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A Lateral Heterojunction Device as a Tool to Study Perovskite-Based Solar Cells

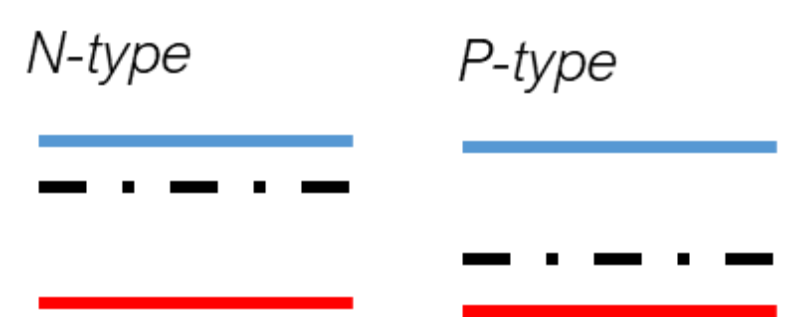
Scope of the work

Study the perovskite (PSK) properties on top of different substrates:

- Surface work function (WF);
- Defect and ion properties;

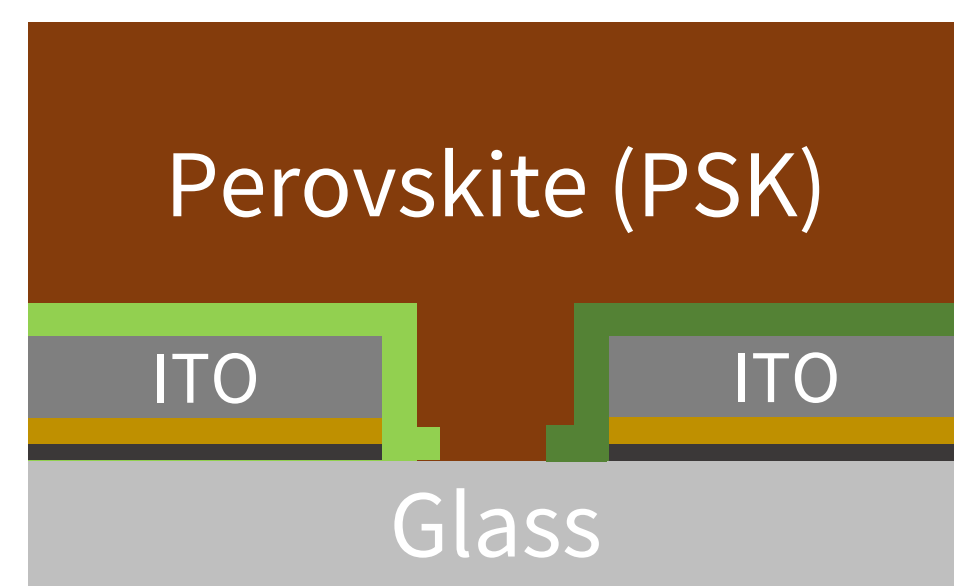
Previous knowledge:

Perovskite WF dependence on the substrate WF



ACS Energy Lett. 2019, 4, 1-7
 S. P. Dunfield et al., (2021).

Cross section view



Previous device allowed to fix an upper limit of the doping density in the PSK layer:

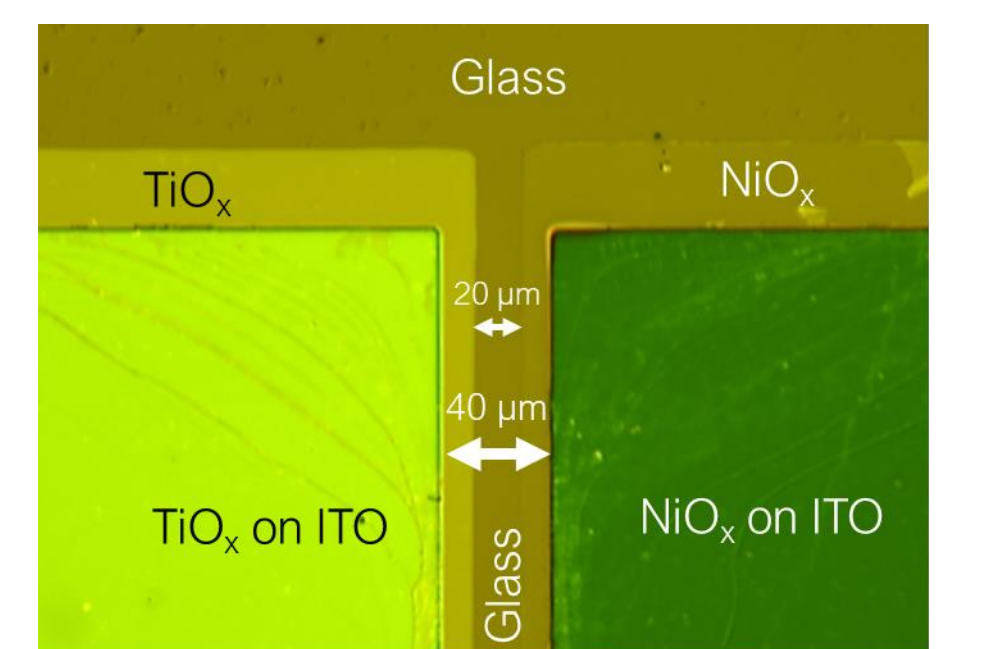
$$N_{\text{dop}} \leq 10^{12} \text{ cm}^{-3}$$

