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Numerical investigation of the effect of interface conditions in HTM-free and standard perovskite solar cells

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Introduction

One of the remaining issues, impeding the commercialization of the low cost and high efficiency perovskite solar cells (PSCs) is the stability of the halide perovskite materials, including the light-induced degradation and the hysteresis effect. The perovskite/TiO_x and perovskite/Au interfaces are numerically investigated, simulating the current-voltage (J-V) and capacitance-voltage (C-V) characteristics. Furthermore, a new approach is proposed for the modelling of Kelvin Probe Force Microscopy (KPFM). It is applied to hetero-structures in dark and under illumination, aiming at estimating the surface states on the top of the electron transport materials and understanding the charge carrier behavior inside the cells.

Basic equations used for the numerical simulation[1]

Coupled continuity and Poisson equations

$$\frac{\partial n}{\partial t} = \frac{1}{q} \text{div} \vec{J}_n + G_n - R_n$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q} \text{div} \vec{J}_p + G_p - R_p$$

$$\Delta \Psi = -\frac{\rho}{\epsilon}$$

Drift diffusion currents

$$\vec{J}_n = -qn\mu_n \vec{E}_n + qD_n \nabla n(x)$$

$$\vec{J}_p = -qp\mu_p \vec{E}_p - qD_p \nabla p(x)$$

Recombination rates

$$R_{bi} = k_{bi}(np - n_i^2)$$

$$R_{SRH} = \frac{pn - n_i^2}{\tau_p(n + n_i) + \tau_n(p + n_i)}$$

HTM-free PSCs

Yong HUANG et al, EPJ Photovoltaics 8, 85501 (2017)

Materials parameters

	χ (eV)	E_g (eV)	N (cm ⁻³)	m_e^* & m_h^* (m_0)	ϵ_r (ϵ_0)
CH ₃ NH ₃ PbI ₃	3.9	1.6	4e16*	0.23&0.26	70
TiO ₂	4.1	3.3	1e19 [2]	5.6&5.6 [3]	31

* indicates fitting parameters

[1] Silvaco Inc., ATLAS user's manual, Sunnyvale, CA, 2012.

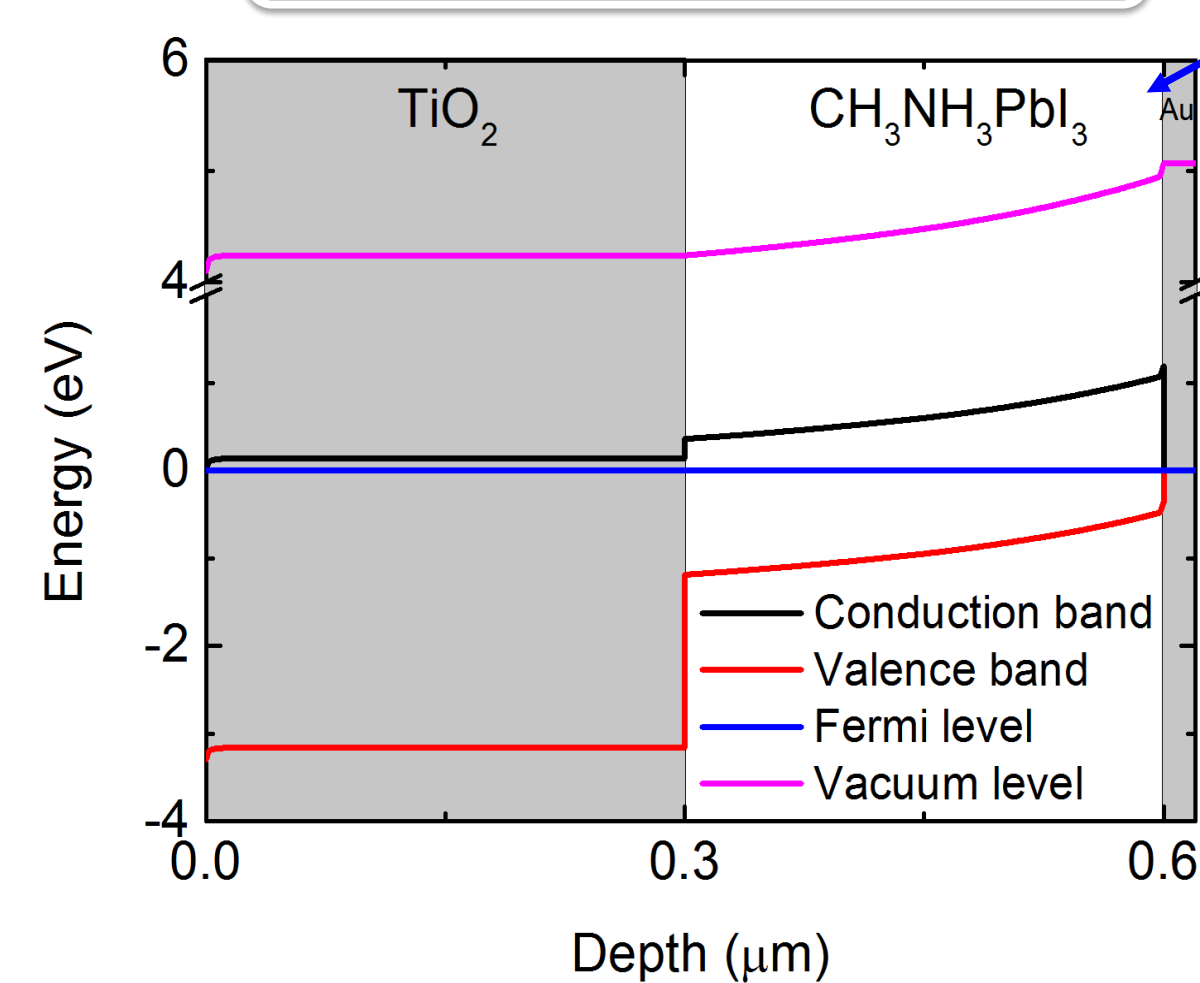
[2] G. Liu, W. Jaegermann, J. He, V. Sundström, and L. Sun, J. Phys. Chem. B **106**, 5814 (2002).

