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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**

$$\frac{\partial n}{\partial t} = \frac{1}{q} div\overrightarrow{J_n} + G_n - R_n$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q} div\overrightarrow{J_p} + G_p - R_p$$

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

**Drift diffusion currents**

$$\overrightarrow{J_n} = -qn\mu_n\overrightarrow{E_n} + qD_n\nabla n(x)$$

$$\overrightarrow{J_p} = -qp\mu_n\overrightarrow{E_n} - qD_p\nabla p(x)$$

**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)*

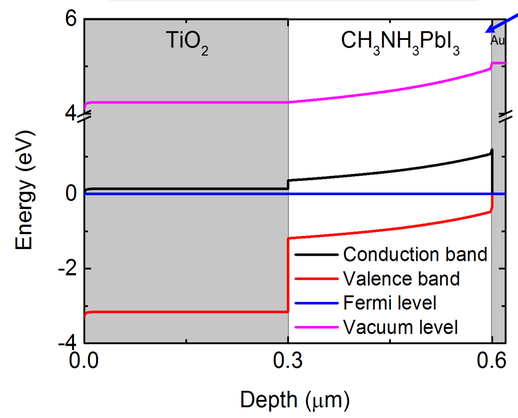
### Materials parameters

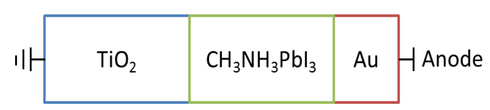
| | χ (eV) | $E_g$ (eV) | N ($cm^{-3}$) | $m_e$*&$m_h$* ($m_0$) | $\varepsilon_r$ ($\varepsilon_0$) |
|---|---|---|---|---|---|
| $CH_3NH_3PbI_3$ | 3.9 | 1.6 | 4e16* | 0.23&0.26 | 70 |
| $TiO_2$ | 4.1 | 3.3 | 1e19 [2] | 5.6&5.6 [3] | 31 |

* *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

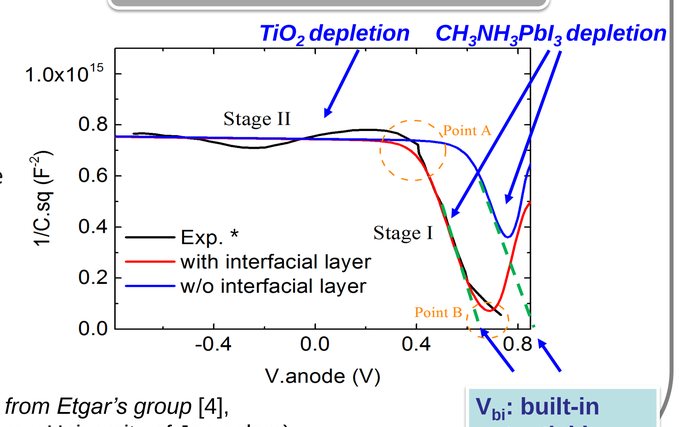



$$\frac{1}{C^2} = \frac{2}{qA^2\varepsilon_0}\frac{1}{N\varepsilon_r}\left(Vbi - Vbias + \frac{kT}{q}\right)$$