LHJ structure and fabrication

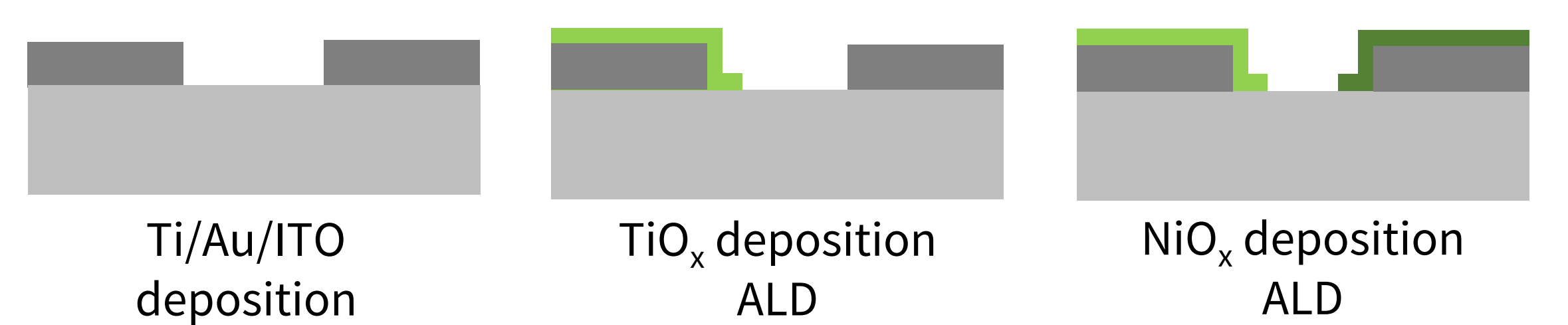
3 photolithography steps to deposit:

- Contact layer: Ti (adhesion to glass) / Au (high conductivity) / ITO (PSK protection);
- Electron transport layer: TiO_x ;
- Hole transport layer: NiO_x .

Top view (optical microscope image)

