Additive effect of ytterbium and neodymium for efficient and stable $CH_3NH_3PbI_3$ perovskite solar cells

THE UNIVERSITY OF SHIGA PREFECTURE
OSAKA GAS CHEMICALS

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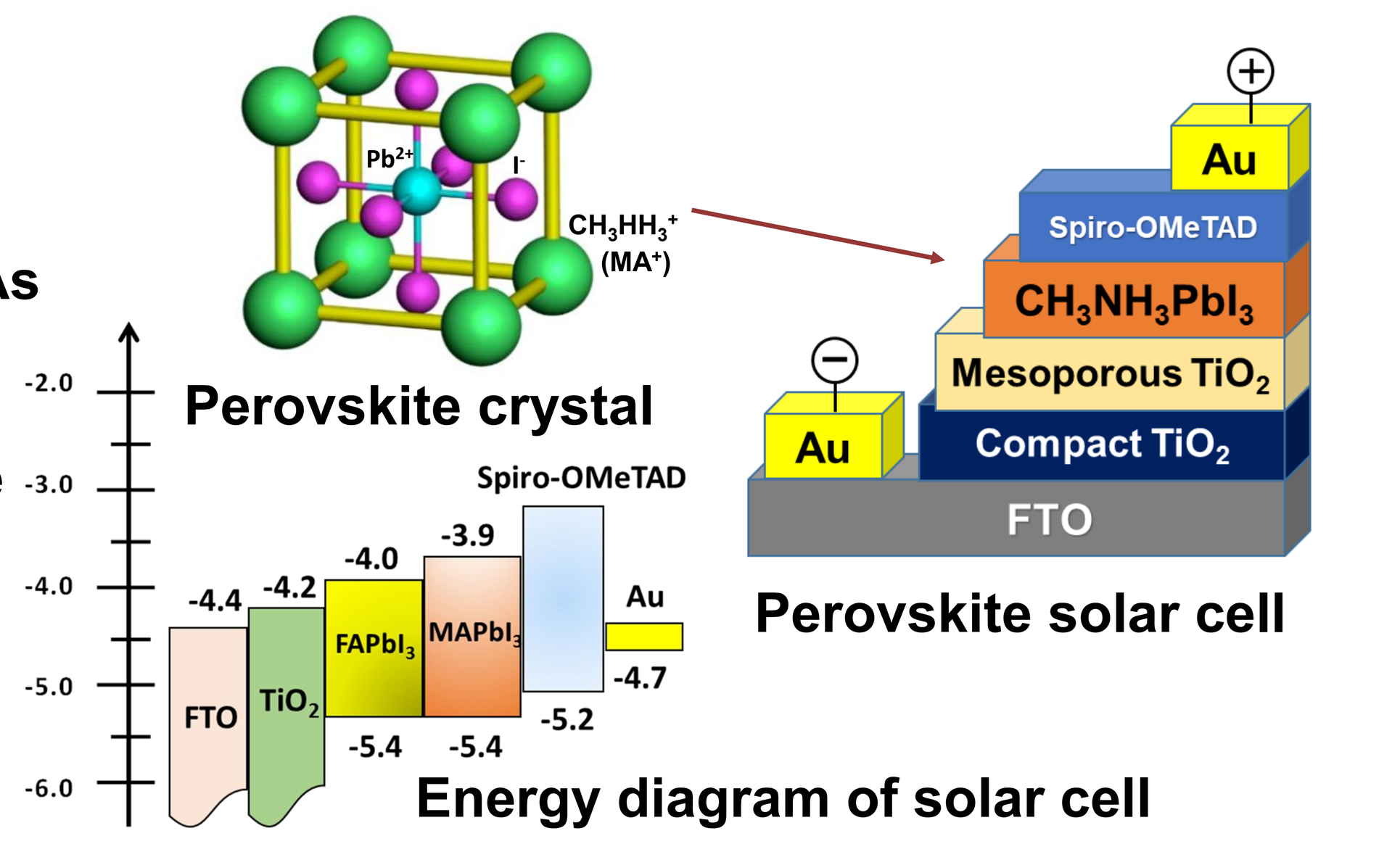
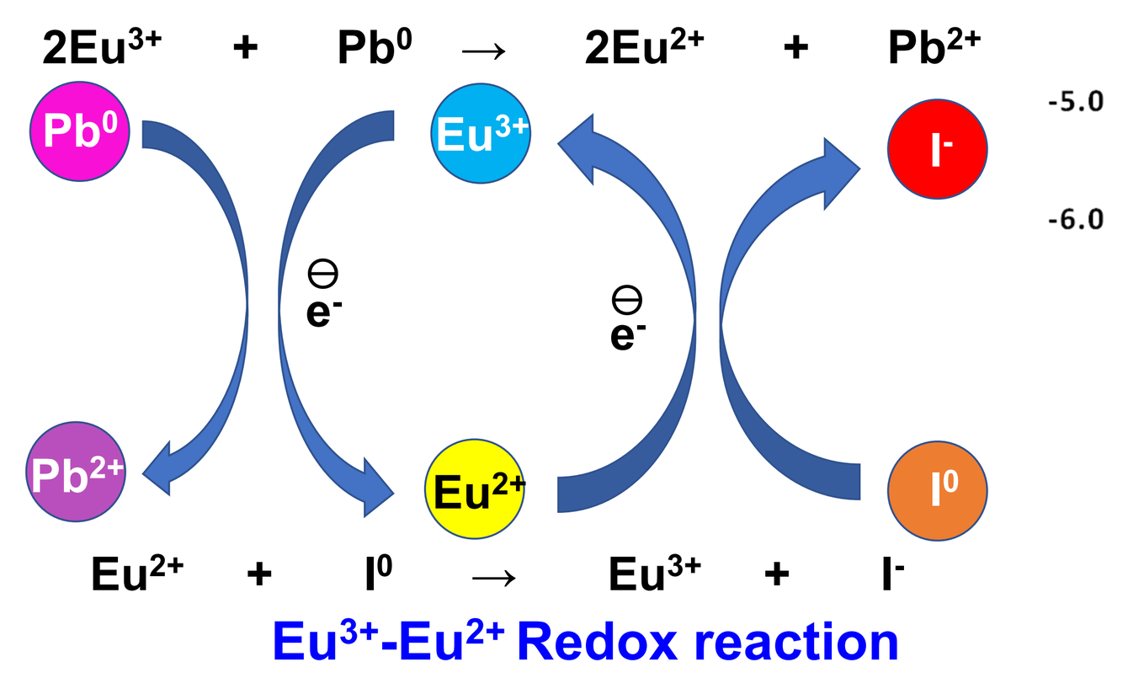
INTRODUCTION & AIM