[3] S. Rühle and D. Cahen, J. Phys. Chem. B **108**, 17946 (2004).

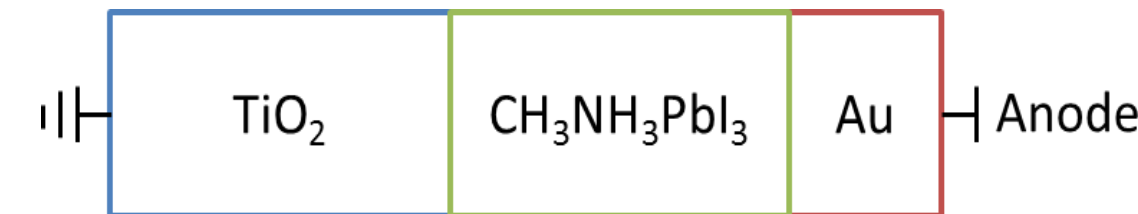
[4] W.A. Laban and L. Etgar, Energy Environ. Sci. **6**, 3249 (2013).

[5] A. Gheno et al, Sol. Energy Mater. Sol. Cells. **161**, 347 (2017).

Static band diagram



Interfacial heavily n-doped layer needed to fit experimental data

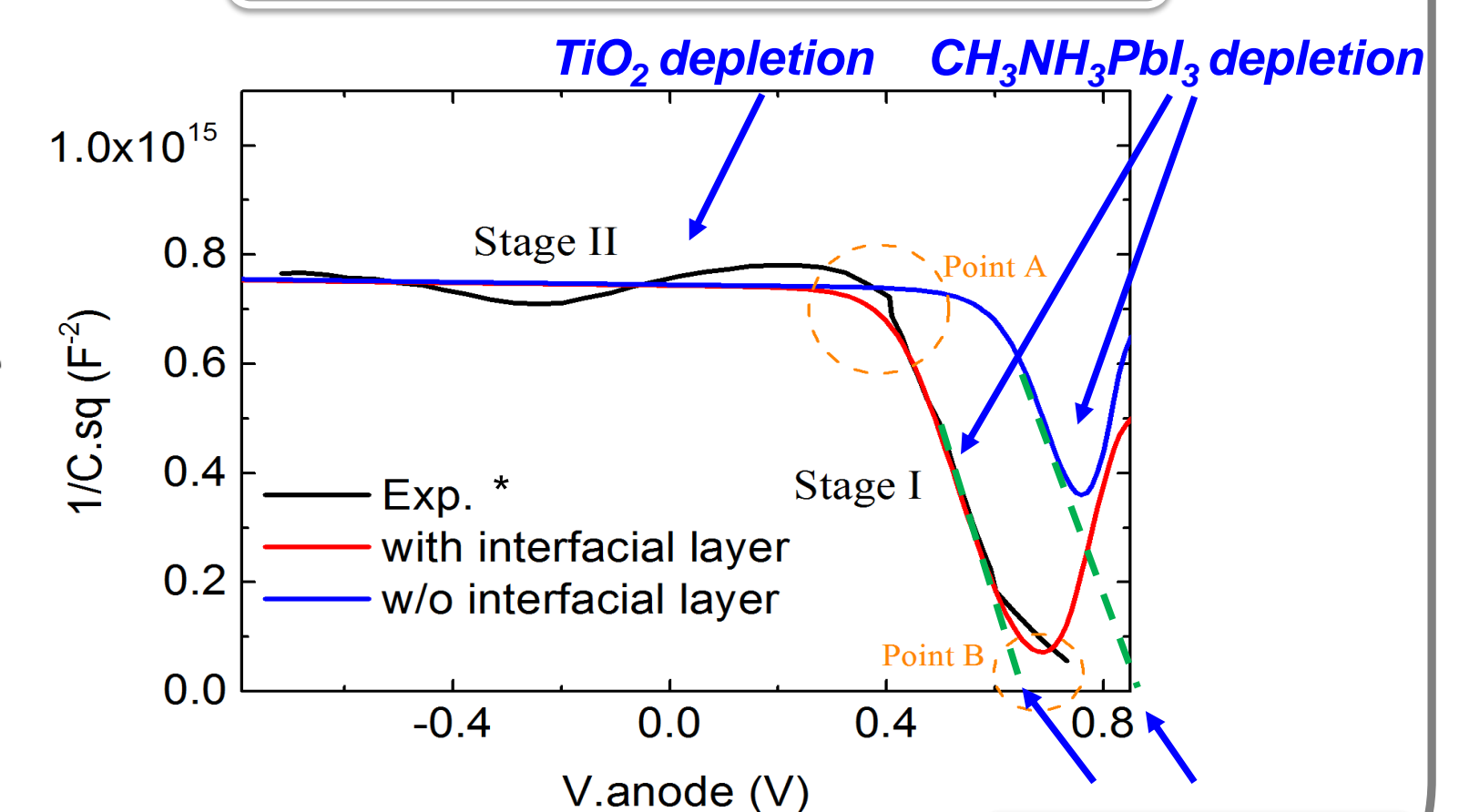


$$\frac{1}{C^2} = \frac{2}{qA^2\epsilon_0 N\epsilon_r} (V_{bi} - V_{bias} + \frac{kT}{q})$$

Equivalent circuit used for capacitance analysis

* Experimental results from Etgar's group [4], (collaboration with Hebrew University of Jerusalem)

