0.4
0.6
0.8

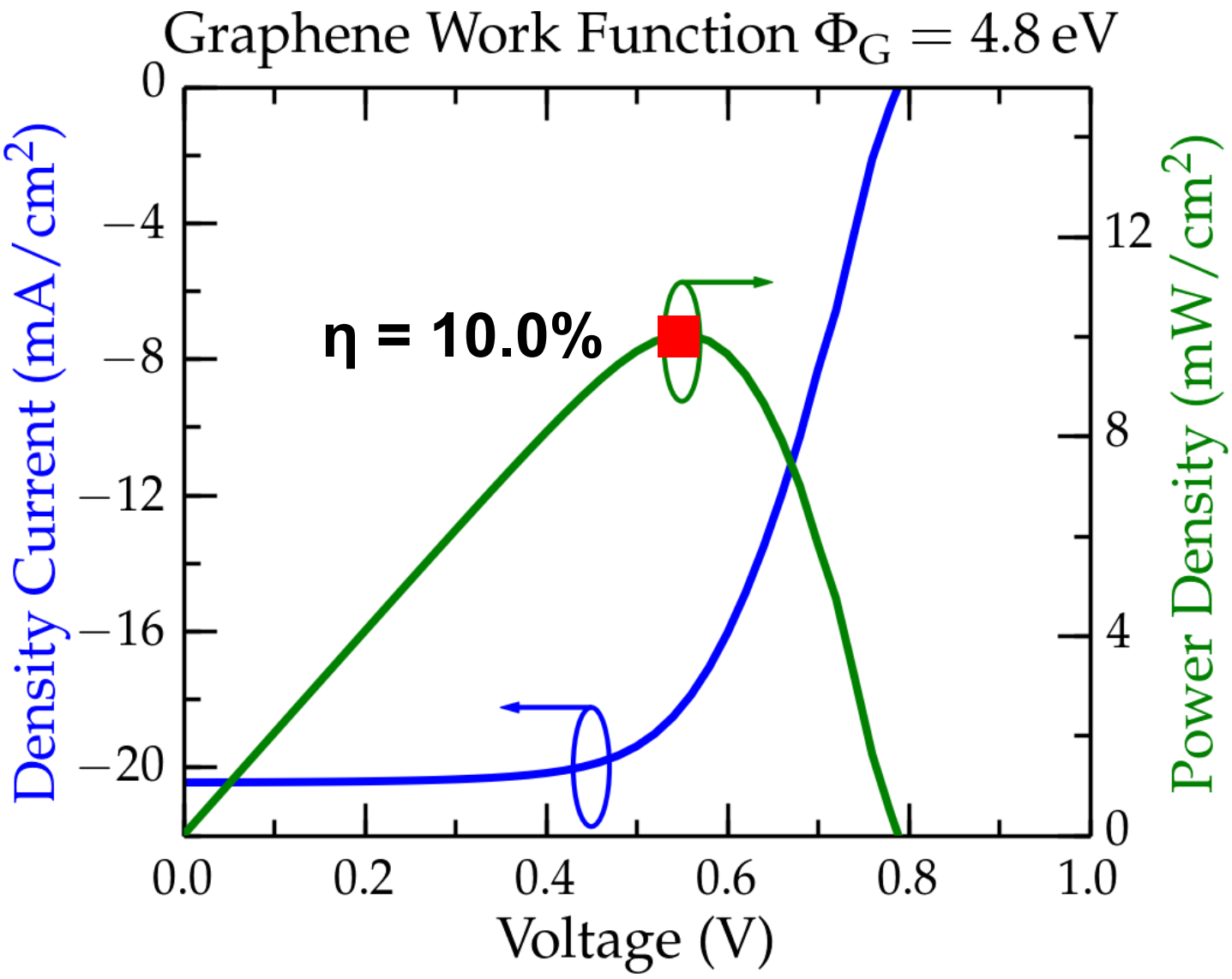

Fill Factor (FF)
1.0
0.8
0.6
0.4
0.2
0.0
ITO
$\Phi_G = 5.1$ eV
$\Phi_G = 4.6$ eV
0
20
40
60
Efficiency (%)
10
8
6
4
2
0
ITO
$\Phi_G = 5.1$ eV
$\Phi_G = 4.6$ eV
0
20
40
60
Series Resistance ($\Omega \cdot cm^2$)