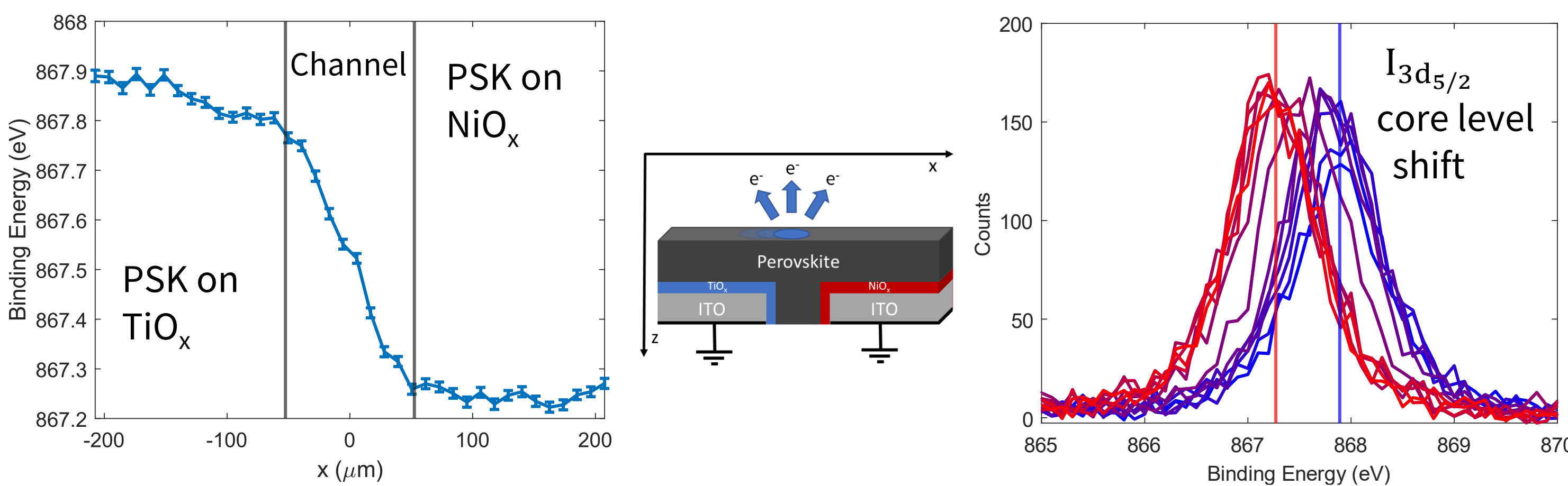


Cross section view



XPS equilibrium characterization

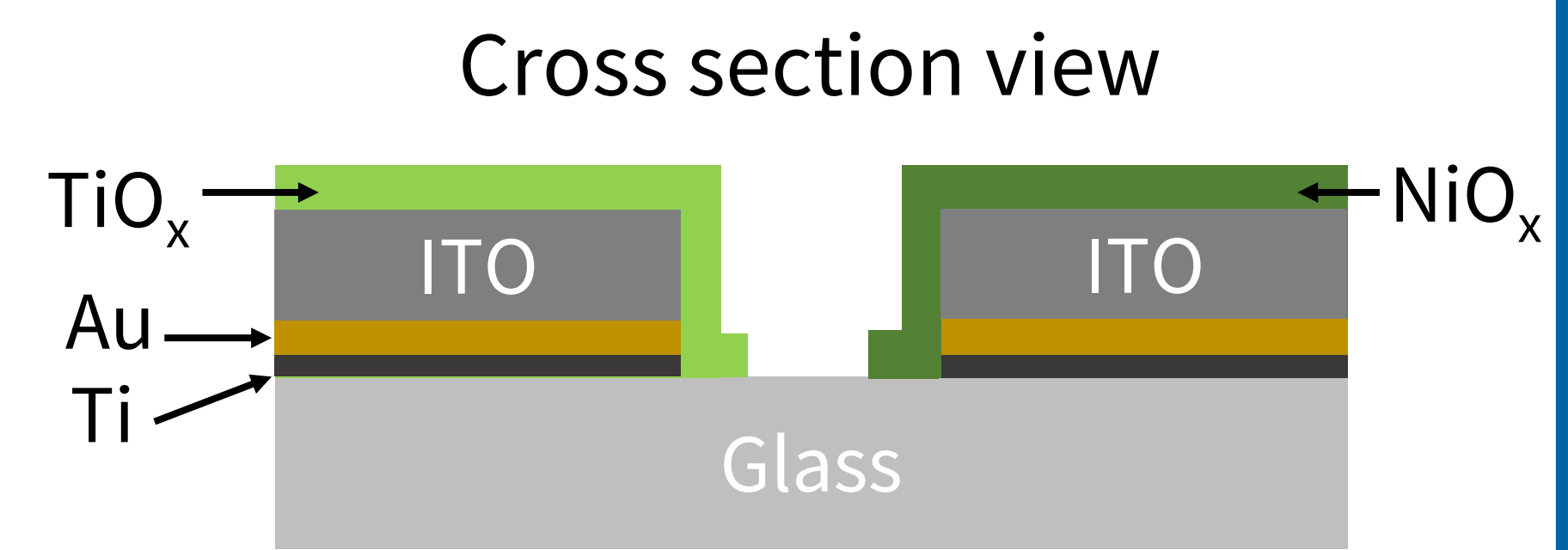
The scan of the X-ray electron collection area (with 10 μm diameter) along the PSK surface, from the TiO_x to the NiO_x side revealed an iodine core level shift of 650 meV, in agreement with the WF difference between the TiO_x and the NiO_x surface.



KPFM substrate characterization

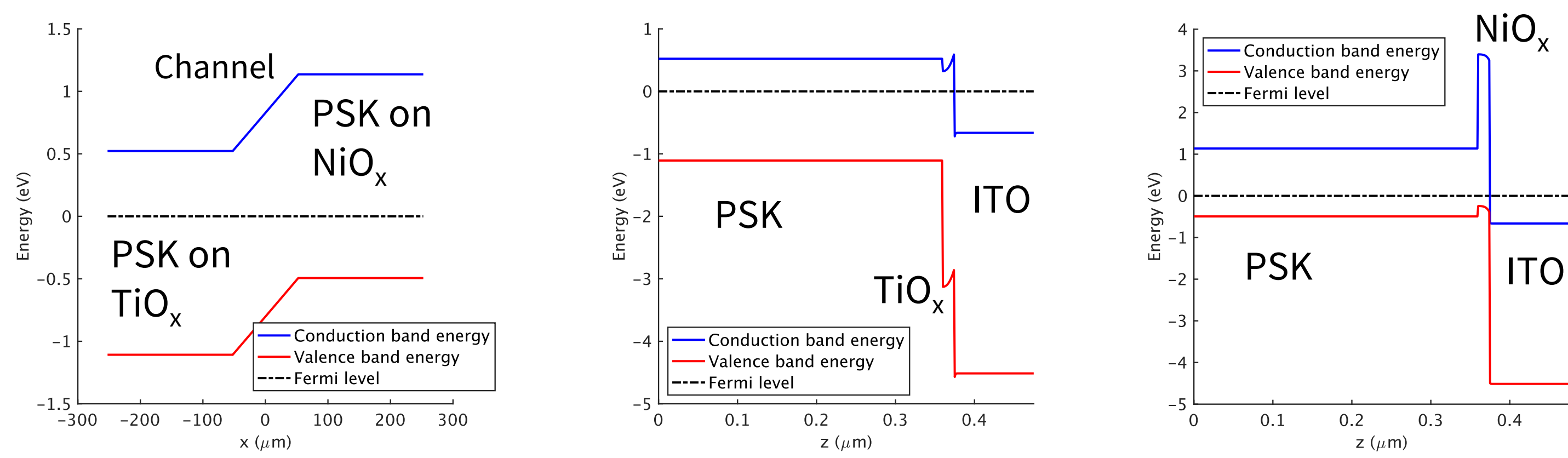
Work functions (KPFM)