Capacitance-voltage



V_{bi}: built-in potential loss

Kelvin Probe Force Microscopy

Yong HUANG et al, OQE, submitted

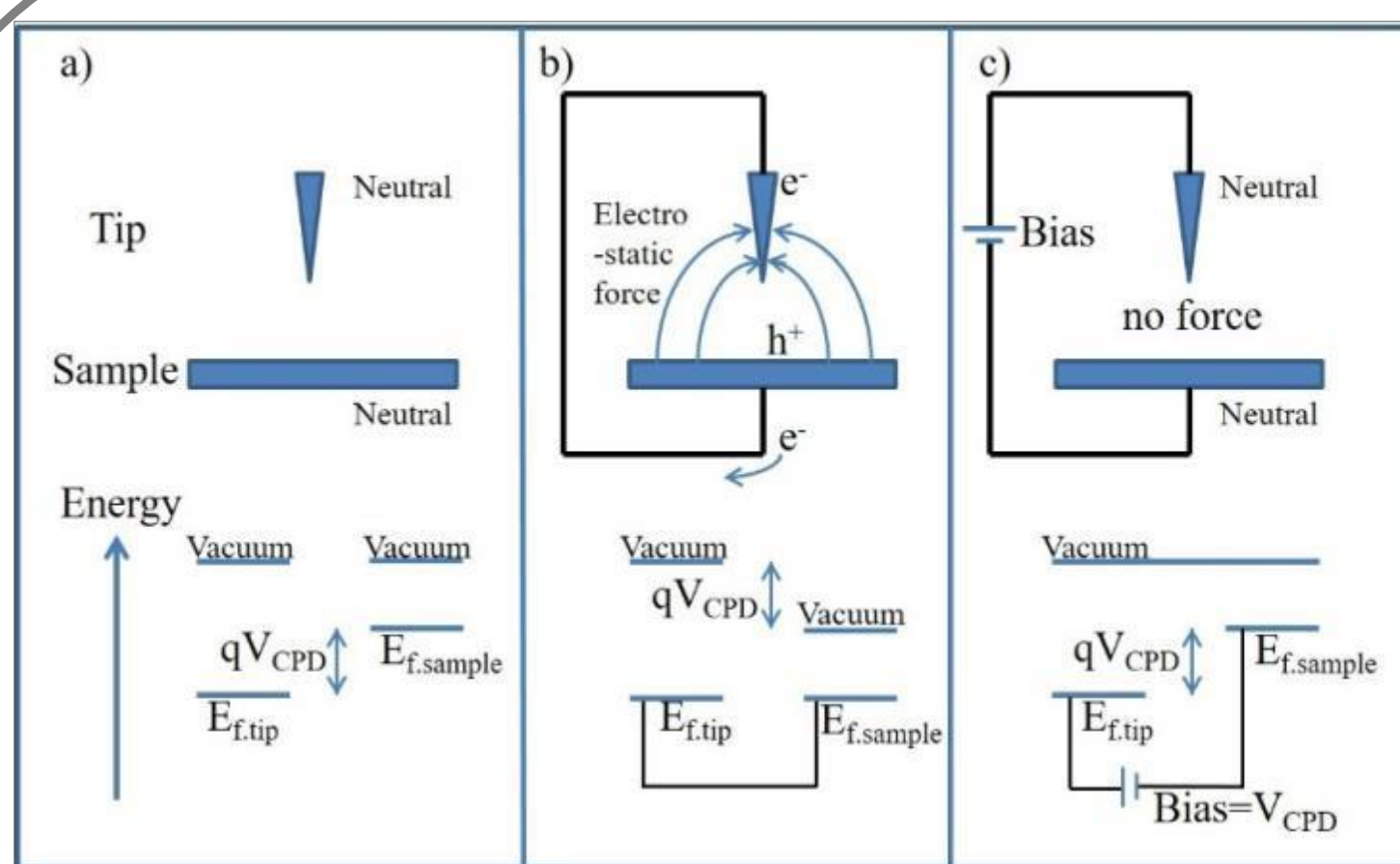


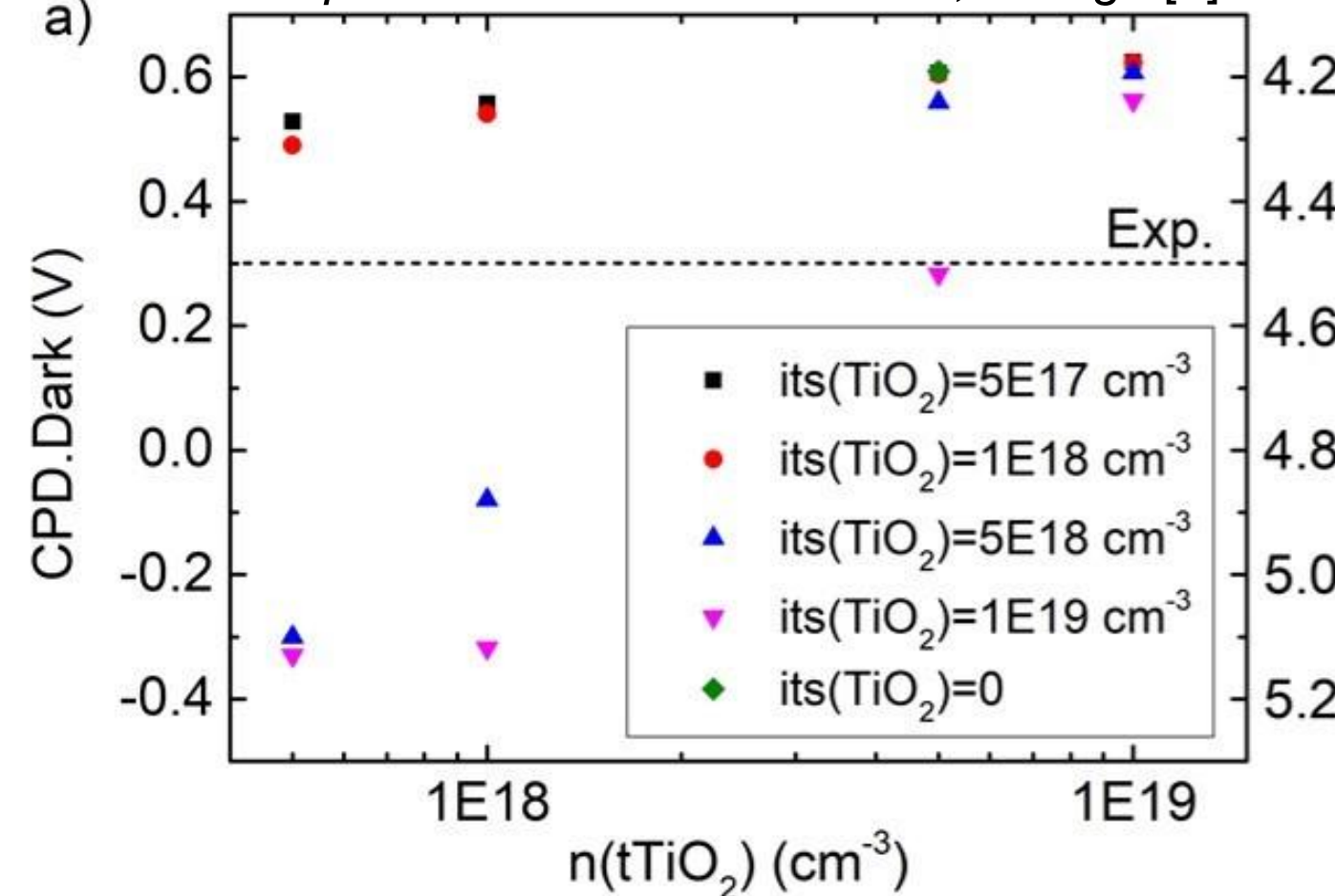
Illustration of the basic measurement setup of Contact Potential Difference (CPD). Tip and sample are a) separated, b) connected at short circuit and c) under bias of V_{CPD}.