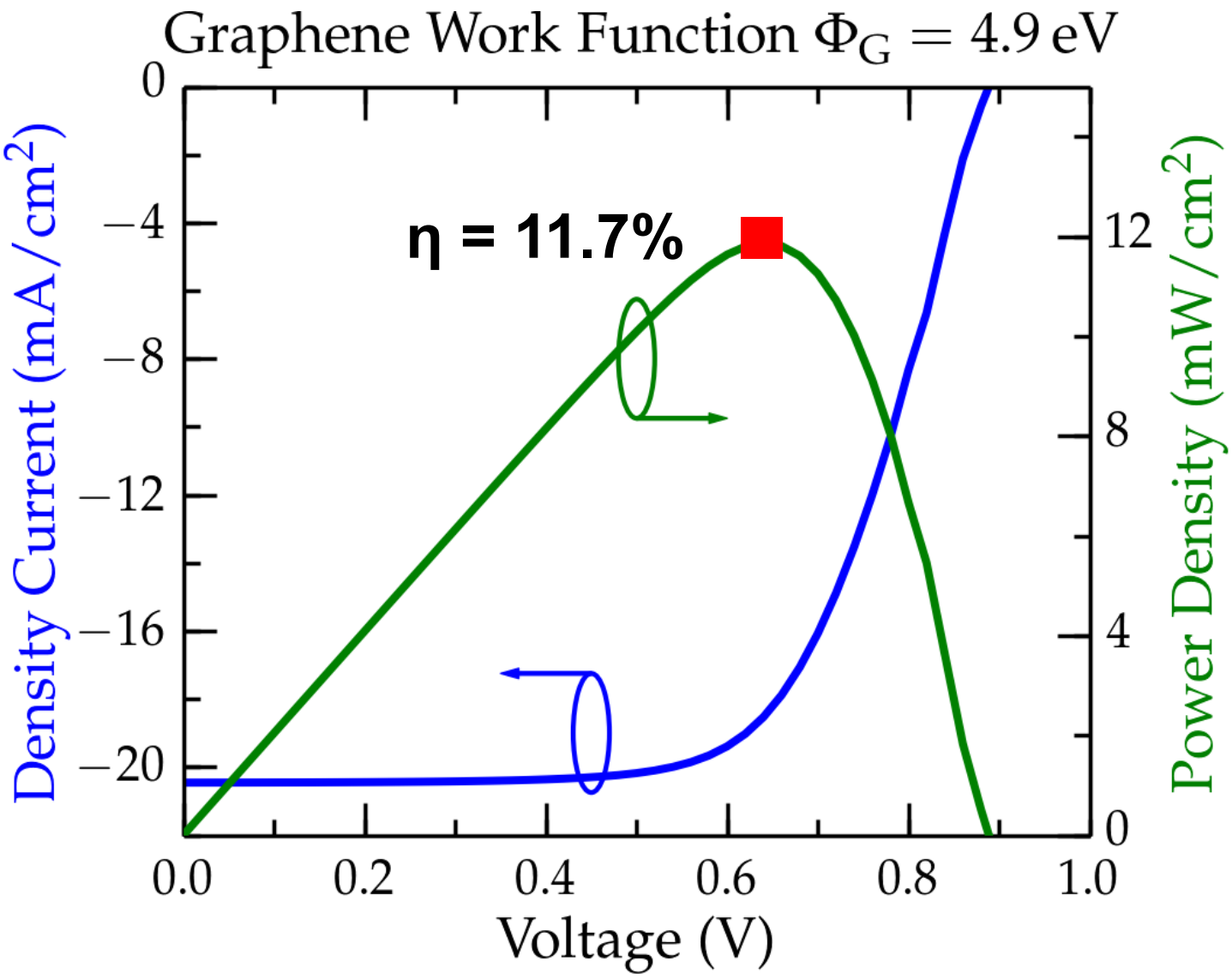
Perovskite

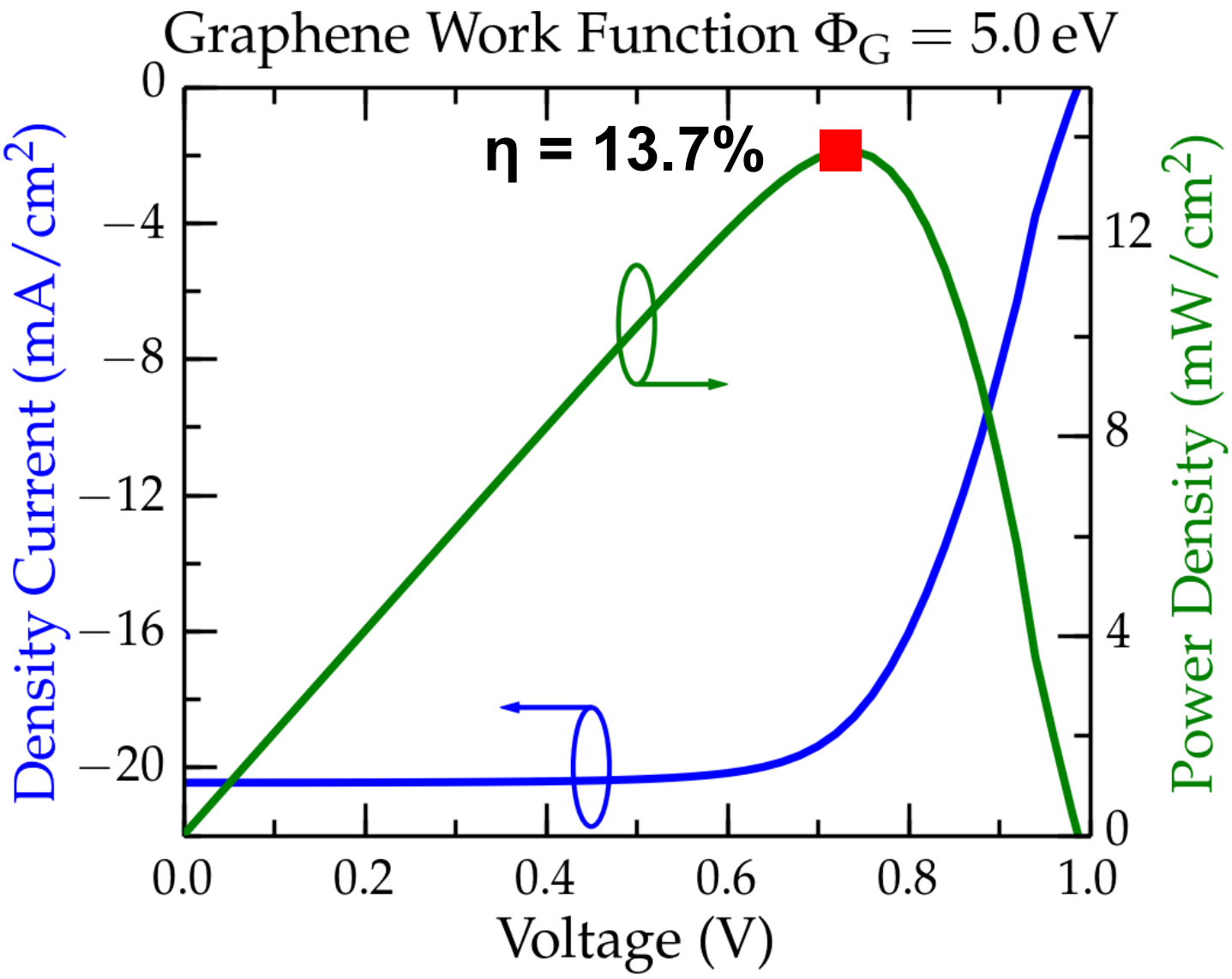
Calibration with experiments

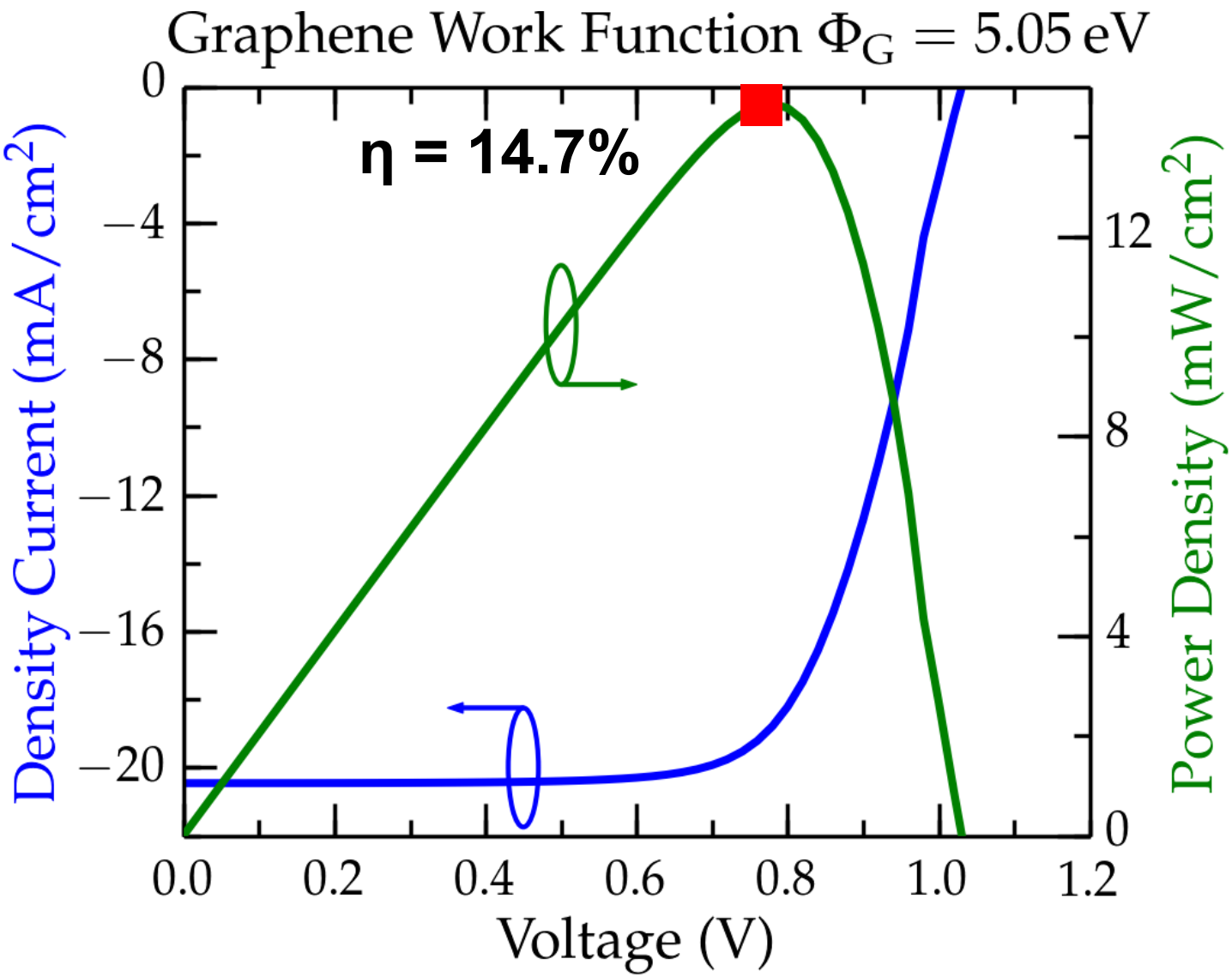


Exp: You et al., ACS Nano 8, 1674, 2014

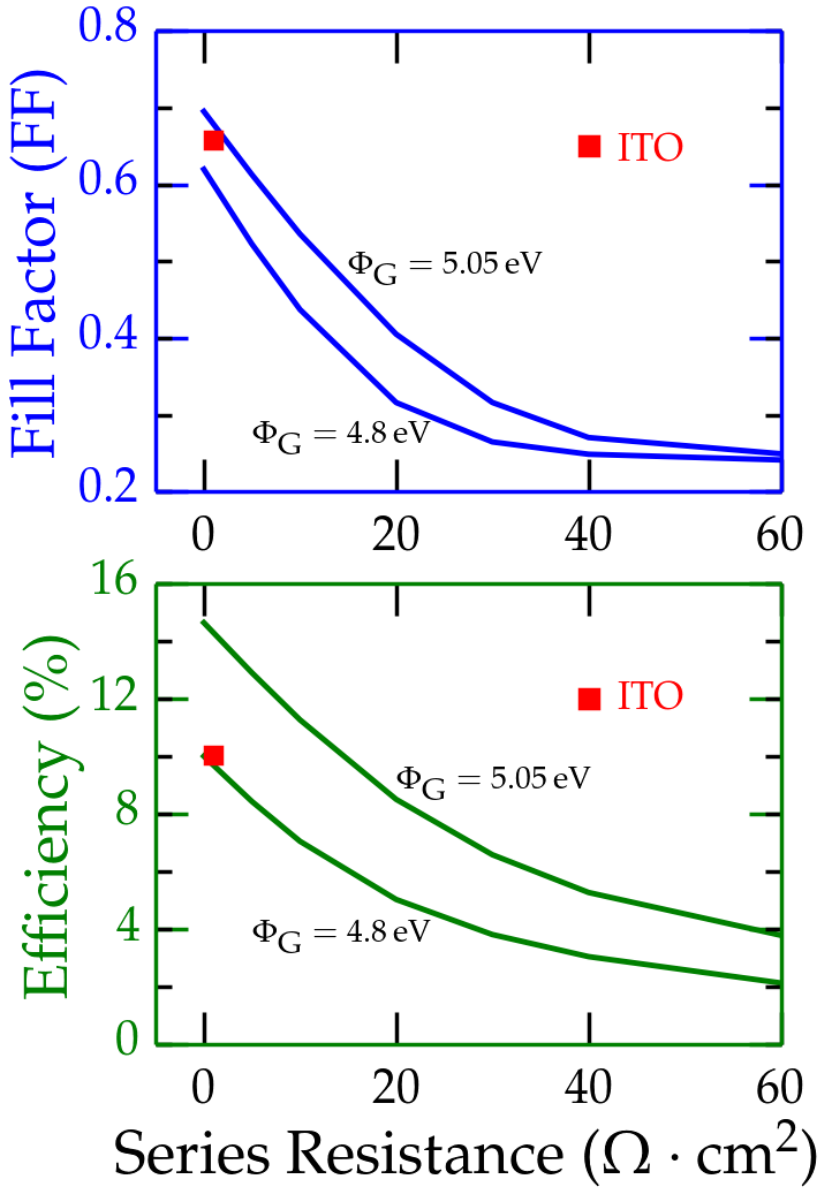

Graphene Work Function $\Phi_G = 4.8\,eV$
η = 10.0%
Density Current (mA/cm^2)
