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# Electronic Properties of Metal Halide Perovskites and their Interfaces with Charge Extraction Layers in Lateral Heterojunction Configuration

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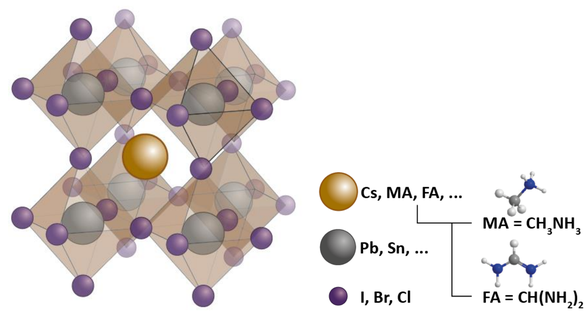
# Electronic Properties of Metal Halide Perovskites and their Interfaces with Charge Extraction Layers in Lateral Heterojunction Configuration

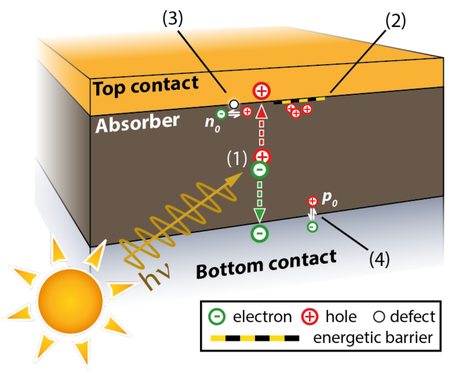
## Metal Halide Perovskites: Applications and Interfaces

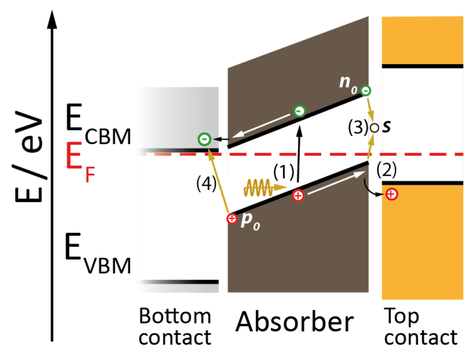



Hybrid organic-inorganic metal halide perovskite (MHP) with complex chemical structure $ABX_3$

Semiconductor with unique combination of optoelectronic and mechanical properties[1]

Breakthrough application in photovoltaics: **Perovskite solar cells (PSC)**




Relevant loss-channels:

(1) Photoexcitation and transport to interface

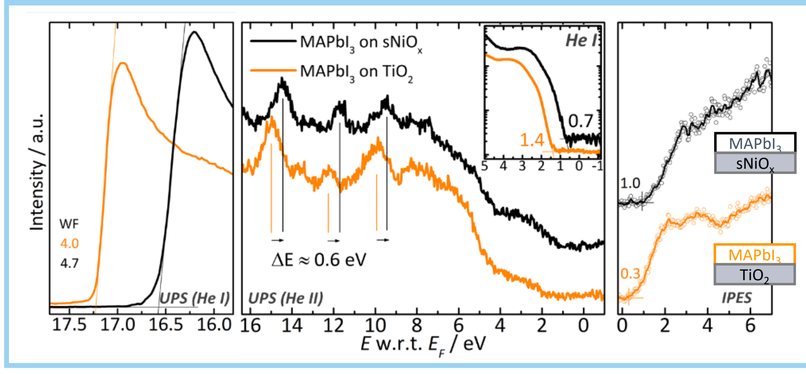
(2) Band misalignment of as barrier for charge extraction

(3) Recombination at interface defect states

(4) Back-recombination

**Predominantly losses at interface[2,3]**

## Substrate-dependent Fermi Level Alignment and Lateral Heterojunction (LHJ)

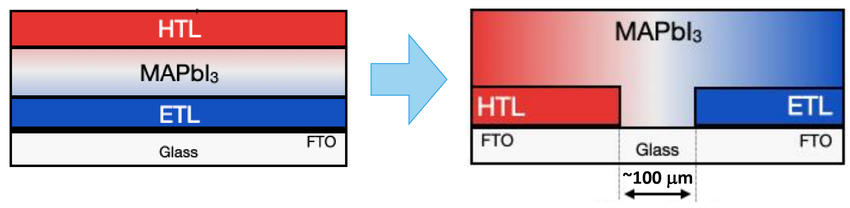



Combined ultraviolet and inverse photoemission spectroscopy (UPS/IPES)[4]:

Optoelectronic properties of MHP can be altered by the substrate (or selective contact) underneath

Position of Fermi level ($E_F$) at the surface of the perovskite film ($MAPbI_3$, 400 nm) changes on different substrate, with $E_F$ close to the perovskite conduction band on $TiO_2$ and in a mid-gap position on NiO

