Fabrication and characterization of perovskite solar cells using metal phthalocyanines and naphthalocyanines

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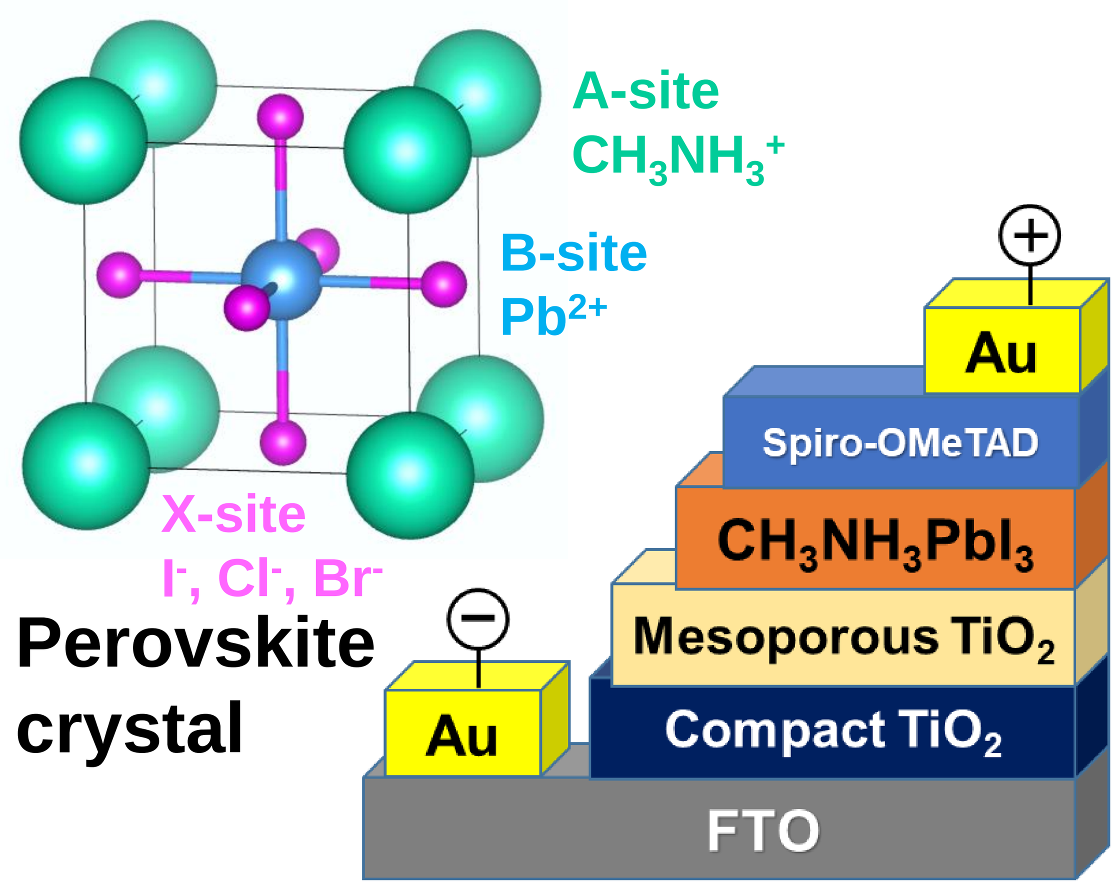
INTRODUCTION

Perovskite solar cell

Photoelectric characteristics
Crystal structures, elements
⇒ Performance control
Subject: Stability of performance