Power Density (mW/cm^2)
Voltage (V)
0
−4
−8
−12
−16
−20
12
8
4
0
0.0
0.2
0.4
0.6
0.8
1.0


Graphene Work Function $\Phi_G = 4.9$ eV
η = 11.7%
Density Current (mA/cm^2)
Power Density (mW/cm^2)
Voltage (V)
0
−4
−8
−12
−16
−20
12
8
4
0
0.0
0.2
0.4
0.6
0.8
1.0


Graphene Work Function $\Phi_G = 5.0$ eV
η = 13.7%
Density Current (mA/cm^2)
Power Density (mW/cm^2)
0
−4
−8
−12
−16
−20
12
8
4
0
0.0
0.2
0.4
0.6
0.8
1.0
Voltage (V)


Graphene Work Function $\Phi_G = 5.05\,eV$
η = 14.7%
Density Current (mA/cm²)
Power Density (mW/cm²)
Voltage (V)
0
−4
−8
−12
−16
−20
12
8
4
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2

PHJ with Perovskite

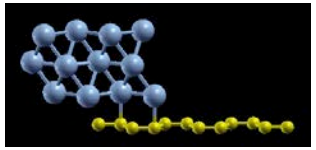


- **Take home message:**

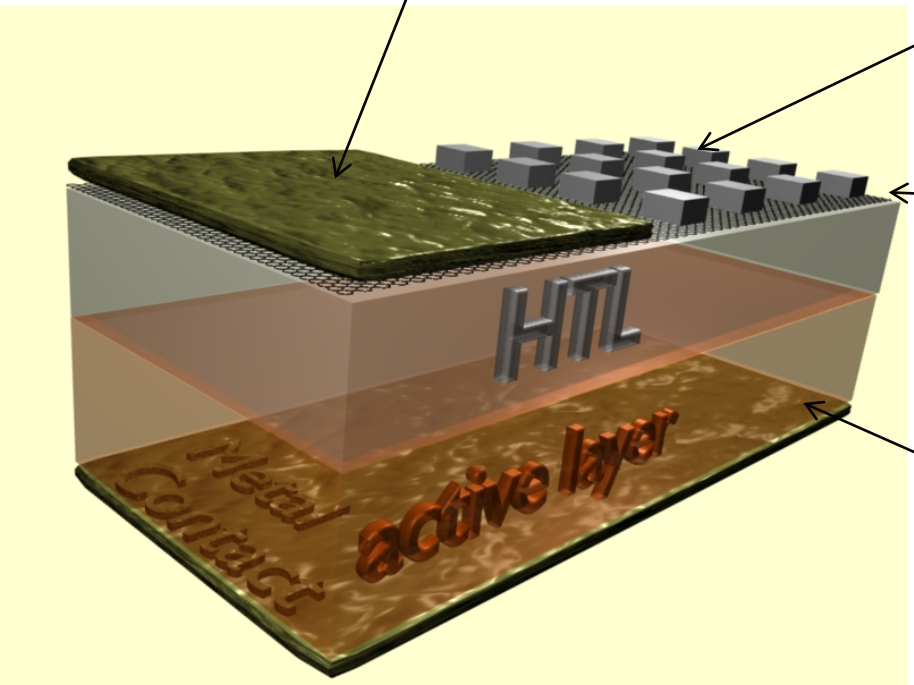
- **Figure of merits (FF and PCE) are really sensitive on the contact resistance**

- **WF tuning plays an important role in SC design (SC less sentive on WF than on contact resistance)**