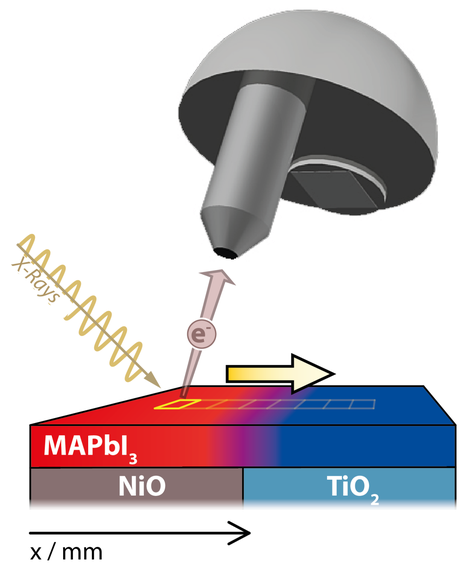
**Need to track interface formation and energy level alignment**

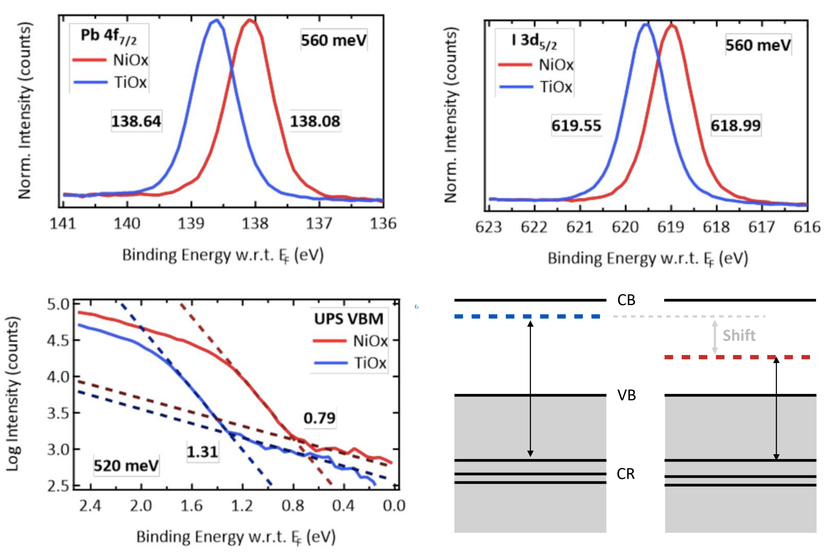


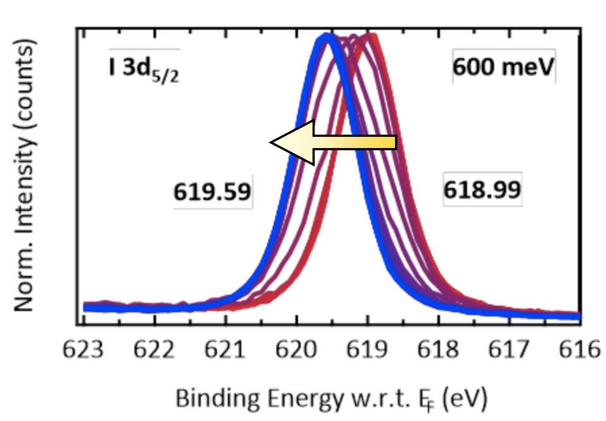

Transition from common, vertically stacked sample geometry to lateral heterojunction architecture[5]

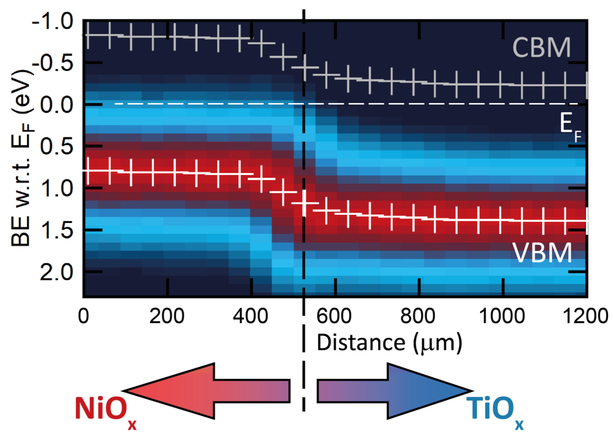
**Access to surface electronic and chemical properties across channel**