Perovskite solar cell

Crystal structure, mole ratio
V_{oc} > 1.0 V Si, E_g ≈ 1.6 eV,
Conversion efficiency η ≈ Si, GaAs
Wavelength (300 - 800 nm)
Easy fabrication process
Decomposition in air atmosphere
Subject: Stability





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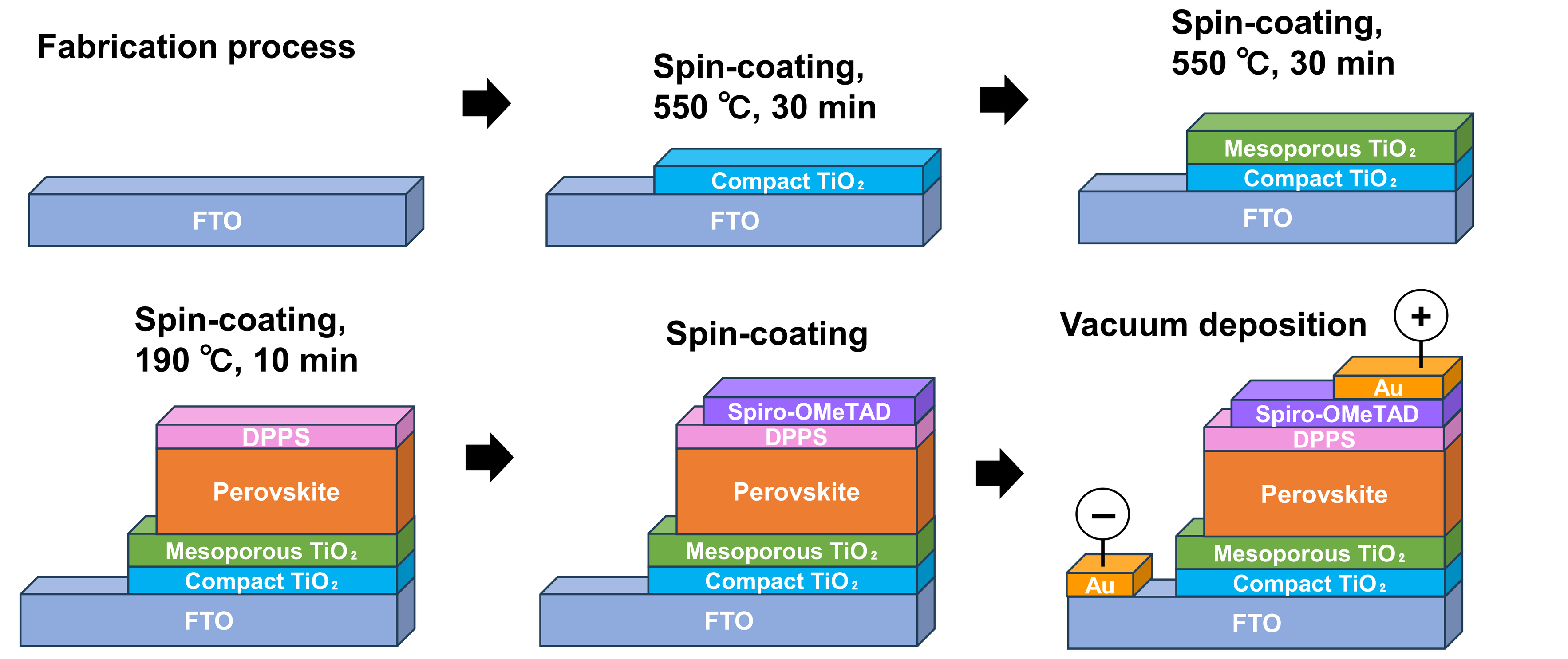
Lanthanide: Eu (III), Sm (III), Tb (III), Gd (III), Nd (III), Yb (II)