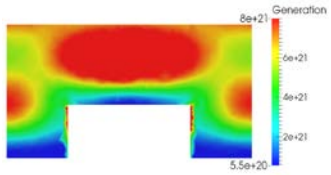
Investigated issues



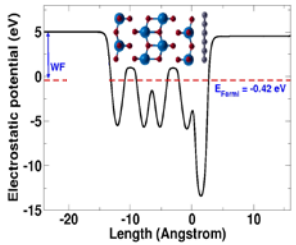
Understanding the role of graphene/metal contact



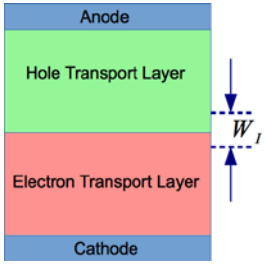
Light management



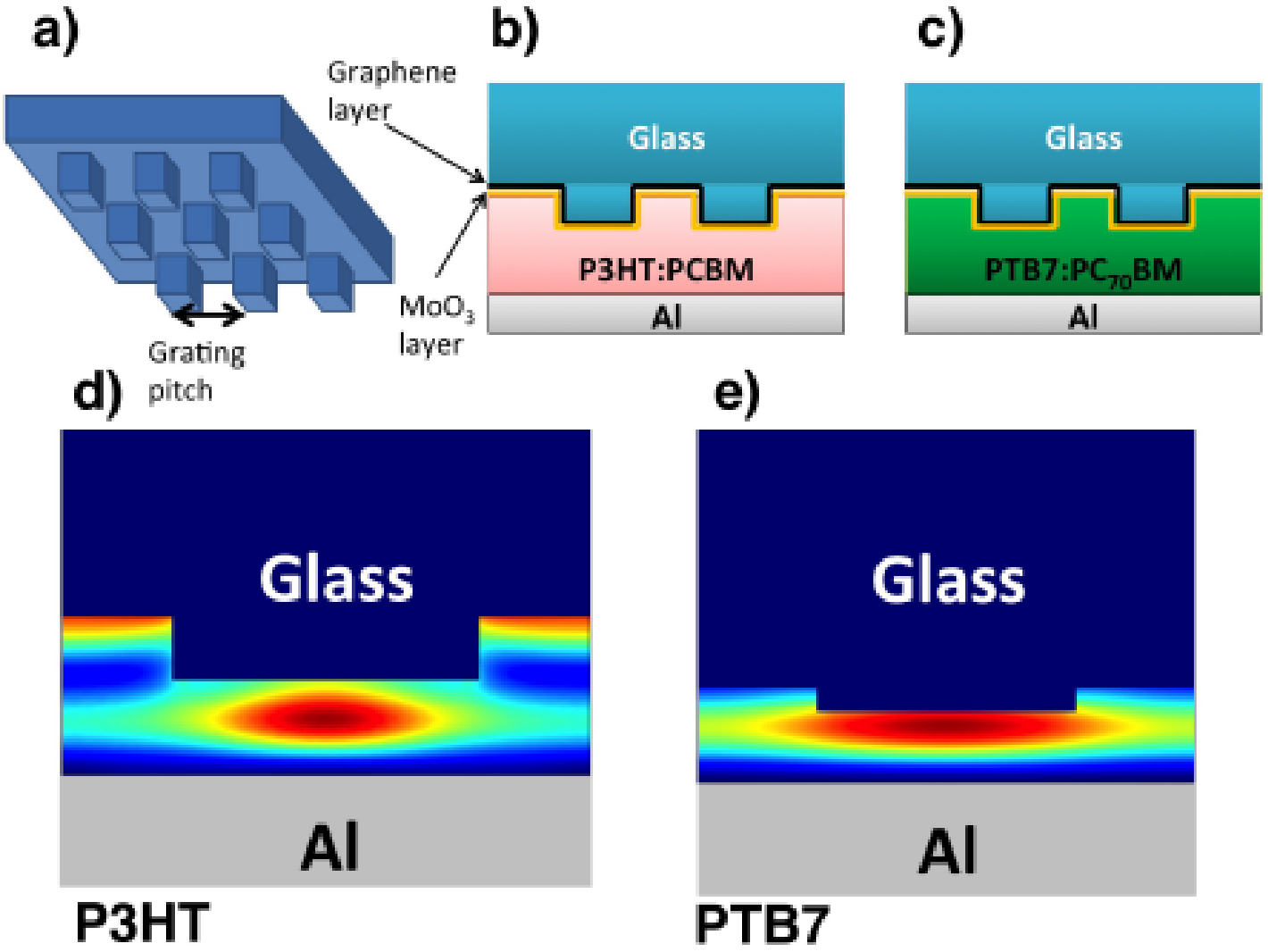
Work-function tuning of graphene



Sensitivity of solar cell to design parameters

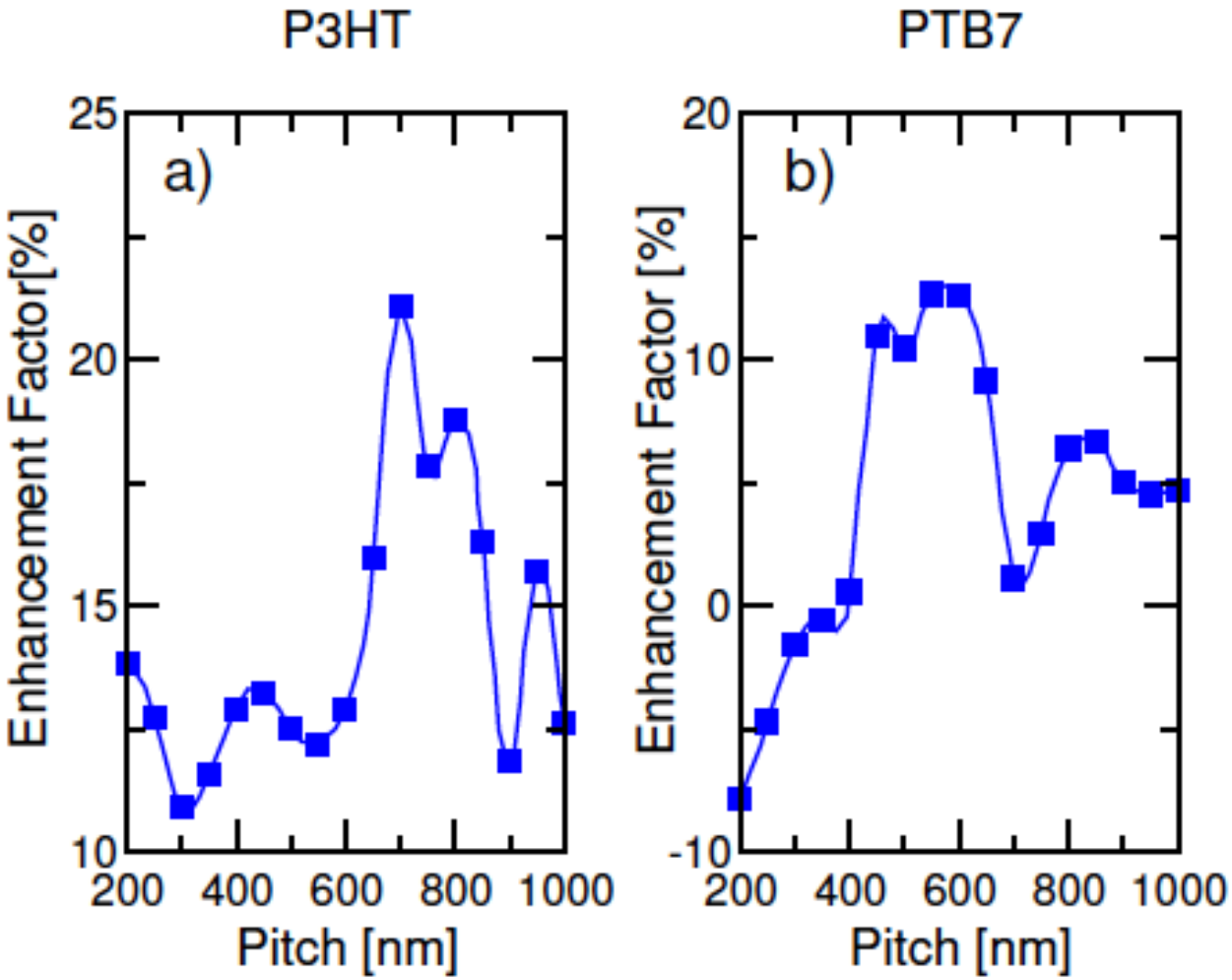