Equivalent circuit used for capacitance analysis

### Capacitance-voltage




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

## Kelvin Probe Force Microscopy

*Yong HUANG et al , OQE, submitted*

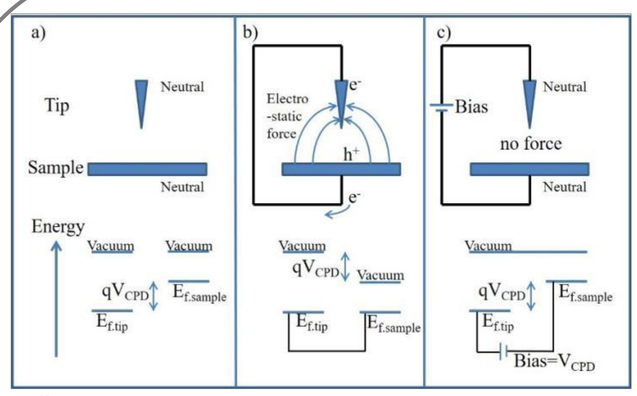
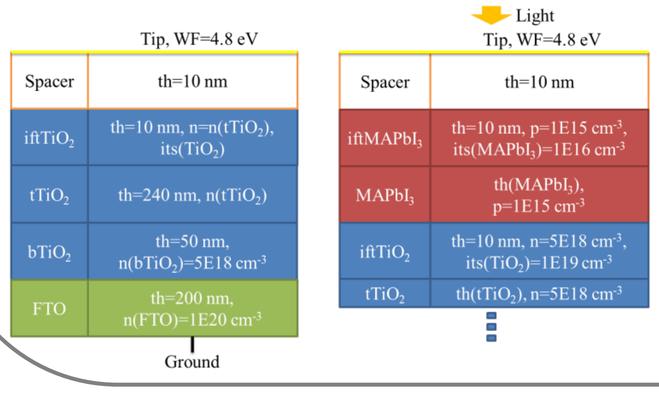


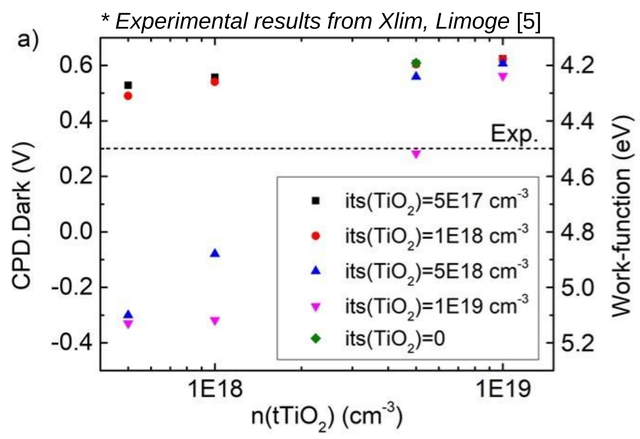

Illustration of the basic measurement setup of Contact Potential Difference (CPD). Tip and sample are a) separated, b) connected at short circuit and c) under bias of $V_{CPD}$.

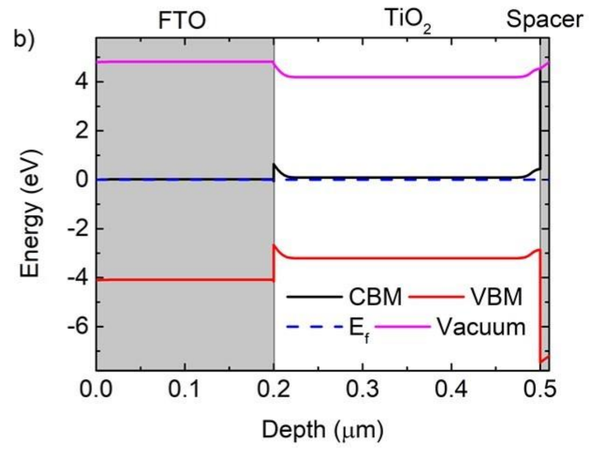
$$V_{CPD} = \frac{E_{f.tip} - E_{f.sample}}{q}$$