Ln-doped $CsPbX_3$
Ln-double perovskite crystal
Subject: band gap expansion

Optical and photovoltaic application

AIM Co-additive affect of Yb/Nd on photovoltaic properties of perovskite solar cell

METHOD

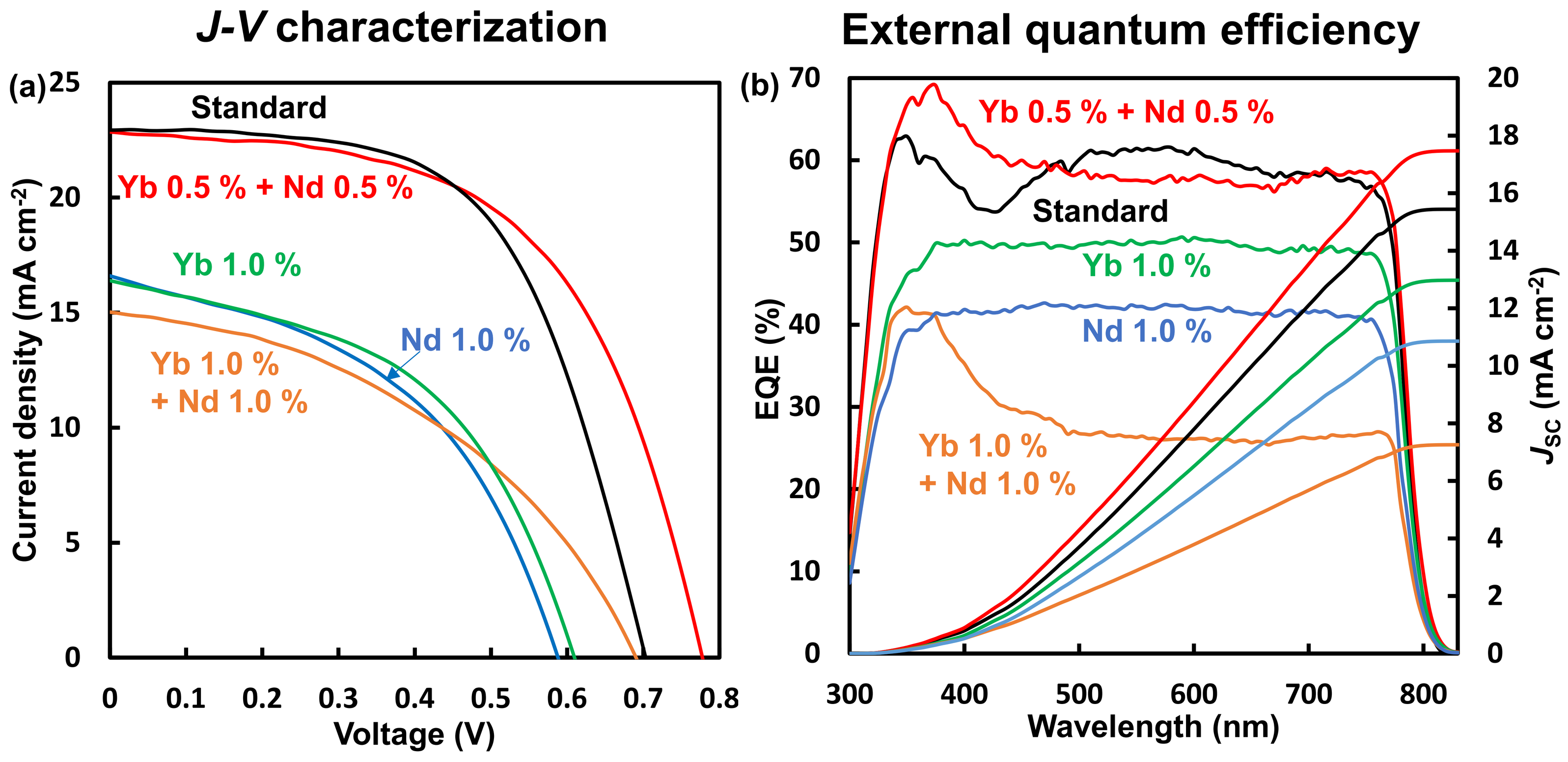


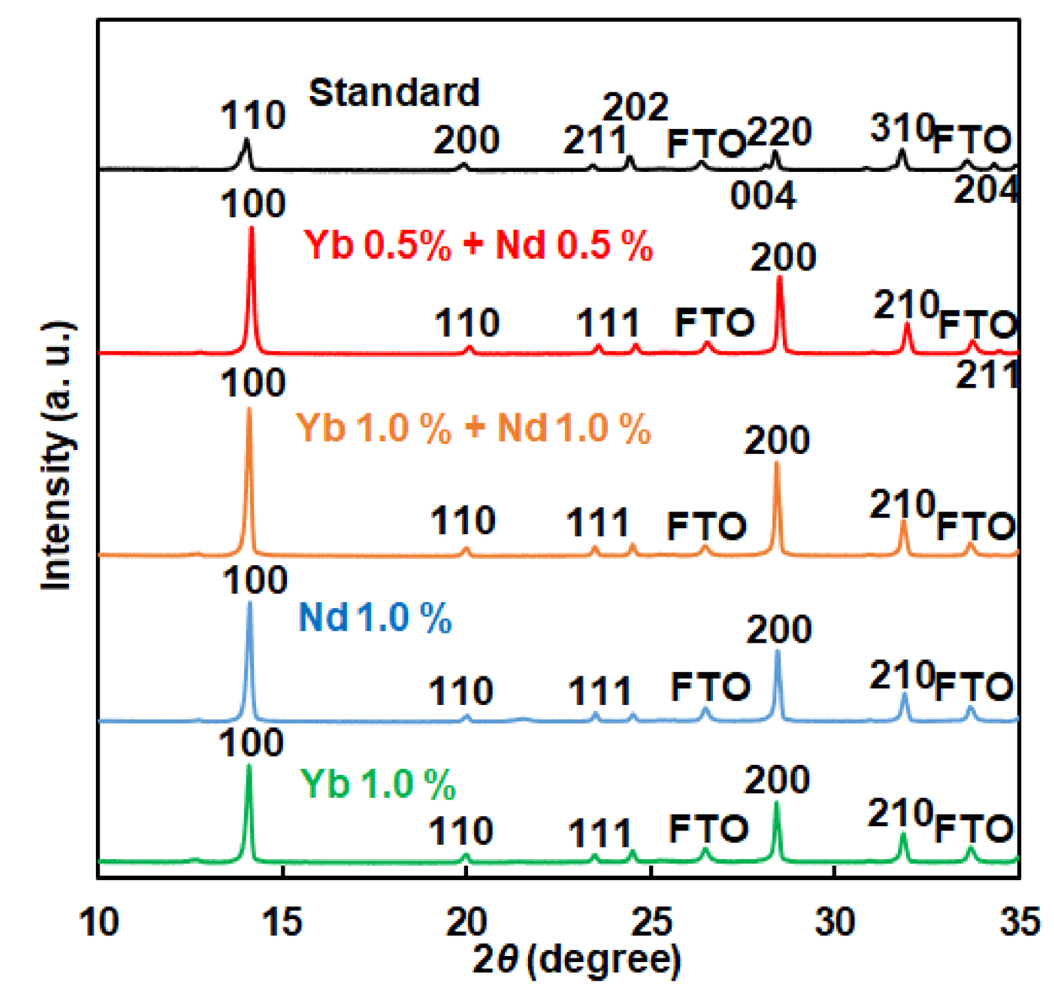
DPPS: Decaphenylcyclopentasilane (Osaka Gas Chemicals Co. Ltd, SI-30-15)