ITO	4.95 eV
NiO_x	≥ 5.10 eV
TiO_x	≤ 4.50 eV

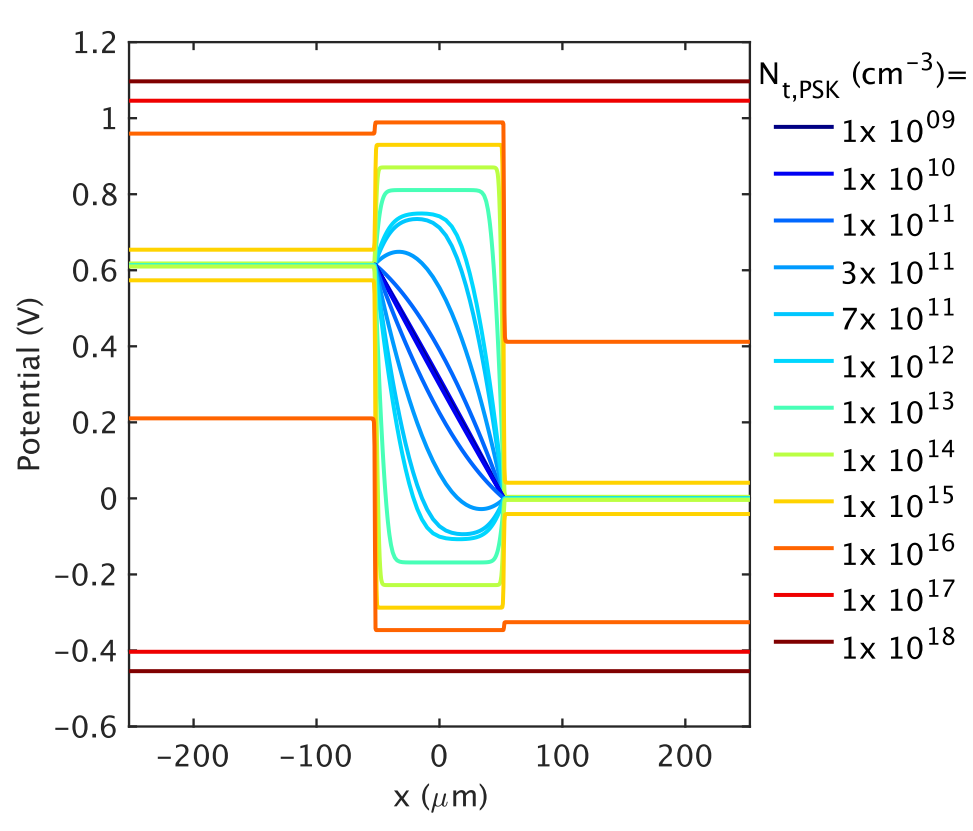


$$\Delta_{WF} = WF_{\text{NiO}_x} - WF_{\text{TiO}_x} \geq 0.6 \text{ eV}$$

Drift-Diffusion model: band diagrams for intrinsic perovskite