## Photoelectron Spectroscopy across LHJ channel



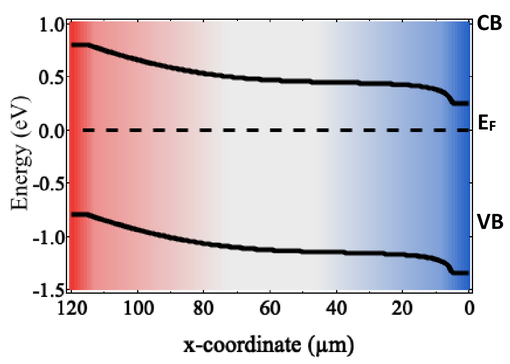



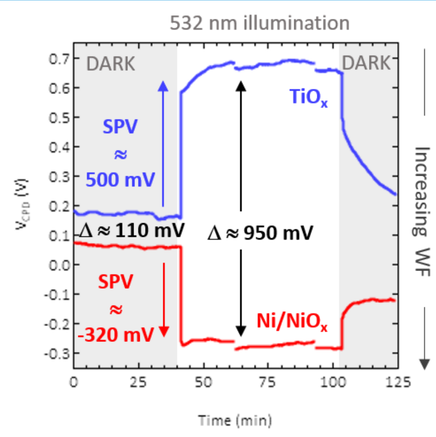



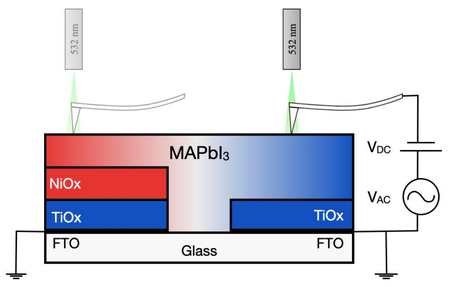

- Lateral contact design as in interdigitated back contacts
- Perovskite deposition on top
- XPS/UPS data acquisition at end points
- Scanning PES (XPS, I $3d_{5/2}$) across lateral heterojunction (LHJ)

- Drift-diffusion modelling to determine origin of surface potential[5,6]
- Observed profile of surface potential requires low doping concentration in MHP ($<10^{13}$ $cm^{-3}$)

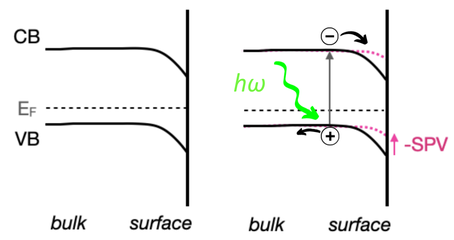



## Complementary Kelvin Probe Force Microscopy

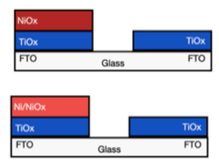



- Assess surface potential / work function
- Measurement in dark and under illumination to capture surface photovoltage (SPV)
- Significant difference in SPV between MHP on $TiO_x$ vs MHP on $NiO_x$ indicates **change of carrier extraction at interface**[5]



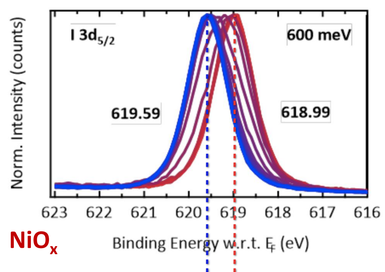

## Modified Charge Selectivity at $NiO_x$ Contact

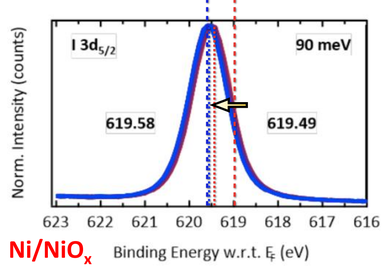


Fully oxidized $NiO_x$ at 300°C / 120 min anneal



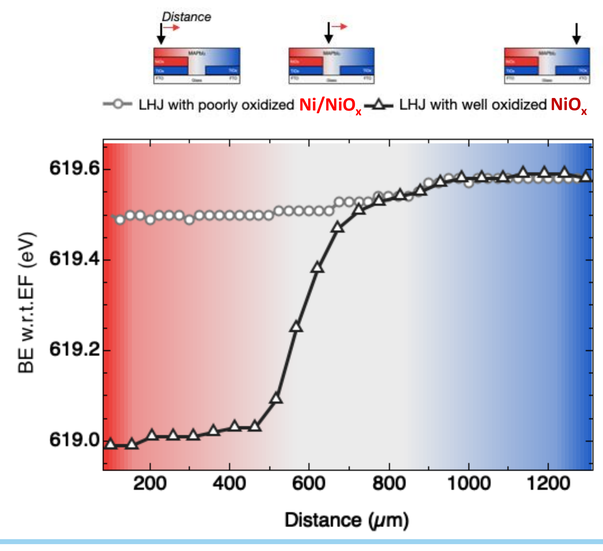
Oxygen-deficient Ni/NiOx at 275°C / 30 min anneal




Adaptation of contact selectivity by variation of $NiO_x$ oxidation level through controlled annealing

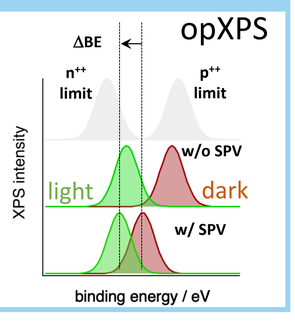
**Reduced shift of $E_F$ in gap for poorly oxidized $Ni/NiO_x$** in line with results of higher recombination seen in photoluminescence measurements[5]




## Conclusion and Next Steps

- Charge selective contacts shift the Fermi level in metal halide perovskites (MHPs)
- Effect is readily observable because of low defect and doping concentrations in the MHP
- Contact selectivity determines carrier extraction across MHP/contact interfaces
- Tailoring charge selective contacts to design MHP-based lateral heterojunction devices

- Operando measurements[7] (opXPS & KPFM) to track dynamic effects and potential ion migration
- Access to buried interfaces via HAXPES measurements

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