$$V_{CPD} = \frac{E_{f,tip} - E_{f,sample}}{q}$$

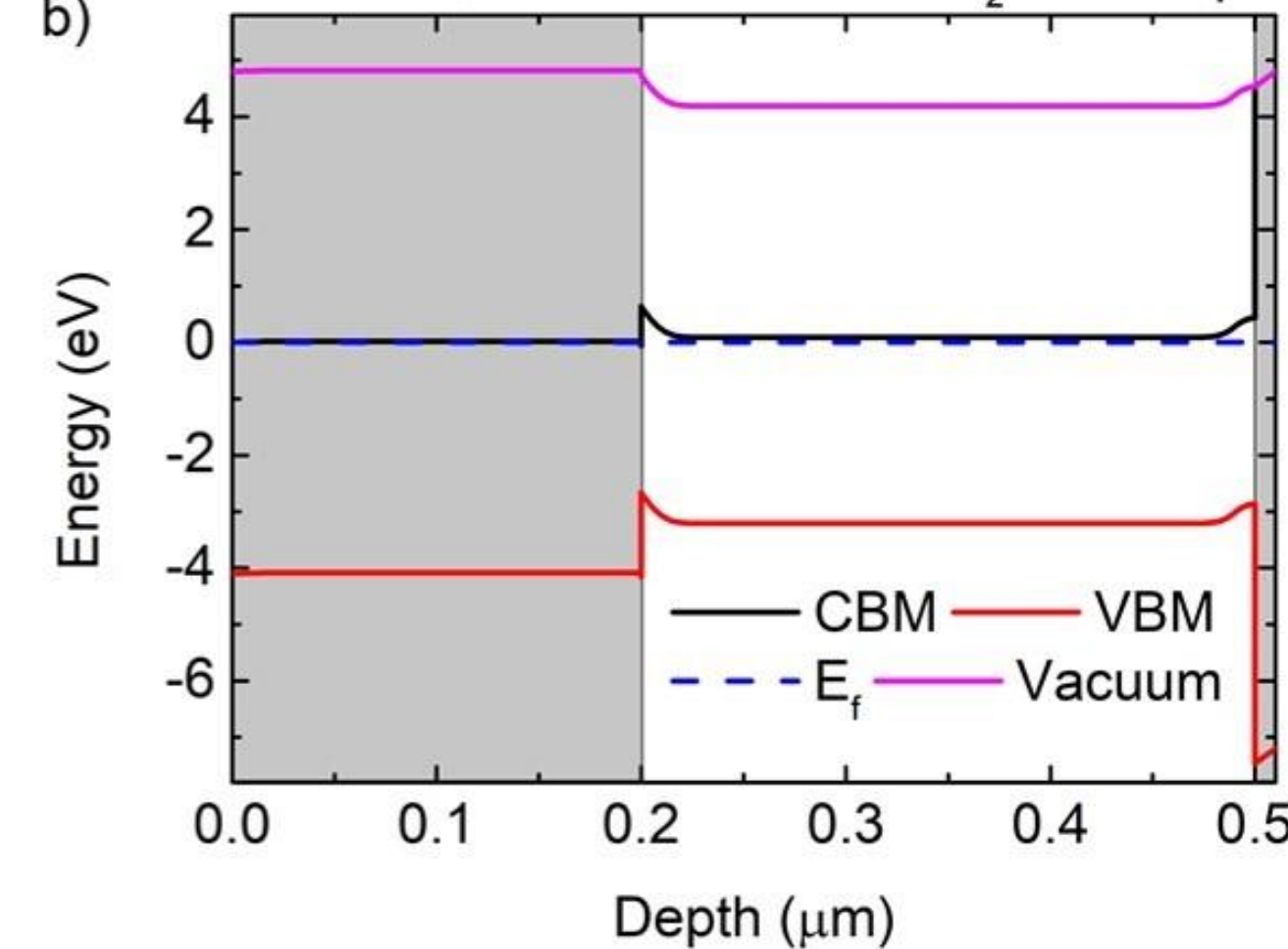
V_{CPD} measured by KPFM, E_{f,tip} is known.

Spacer	th=10 nm	Tip, WF=4.8 eV
iftTiO ₂	th=10 nm, n=n(tTiO ₂), its(tTiO ₂)	Light Tip, WF=4.8 eV
tTiO ₂	th=240 nm, n(tTiO ₂)	
bTiO ₂	th=50 nm, n(bTiO ₂)=5E18 cm ⁻³	Light Tip, WF=4.8 eV
FTO	th=200 nm, n(FTO)=1E20 cm ⁻³	