Actual Potential

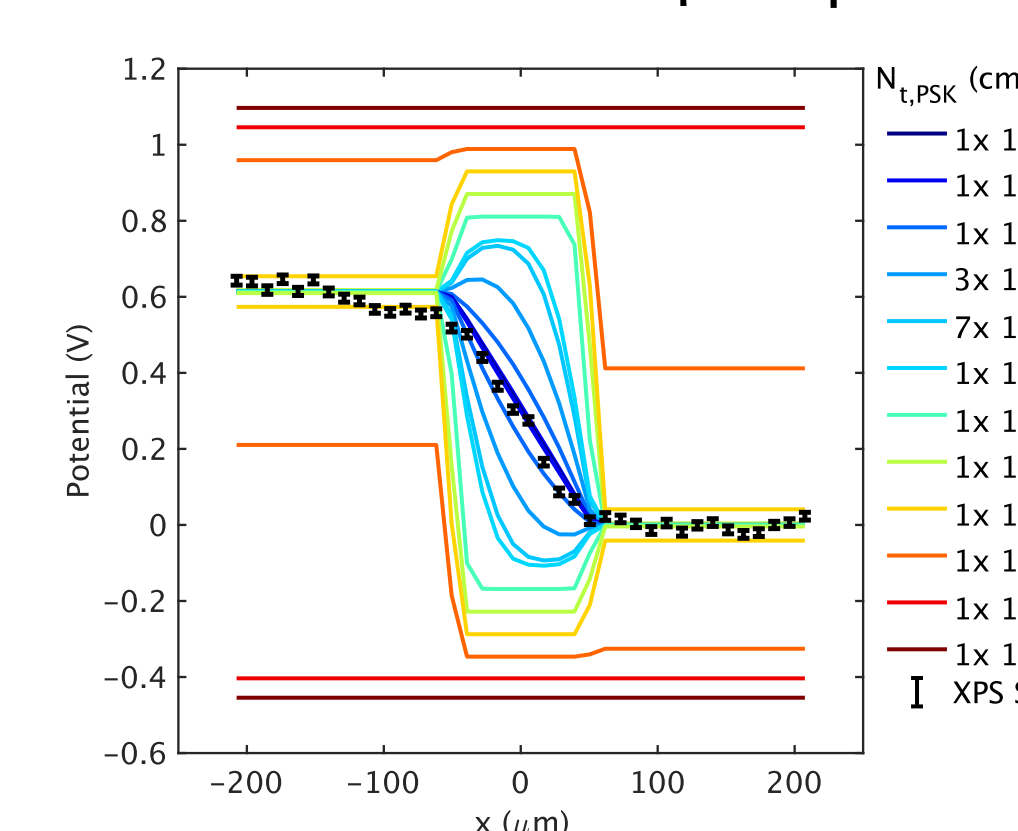


Surface Potential as a function of PSK doping density

Conclusion:

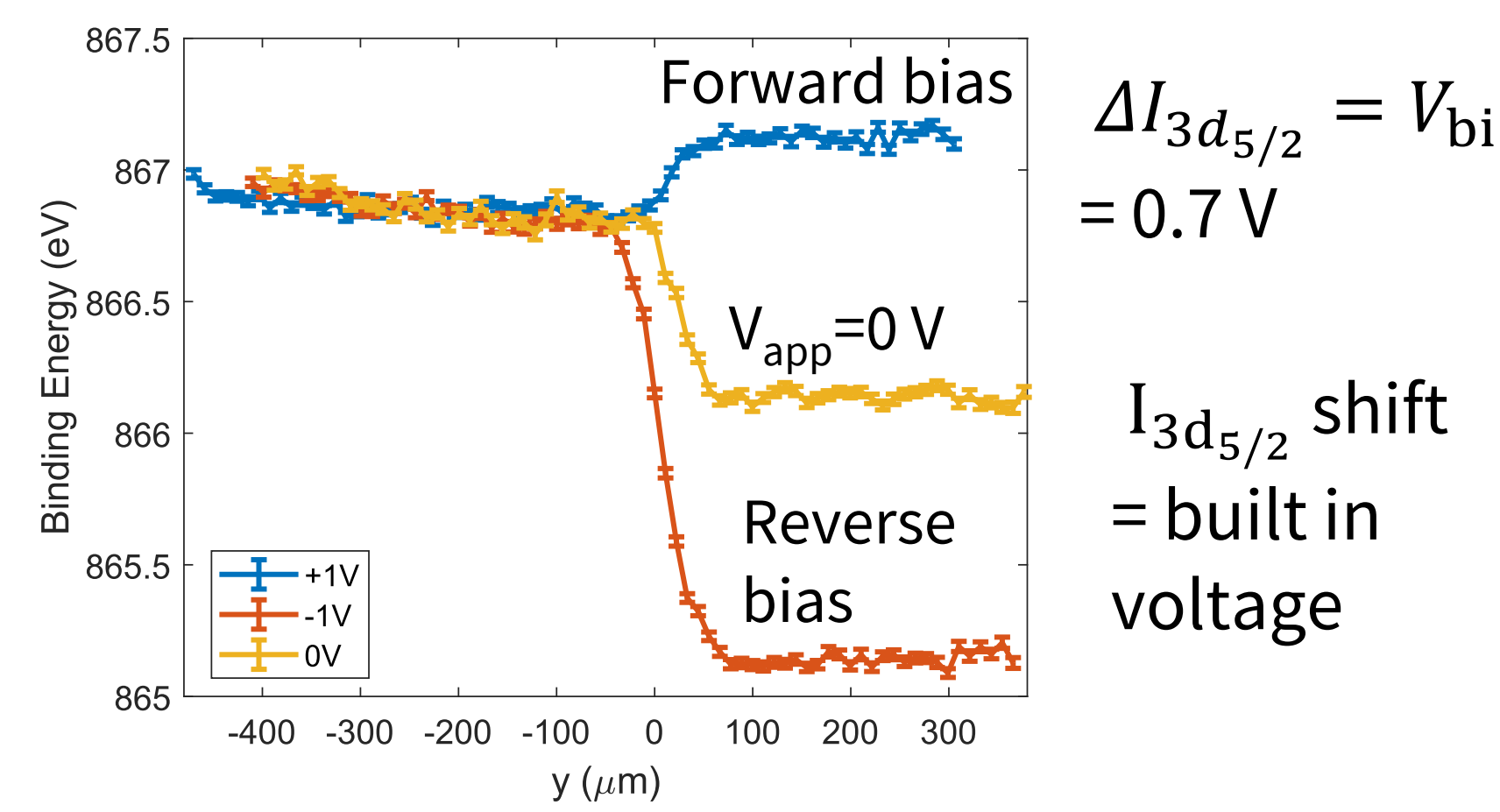
$$N_{\text{dop}} \leq 10^{11} \text{ cm}^{-3}$$