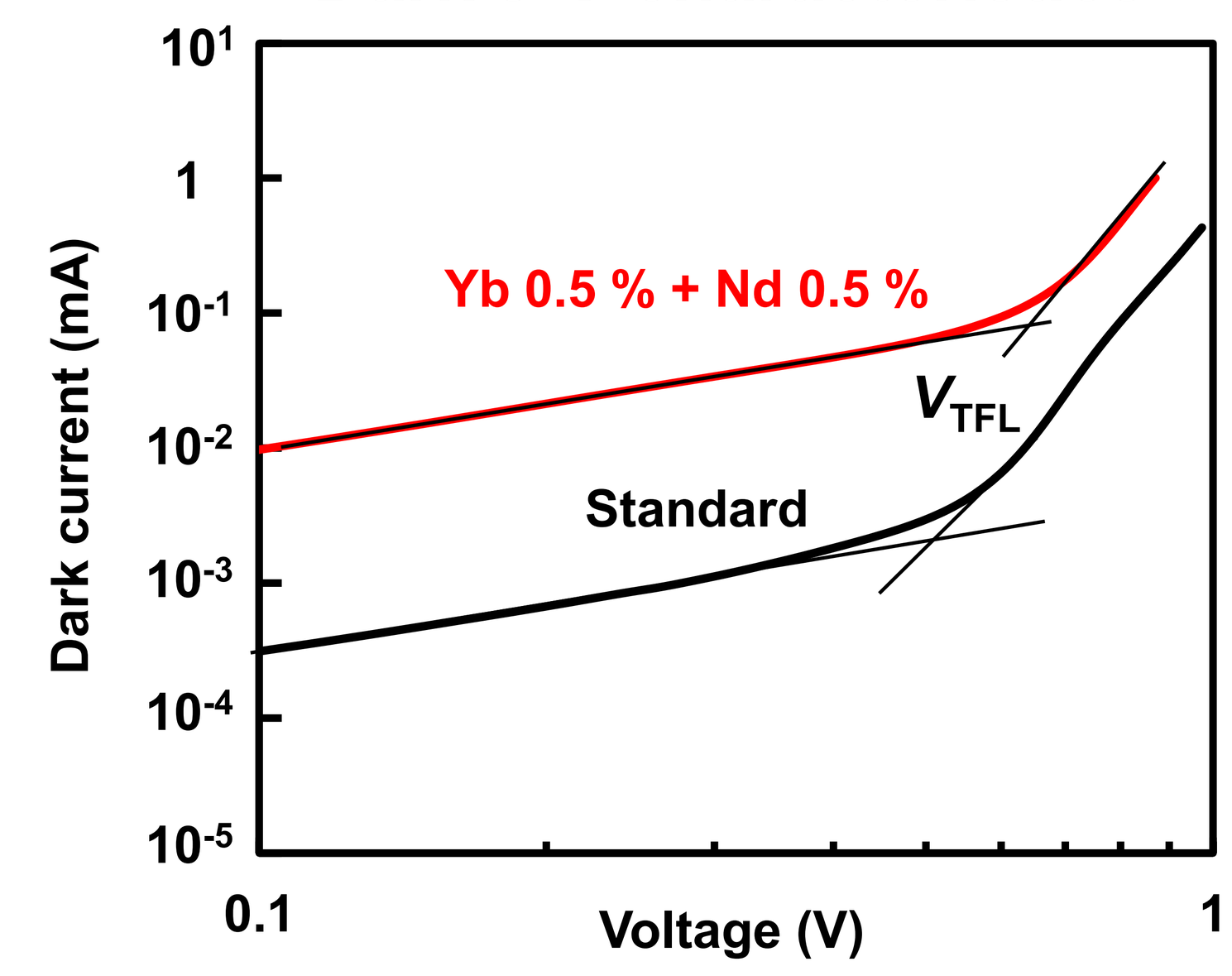
Experiments and calculation

Photovoltaic characterization (San-ei Electric XES-3015, Enlitech QE-R3011)
X-ray diffraction pattern (Bruker AXS D2 PHASER), SEM/EDX (SEM, Jeol, JSM-6010PLUS/LA)
First-principles calculation (Quantum Espresso), Device simulation (SCAPS-1D)

RESULTS & DISCUSSION







Photovoltaic parameters of the doped perovskite solar cells.