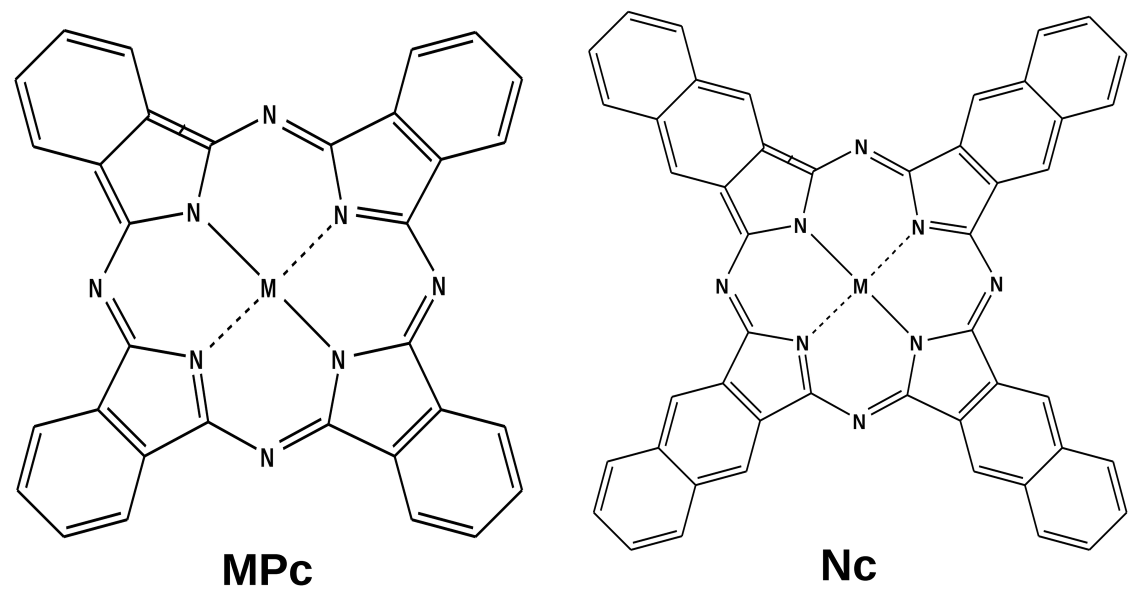
Perovskite solar cell

Hole-transporting materials

Conventional hole-transporting materials
Spiro-OMeTAD: Dopant needed, reducing
Durability ⇒ Performance graduated

Metal phthalocyanine (MPc)
Naphthalocyanine (Nc)

Semi-conductive materials
Heat and weather resistance, Low cost
Central metal and chemical groups
⇒ Control of *Eg* and wavelength

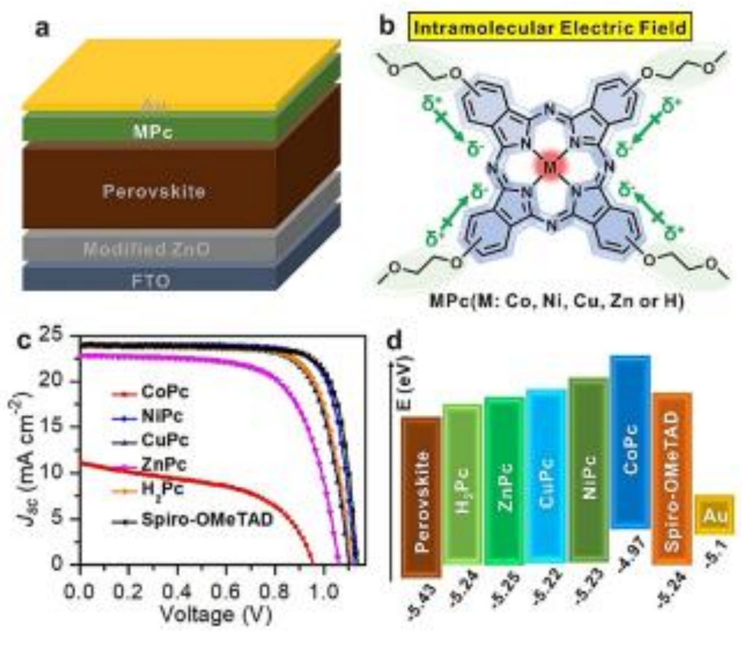


Molecular structure of MPc and Nc

Purpose

Incorporation of MPc and Nc in the perovskite solar cells are investigated to improve the photovoltaic properties and stability of performance.