Convolution with 10 μm spot size

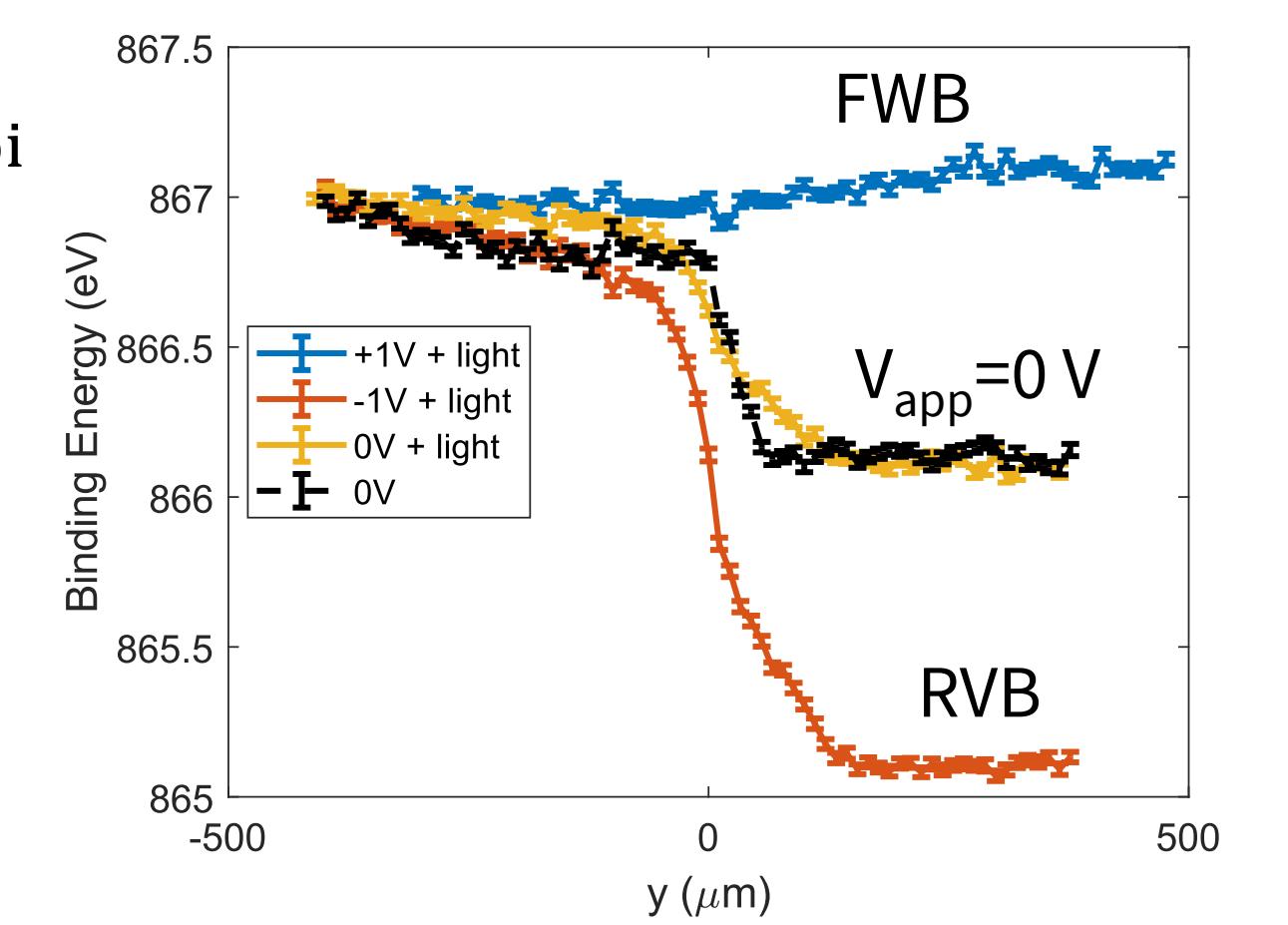


XPS under Light and Voltage bias

Scan in the « dark »