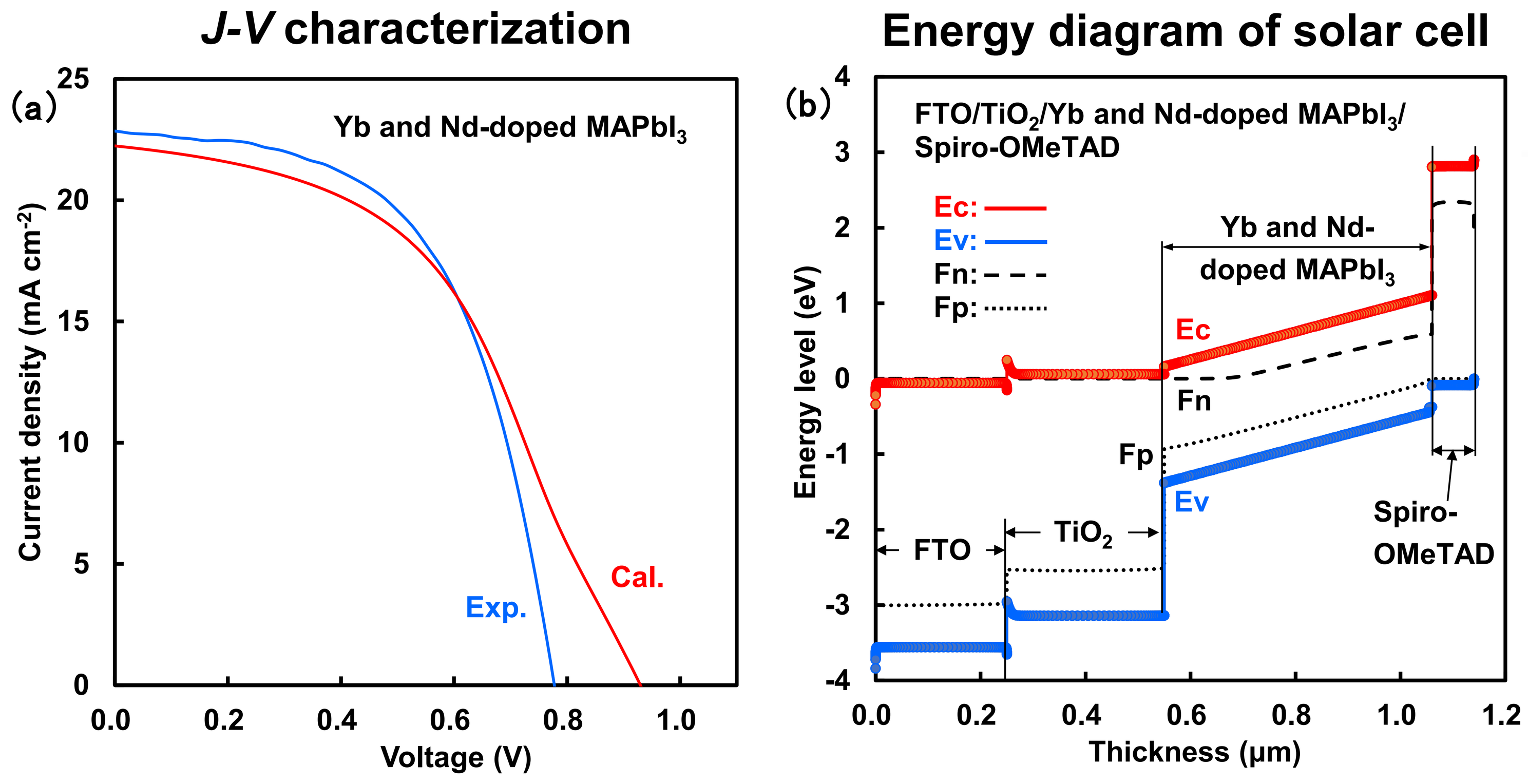
Device	J_{SC} (mA cm^{-2})	V_{OC} (V)	FF	R_s (Ω cm^2)	R_{sh} (Ω cm^2)	η (%)	η_{ave} (%)	E_g (eV)
Standard	22.9	0.702	0.588	7.42	3250	9.49	7.55	1.55
Yb 0.5 %, Nd 0.5 %	22.8	0.777	0.562	6.35	585	10.0	7.19	1.54
Yb 1.0 %, Nd 1.0 %	16.4	0.609	0.486	2.80	140	4.85	3.69	1.54
Nd 1.0 %	16.6	0.588	0.458	3.00	117	4.47	3.60	1.54
Yb 1.0 %	15.0	0.690	0.458	2.02	217	4.36	3.98	1.54

Measured crystal parameters of the doped perovskite compounds.

Device	Lattice constant (Å)	V (Å^3)	I_{110}/I_{310} I_{100}/I_{210}	Crystallite size (Å)
Standard	a = 8.872(2), c = 12.667(3)	997.0	1.4	380
Yb 0.5 %, Nd 0.5 %	6.248(5)	243.9	4.2	671
Yb 1.0 %, Nd 1.0 %	6.279(2)	247.6	4.1	704
Nd 1.0 %	6.270(0)	246.5	4.3	640
Yb 1.0 %	6.284(2)	248.1	3.4	659