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

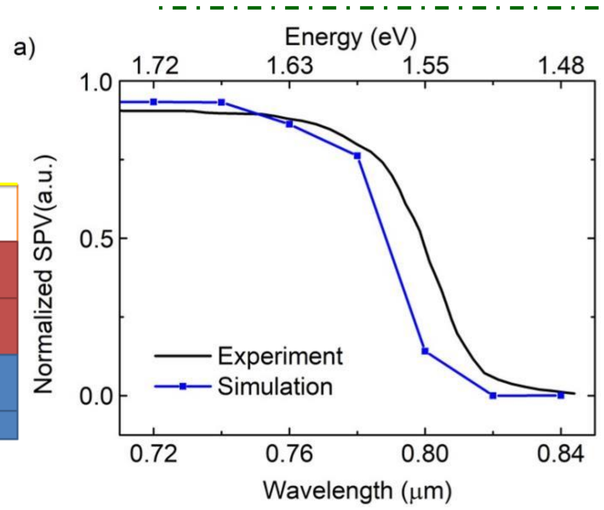


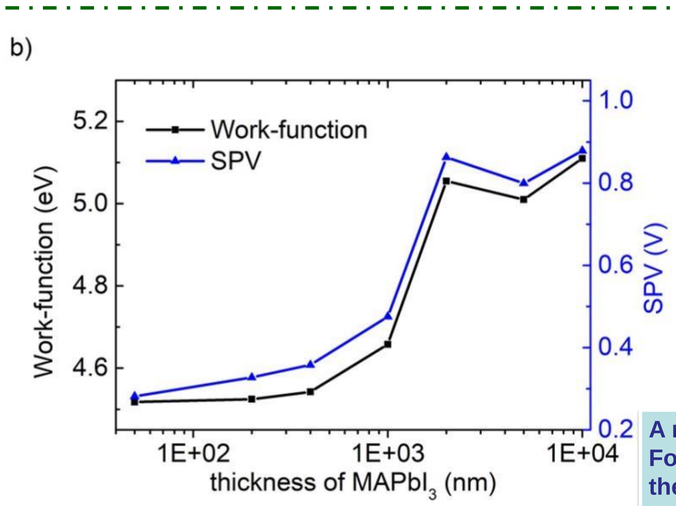

* *Experimental results from Xlim, Limoge* [5]




a) Static Contact Potential Difference (CPD.Dark) and work-function as a function of the doping level, n(t$TiO_2$) and the surface trap density, its($TiO_2$). b) Schematic representation of the static band alignment with acceptor-like trap density equal to 1E19$cm^{-3}$ on the top of a 5E18$cm^{-3}$ doped $TiO_2$.



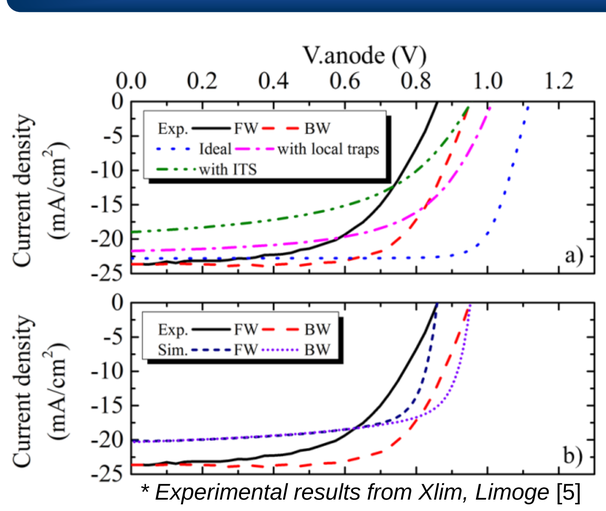

a) Experimental and simulated Surface Photovoltage (SPV). The simulated light power is 1 W/$cm^2$. b) Computed surface work-function and Surface PhotoVoltage (SPV) as a function of the thickness of $CH_3NH_3PbI_3$. The external light source is one sun.

**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/$TiO_2$ and FTO/$TiO_2$/$MAPbI_3$ structures. Unexpected surface states on the top of $TiO_2$ layer are inferred by the combination of theoretical computation and experimental results. The basic applications of KPFM under illumination are analyzed as well.**

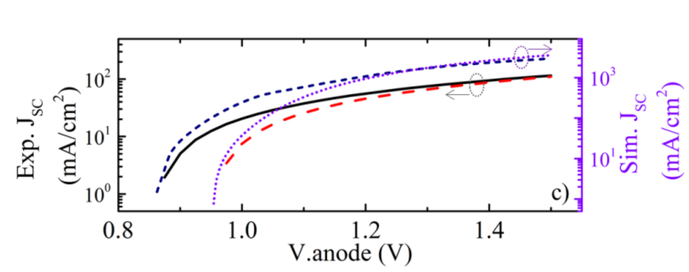
## $V_{oc}$ Losses in PSCs

*Yong HUANG et al , NUSOD international conference (2017)*

a) Experimental J-V properties of $TiO_x$/$MAPbI_3$/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.




* *Experimental results from Xlim, Limoge* [5]




**The $V_{OC}$ loss of standard $TiO_x$/$CH_3NH_3PbI_3$/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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