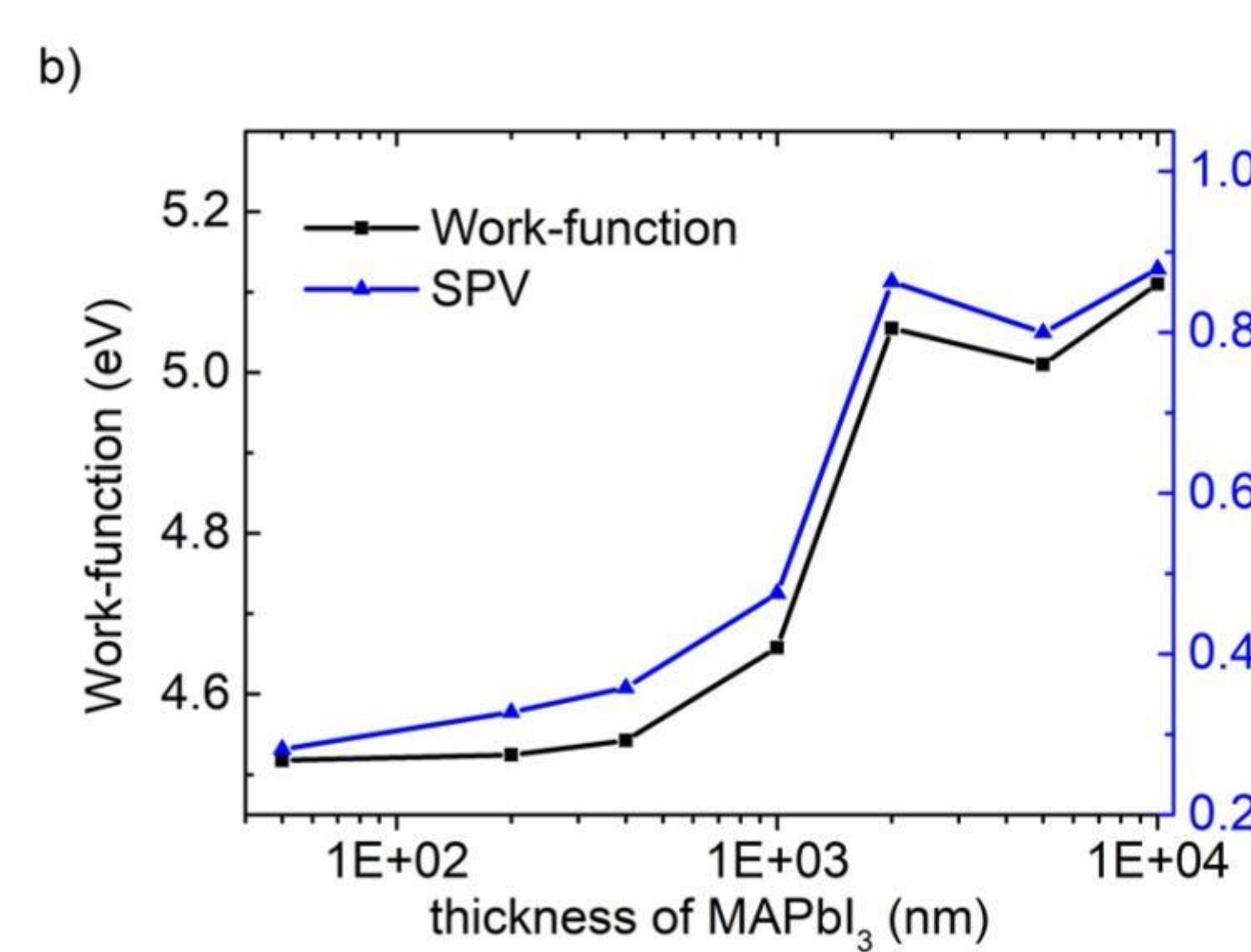
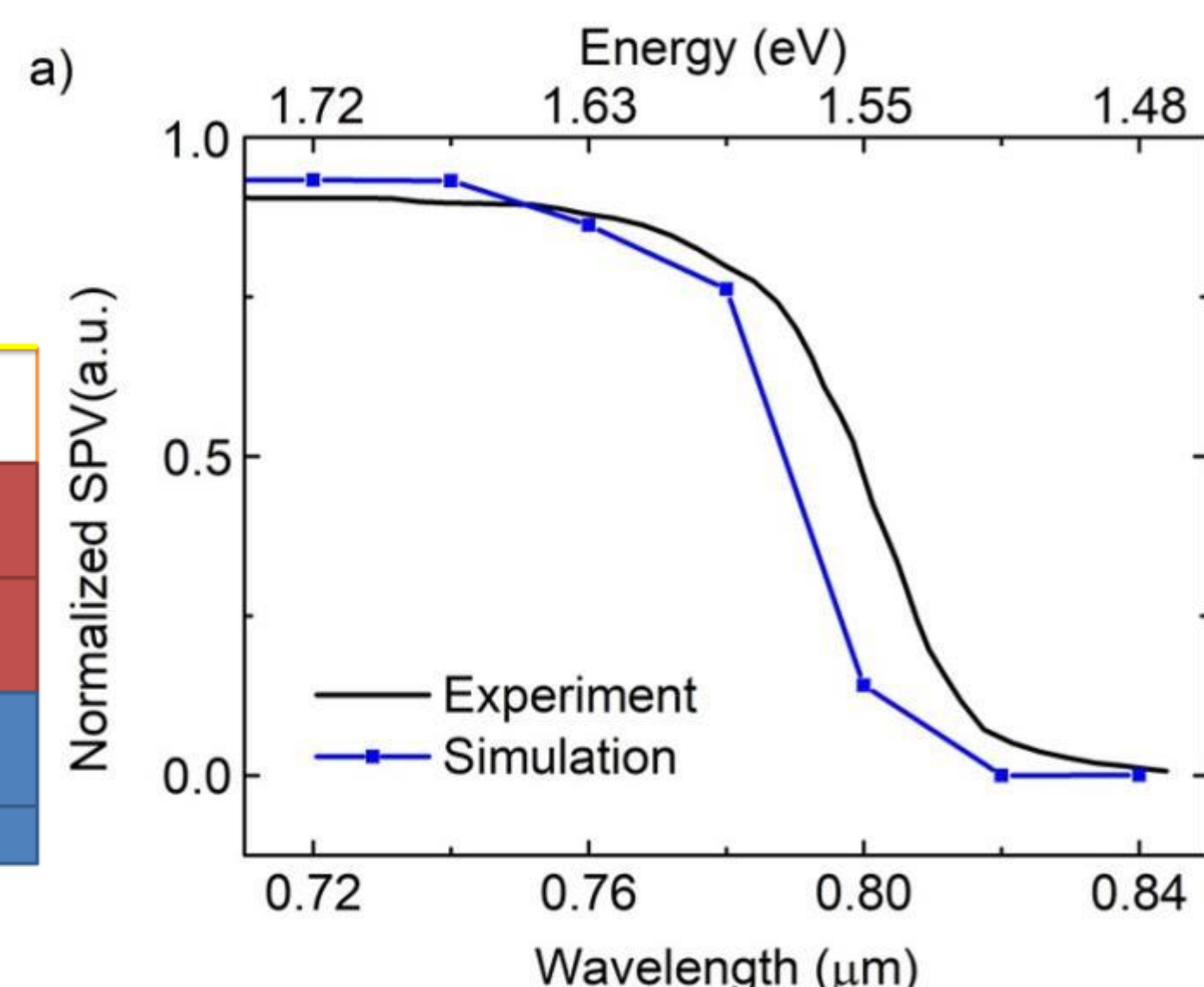
* Experimental results from Xlim, Limoge [5]