Additive effect of MPs



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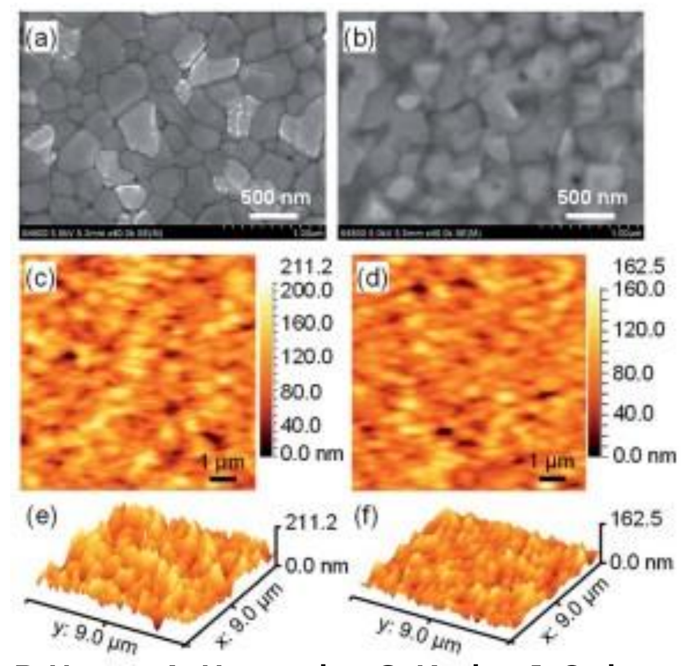

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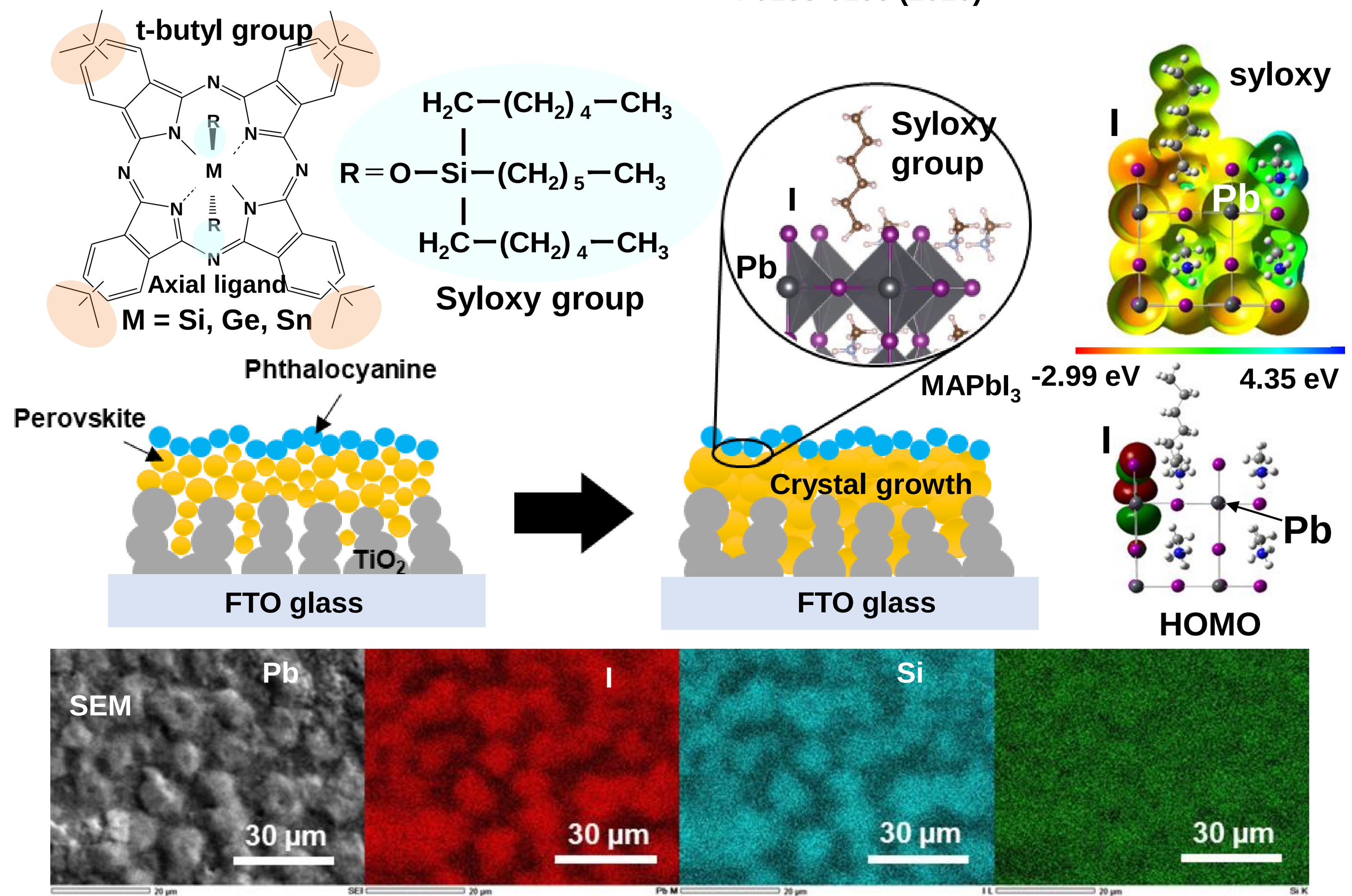