Light management: grating of the graphene electrode

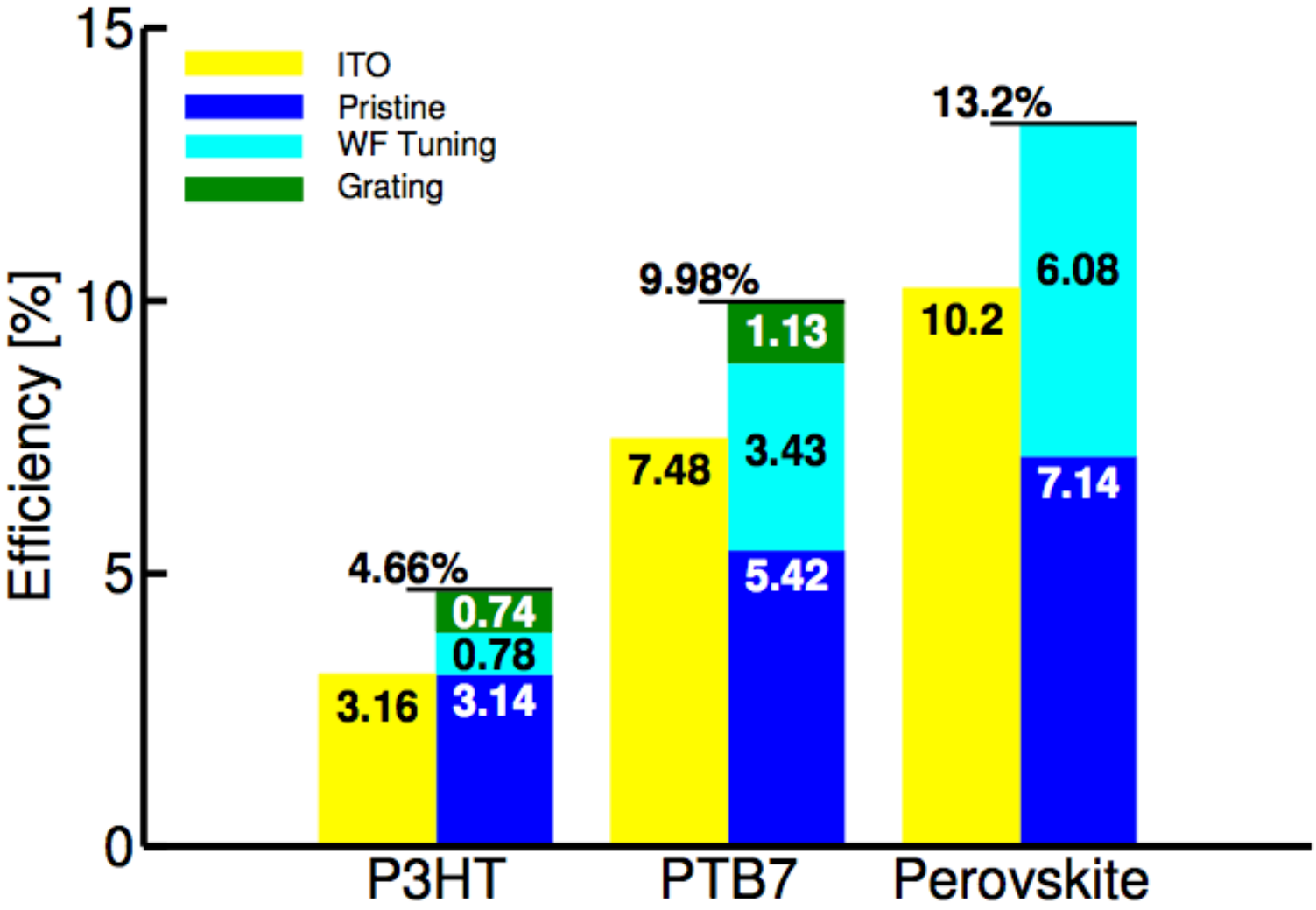


Comsol multiphysics considering complex refractive index

Enhancement factor up to 21%



All effect combined



Conclusion

- We have performed a detailed investigation of graphene-based organic solar cells with multi-scale simulations [ab-initio + DD + electromagnetics]

- Graphene-based solar cells can outperform ITO-based solar cells

ONLY IF

- The series resistance of the graphene layer can be minimized

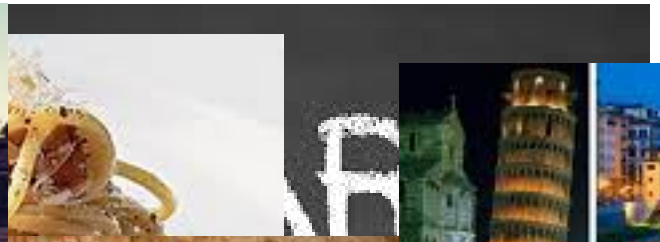
just a sec……..

just a sec……..

just a sec……..

just a sec……..

just a sec……..









just a sec……..

just a sec……..

Thank You!

Acknowledgment:

EC FP7 project GO-NEXTS

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