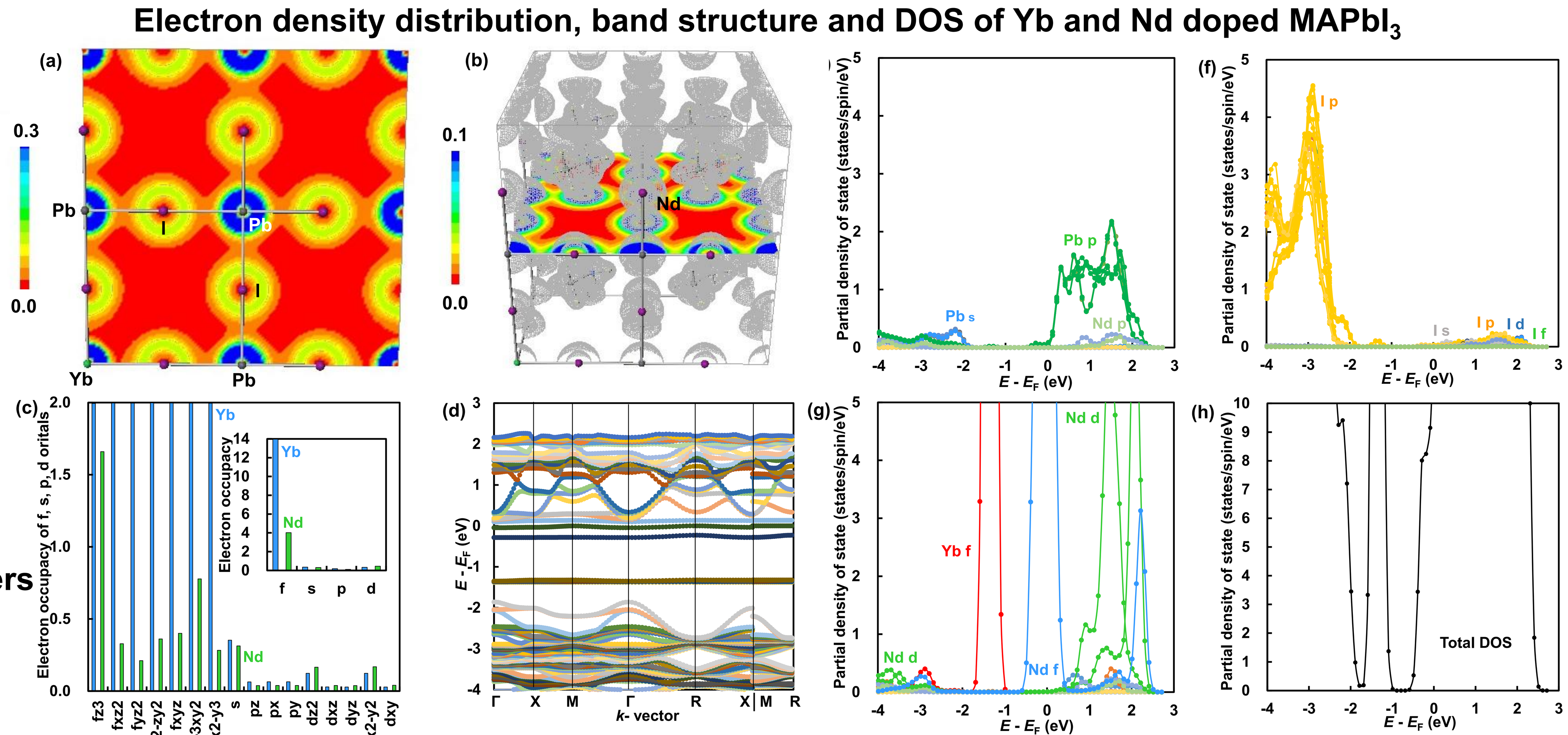
Trap-filled limited voltages (V_{TFL}), and trap density (D_{trap})

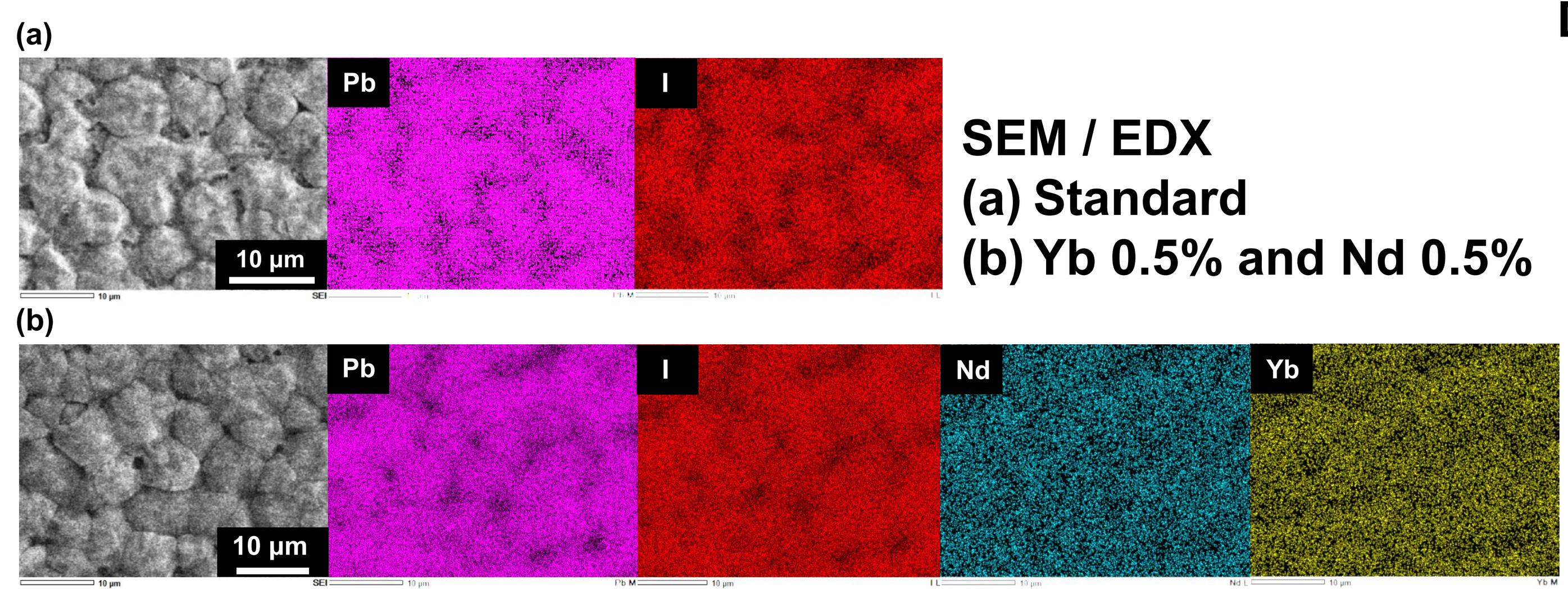
Devices	V_{TFL} (V)	D_{trap} (cm^{-3})
Standard	0.50	1.04 × 10^{16}
Yb 0.5 % + Nd 0.5 %	0.63	1.31 × 10^{16}