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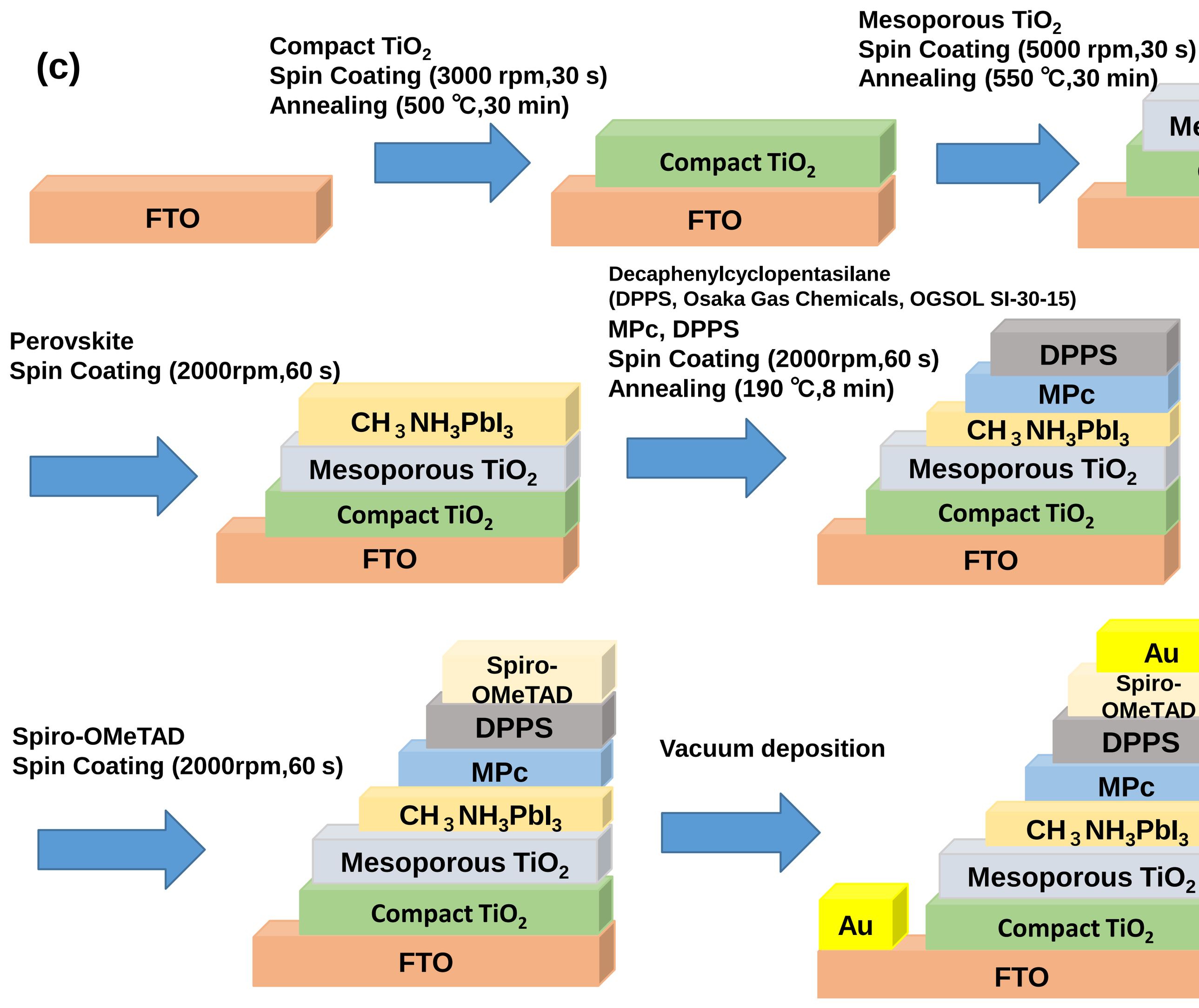
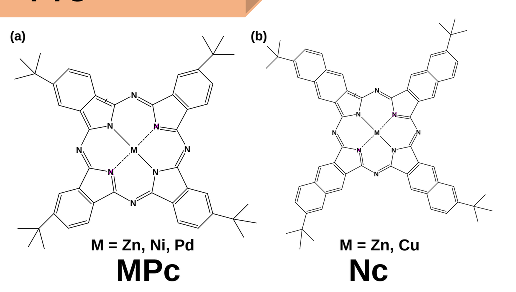
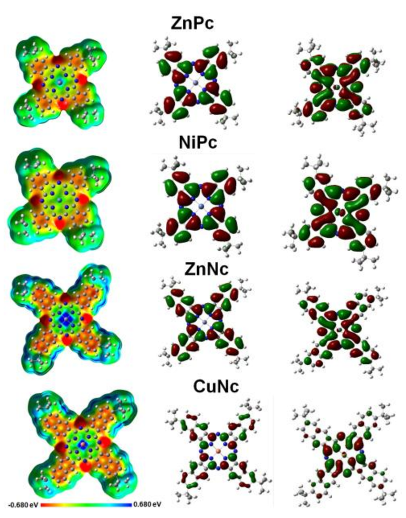
EXPERIMENTS