Scan under illumination

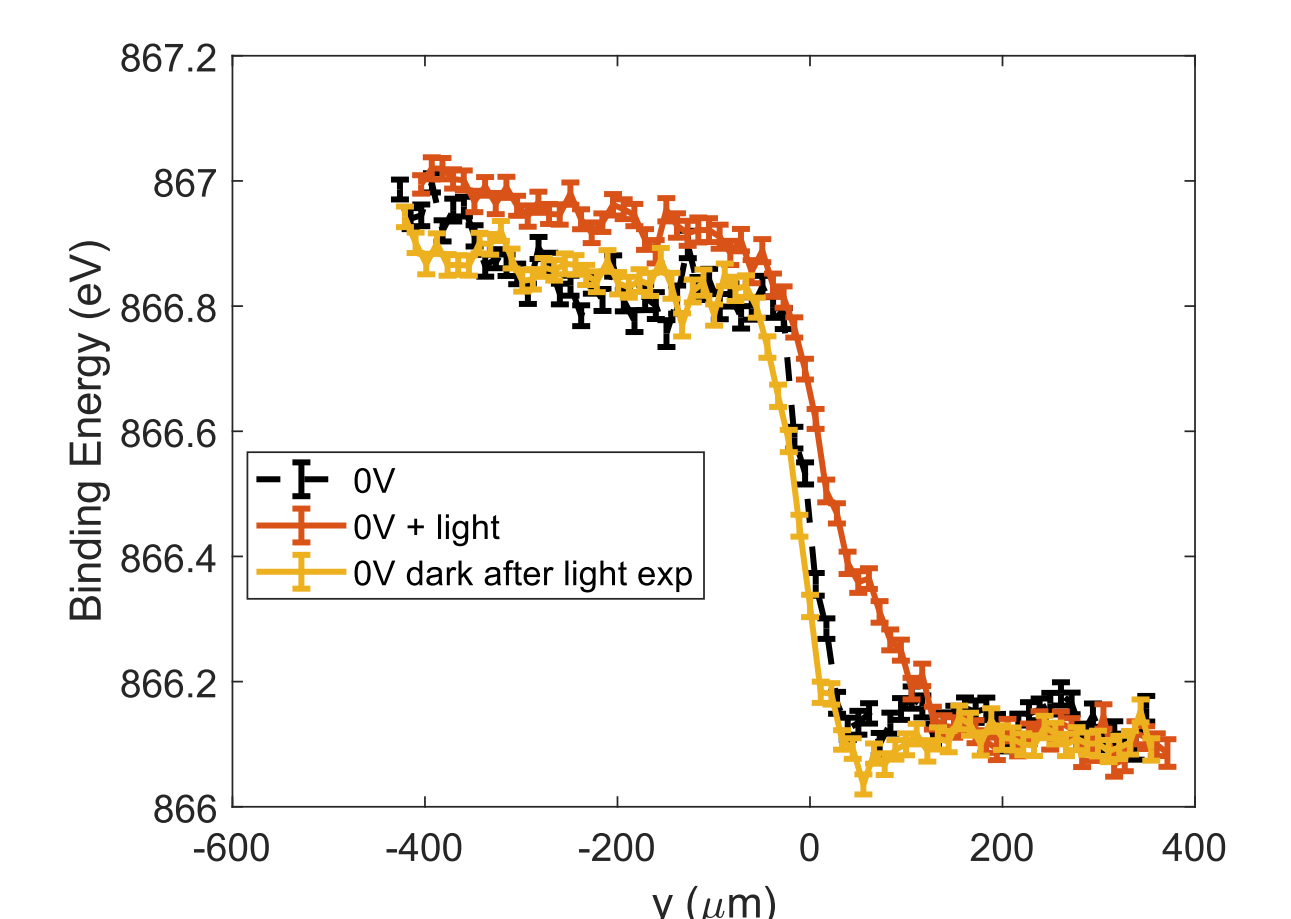
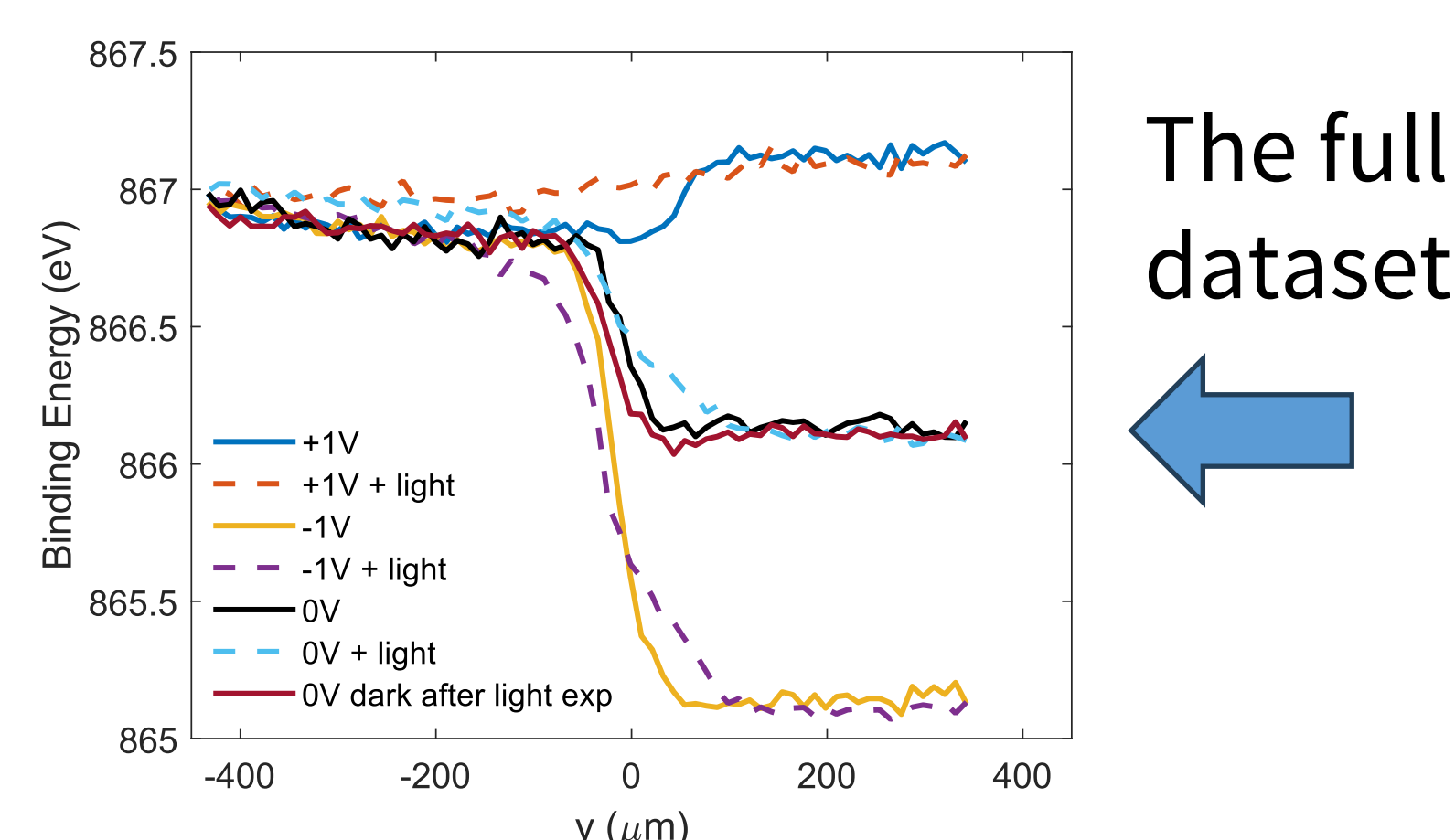


The applied voltage modifies V_{bi} :

$$\text{RV B: } V_{bi} - V_{app} = 0.7 + 1 = 1.7 \text{ V}$$

$$\text{FW B: } V_{bi} - V_{app} = 0.7 - 1 = -0.3 \text{ V}$$

No hysteresis in the dark 0 V scan, after applying light.



CONCLUSIONS

NiO_x and TiO_x - based LHJ device: various PSK channels created between the two contacts (lengths ranging from 10 to 100 μm). Double cation perovskite spin coated on the LHJ: the selective contacts under the PSK determine the potential drop in the PSK (V_{bi}) which can be modulated by an applied bias. PSK doping density measured $\leq 10^{11} \text{ cm}^{-3}$.

Dunfield et al., **Carrier gradients and the role of charge selective contacts in lateral heterojunction all back contact perovskite solar cells**, Cell Reports Physical Science 2, 100520.

Regaldo, D et al, **On the equilibrium electrostatic potential and light-induced charge redistribution in halide perovskite structures**. Prog Photovolt Res Appl. 2022; 1-9.