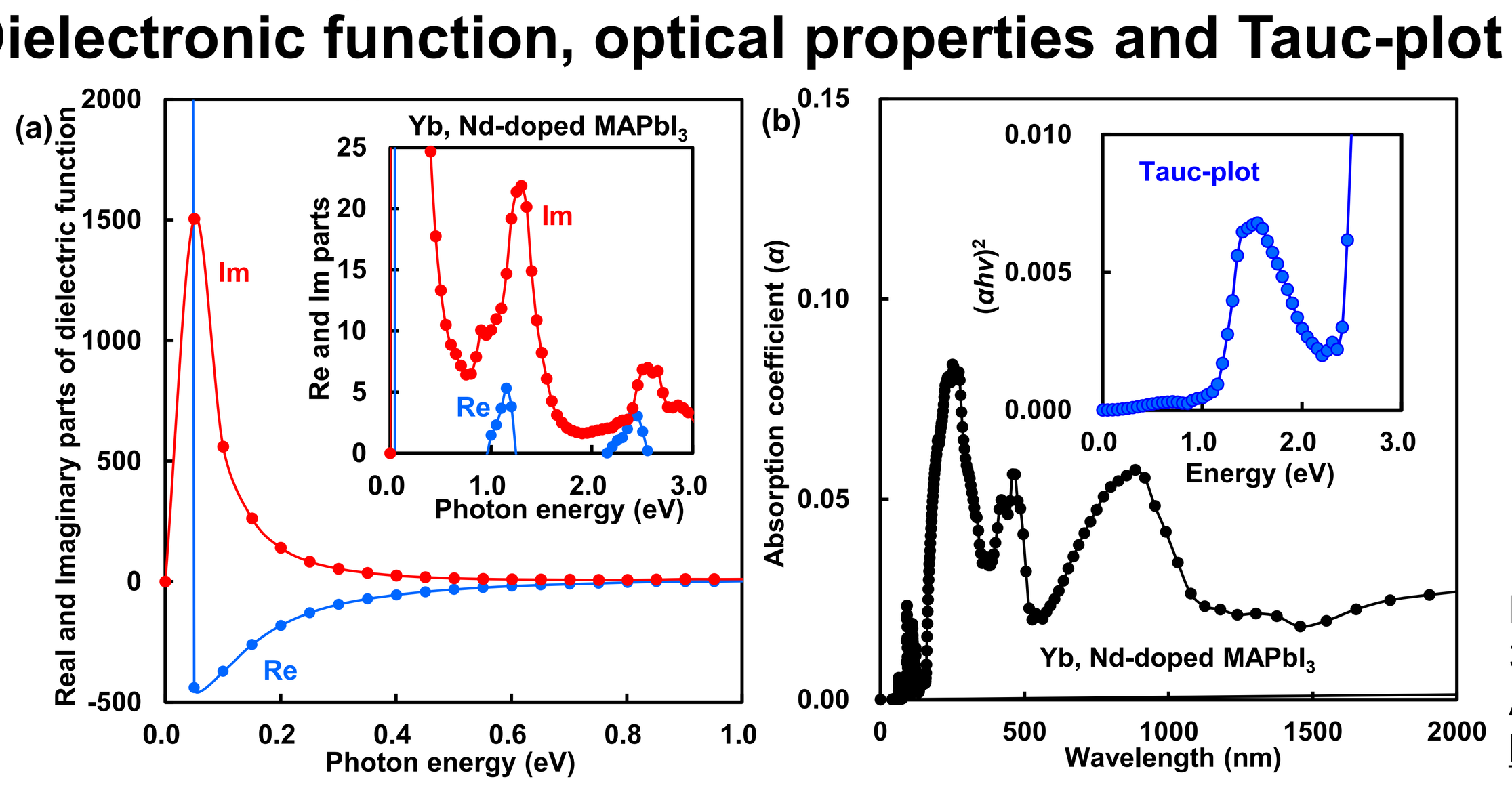
Calculated and experimental results on the photovoltaic parameters

	J_{SC} (mA cm^{-2})	V_{OC} (V)	FF	η (%)
Calculated	22.2	0.930	0.472	9.77
Experiments	22.8	0.777	0.562	10.0





SEM / EDX
(a) Standard
(b) Yb 0.5% and Nd 0.5%



CONCLUSIONS

Addition of Yb^{3+} and Nd^{3+} improved η, crystal orientation and growth, while preventing defect and recombination near the interface.

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