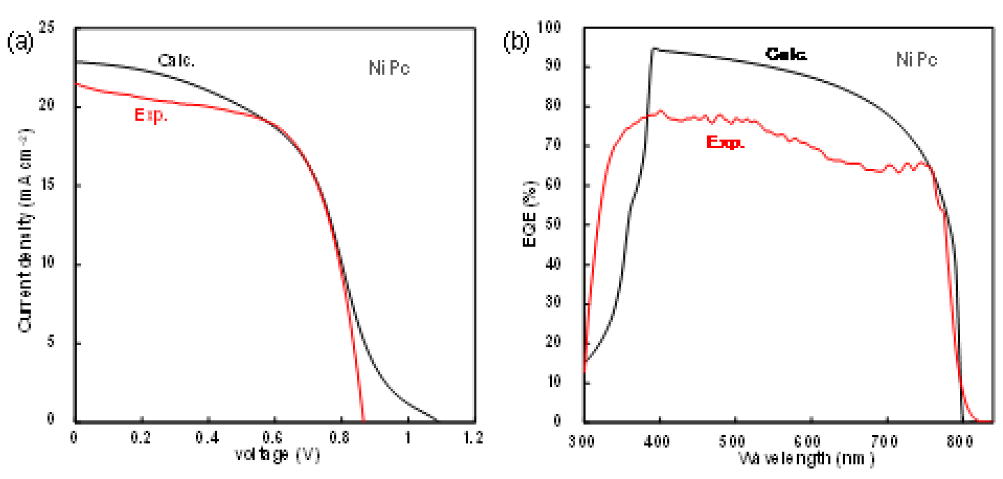


t-butyl metal phthalocyanine (MPc)
t-butyl naphthalocyanine (Nc)