FTO TiO₂ Spacer



a) Static Contact Potential Difference (CPD.Dark) and work-function as a function of the doping level, n(tTiO₂) and the surface trap density, its(TiO₂). b) Schematic representation of the static band alignment with acceptor-like trap density equal to 1E19cm⁻³ on the top of a 5E18cm⁻³ doped TiO₂.



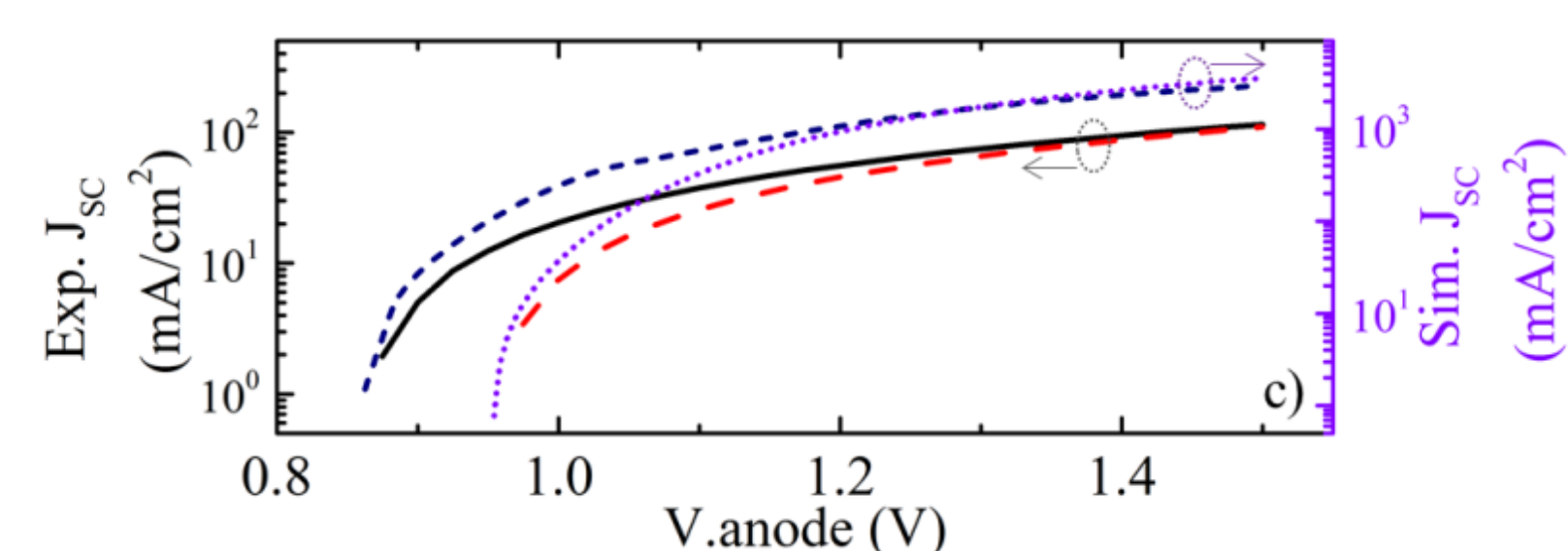
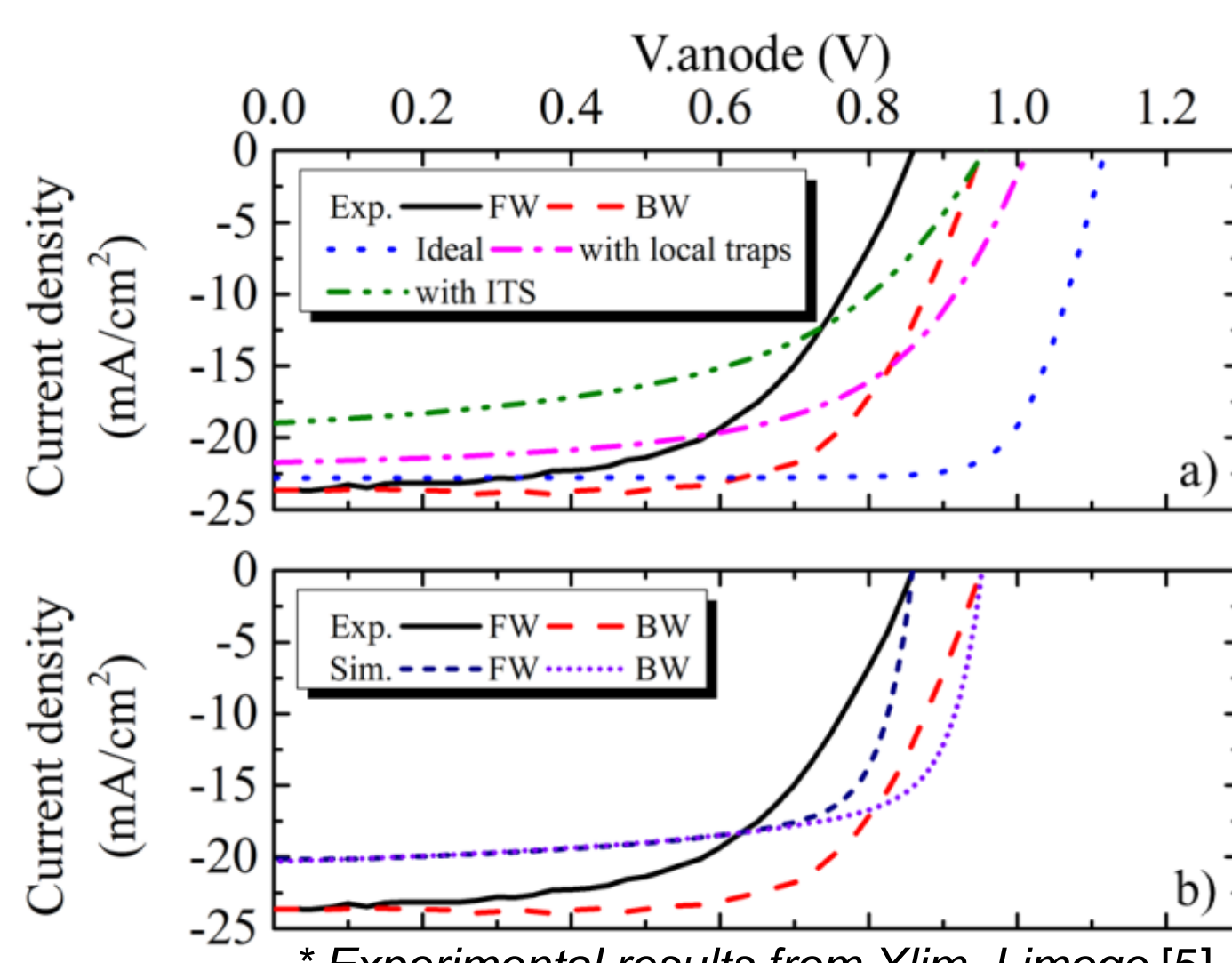
a) Experimental and simulated Surface Photovoltage (SPV). The simulated light power is 1 W/cm². b) Computed surface work-function and Surface PhotoVoltage (SPV) as a function of the thickness of CH₃NH₃PbI₃. The external light source is one sun.

A new approach to modelling Kelvin Probe Force Microscopy for hetero-structures in the dark and under illumination has been presented. The approach has been tested by examining FTO/TiO₂ and FTO/TiO₂/MAPbI₃ structures. Unexpected surface states on the top of TiO₂ layer are inferred by the combination of theoretical computation and experimental results. The basic applications of KPFM under illumination are analyzed as well.

V_{oc} Losses in PSCs

Yong HUANG et al, NUSOD international conference (2017)

a) Experimental J-V properties of TiO_x/MAPbI₃/Spiro-OMeTAD solar cells; black solid and red dash lines indicate forward and backward scan, respectively. The computed ideal case with only bimolecular recombination is drawn as blue dots. The curve shift to violet dash dot line with taking into account the local trap states, and it becomes worse with interface trap states as the green dot dot dash line. b) Experiment data in comparison with the computation with ITS and mobile ions. The tick labels of a) and b) are on the top. c) J-V characteristics of experimental and simulation with mobile ions biased above 0.8V.



The V_{oc} loss of standard TiO_x/CH₃NH₃PbI₃/Spiro-OMeTAD PSCs could mainly come from the local trap-assisted recombination in the bulk, besides the interface trap recombination and ion migration.

Acknowledgements

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