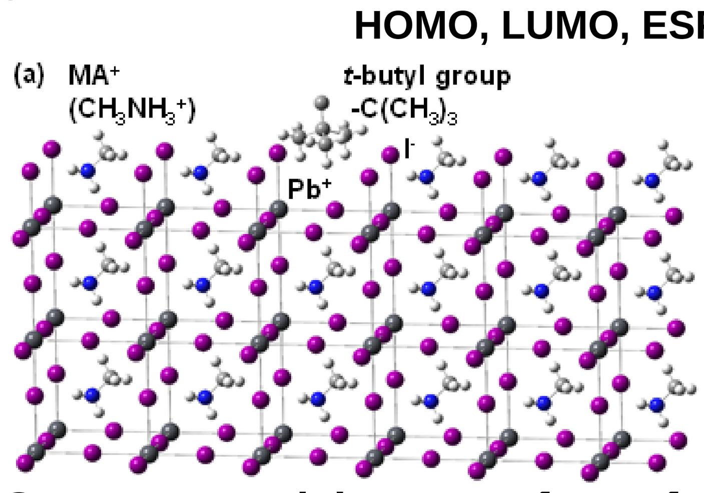
Fabrication of $MAPbI_3$ perovskite solar cell using MPc and Nc



HOMO, LUMO, ESP



(a) Calculated *J-V* characteristics and (b) EQE of the perovskite solar cell using NiPc

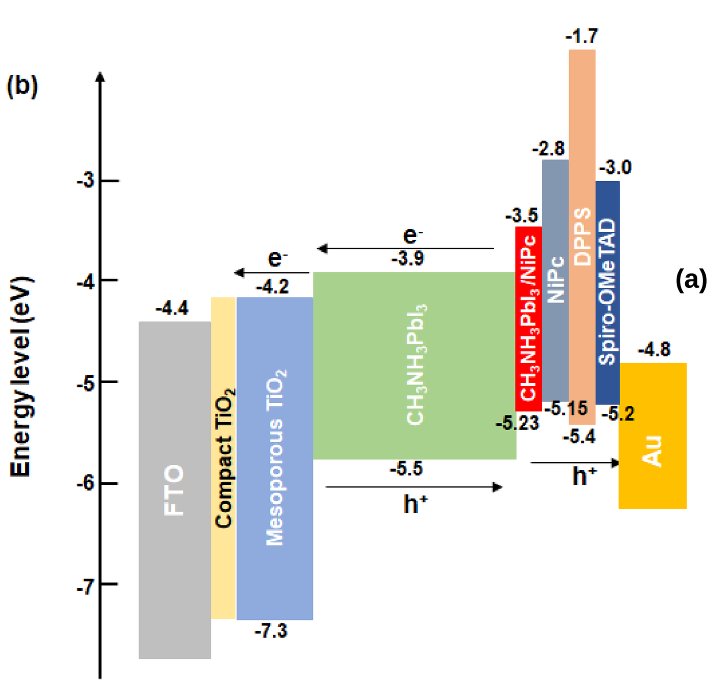


Structure model near surface of the $MAPbI_3$ with *t*-butyl group.

Experimental and calculated results by SCAPS-1D

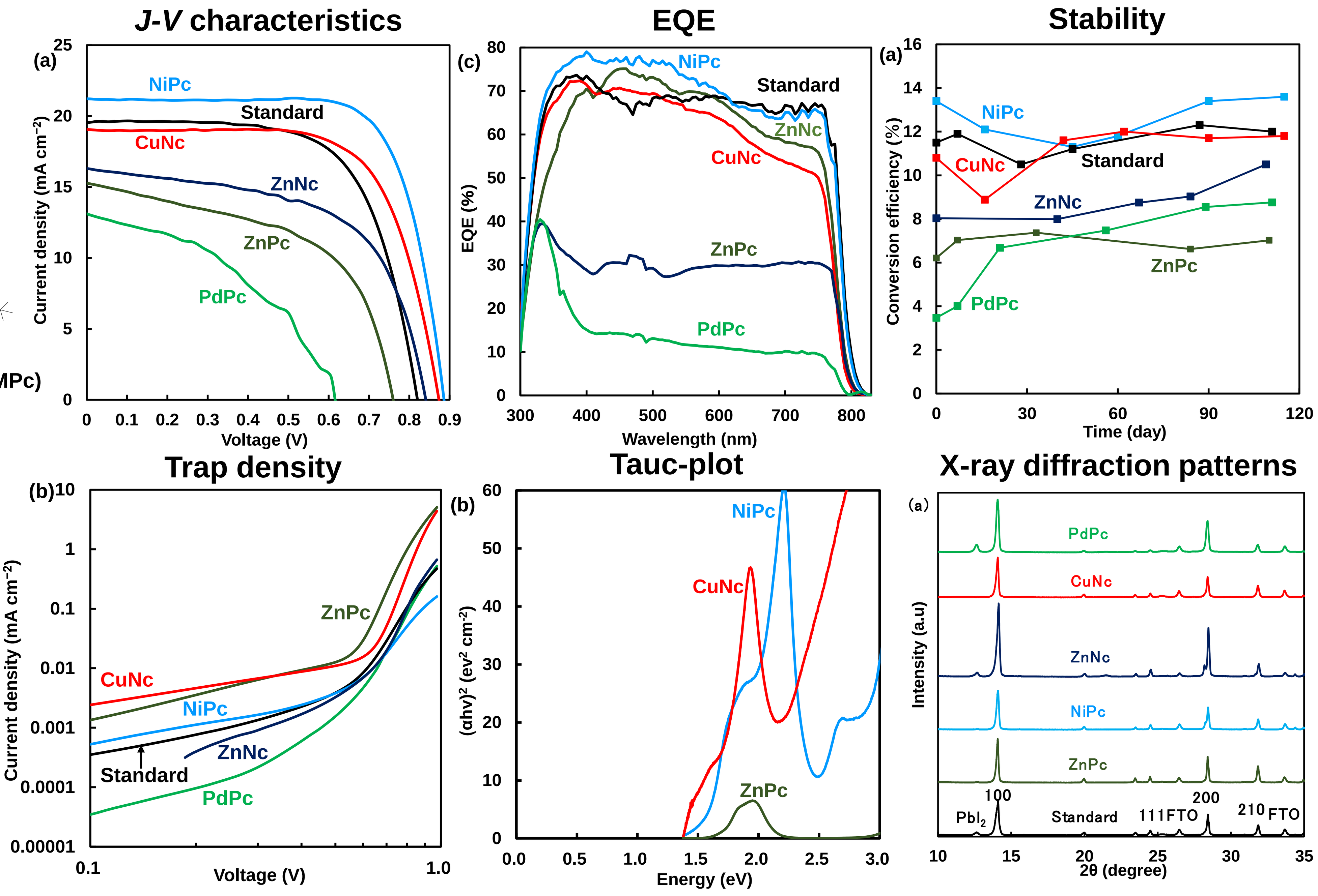
NiPc	*Voc* (V)	*Jsc* (mA cm^{-2})	*FF*	*η* (%)
Exp.	0.865	21.5	0.627	11.6
Calc.	1.092	22.9	0.463	11.6

	FTO	TiO_2	$MAPbI_3$	NiPc	Spiro-OMeTAD
Thickness (nm)	250	400	500	60	100
Bandgap (eV)	3.50	3.2	1.55	1.70	2.9
Electron affinity (eV)	4.40	4.00	3.75	3.06	2.2
Dieelectric permittivity (relative)	9.00	100	22.0	6.392	3.0
CB effective density of state (1/cm^3)	2.2×10^{18}	1.0×10^{20}	3.1×10^{18}	2.5×10^{20}	2.5×10^{20}
VB effective density of state (1/cm^3)	1.8×10^{19}	1.0×10^{20}	3.1×10^{18}	2.5×10^{20}	2.5×10^{20}
Electron thermal velocity (cm/s)	1.0×10^{7}	1.0×10^{7}	1.0×10^{7}	1.0×10^{7}	1.0×10^{7}
hole thermal velocity (cm/s)	1.0×10^{7}	1.0×10^{7}	1.0×10^{7}	1.0×10^{7}	1.0×10^{7}
Electron mobility (cm/V s)	2.0×10^{3}	50	7.80	1.23×10^{-4}	3.5×10^{-4}
Hole mobility (cm/V s)	1.0×10^{2}	50	7.80	4.97×10^{-2}	4.0×10^{-3}
Donor density (1/cm^3)	2.0×10^{19}	1.0×10^{18}	0	0	0
Acceotor density (1/cm^3)	0	0	1.0×10^{16}	1.0×10^{18}	1.0×10^{19}
Defect density (1/cm^3)	1.0×10^{15}	1.5×10^{17}	9.3×10^{15}	1.0×10^{15}	1.0×10^{16}



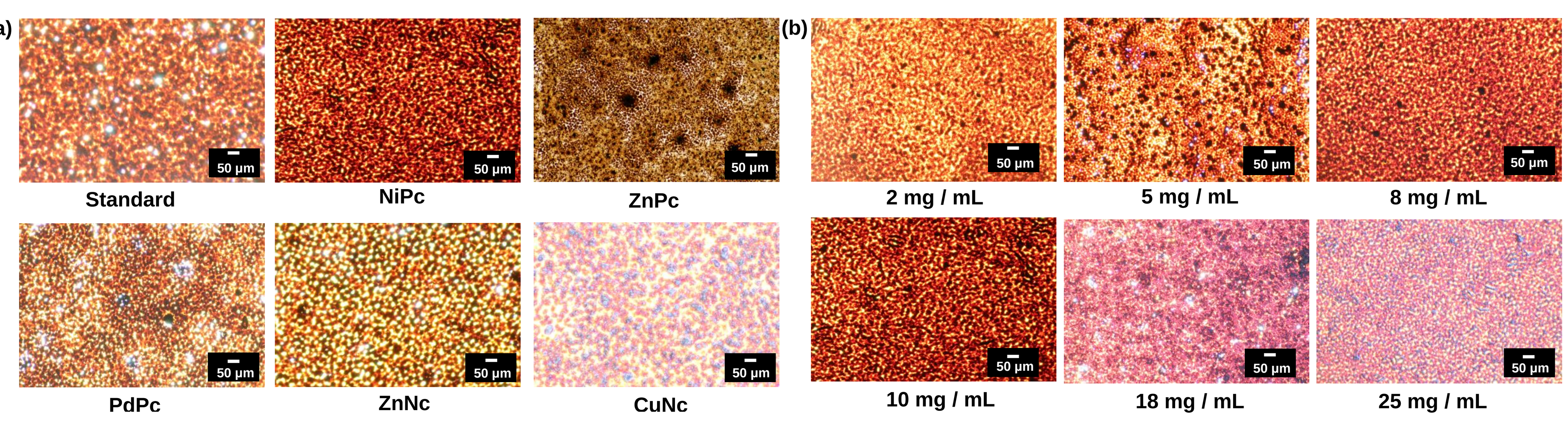
Energy levels of the solar cells using NiPc.

RESULTS & DISCUSSION



Photovoltaic parameters, trap density and crystal parameters

Devices	J_{sc} (mA cm^{-2})	*Voc* (V)	*FF*	R_s (Ω cm^2)	R_{sh} (Ω cm^2)	*η* (%)	η_{ave} (%)	V_{TFL} (V)	D_{trap} (×10^{16} cm^{-3})	Lattice constant (Å)	Crystallite size (Å)	I_{100} / I_{210}
$MAPbI_3$	19.5	0.802	0.664	3.67	7450	10.7	9.03	0.475	0.986	6.274 (1)	429.9	3.21
+NiPc	21.1	0.885	0.726	2.58	38900	13.4	11.5	0.448	0.930	6.274 (1)	451.7	3.54
+ZnPc	15.3	0.760	0.535	3.48	327	6.71	4.70	0.553	1.11	6.274 (2)	506.4	3.30
+PdPc	13.1	0.615	0.430	3.28	209	3.47	2.88	0.501	1.04	6.274 (2)	451.7	4.50
+CuNc	19.1	0.873	0.689	4.45	7790	11.4	9.33	0.527	1.09	6.278 (1)	536.6	3.18
+ZnNc	16.3	0.840	0.586	3.09	306	8.03	5.64	0.659	1.37	6.275 (1)	506.1	5.48



(a) Optical microscopy images of the $MAPbI_3$ layers with MPc and Nc. (b) Effect of the amount of NiPc

CONCLUSION

The photovoltaic performance using NiPc reached *η* at 13.4 %. Incorporation of NiPc passivated the $MAPbI_3$ layer, yielding the crystal growth and optimization with tunning the energy levels near HOMO of NiPc, supporting charge transfer from VB of $MAPbI_3$ to HOMO of NiPc.