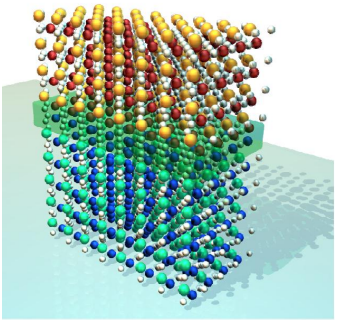
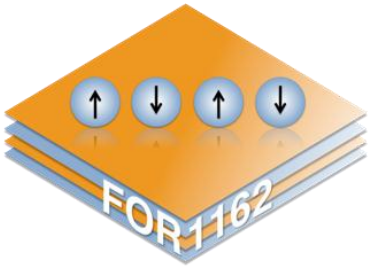
Valence Band Analysis of $LaAlO_3/SrTiO_3$ Heterostructures using Hard X-Ray Photoelectron Spectroscopy

G. Berner, F. Pfaff, A. Müller,
S. Paetel, C. Richter, J. Mannhart,
A. Hloskovskyy, W. Drube, M. Sing and R. Claessen

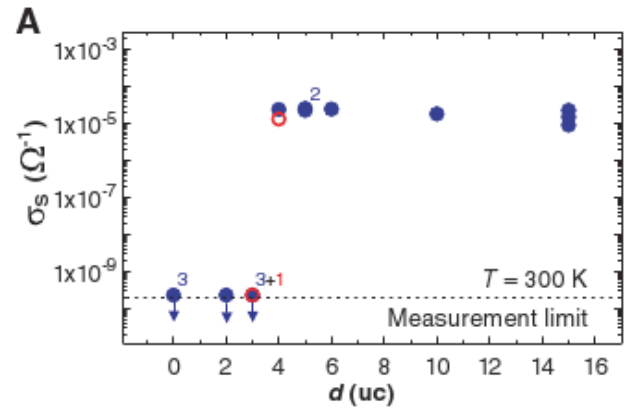


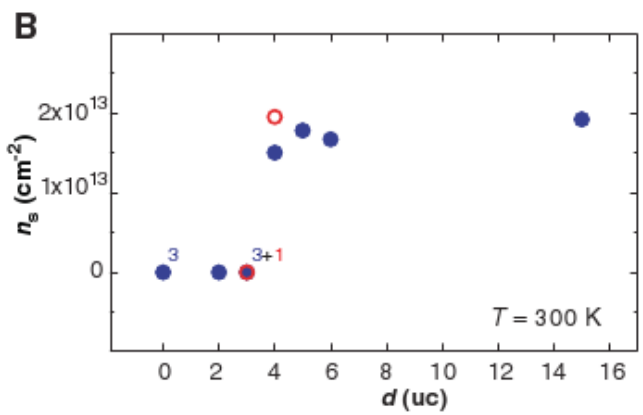


$LaAlO_3/SrTiO_3$ heterostructures

- epitaxial growth by pulsed laser deposition
- more than 3uc LAO:
  formation of **2DEG** at the interface
- electrostatical tuning of the interface properties (field effect)

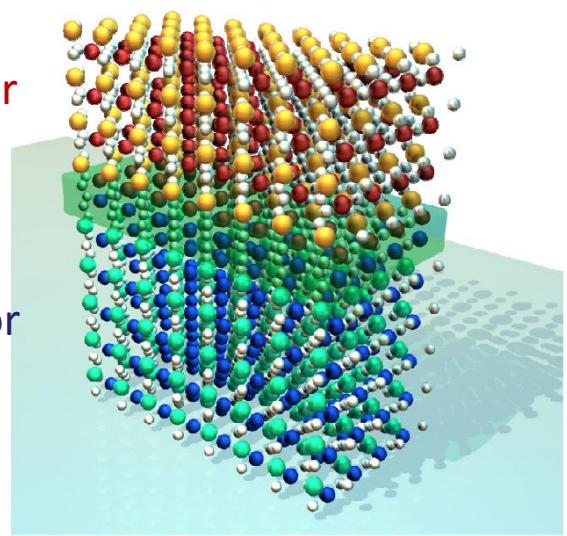
Critical thickness: ≥4uc





$LaAlO_3$:
Band insulator
Δ=5.6eV

$SrTiO_3$:
Band insulator
Δ=3.2eV



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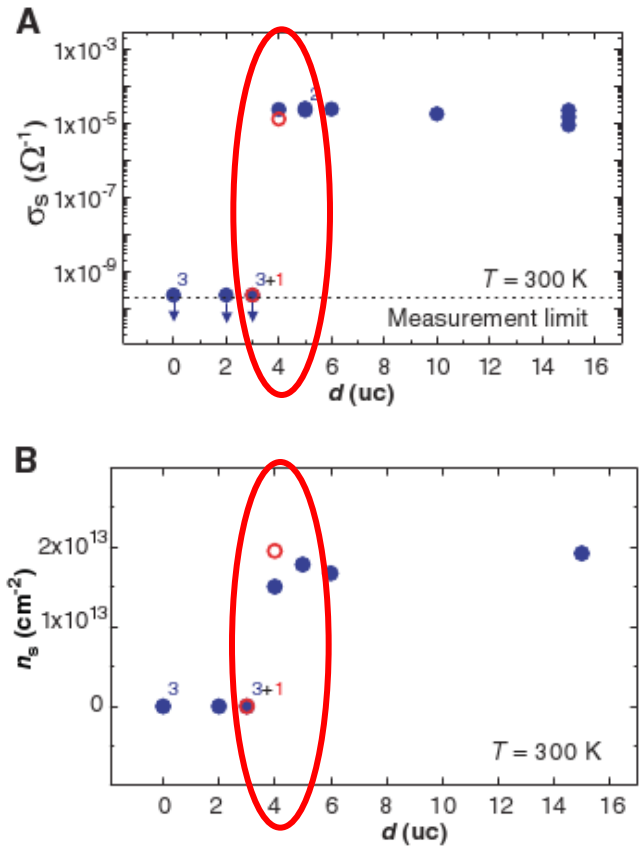

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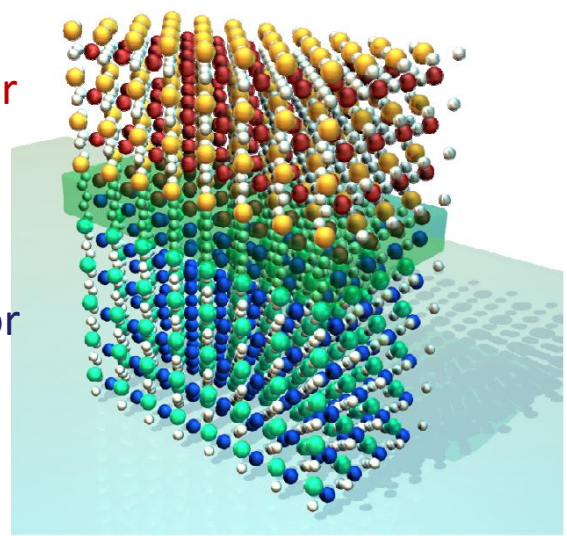
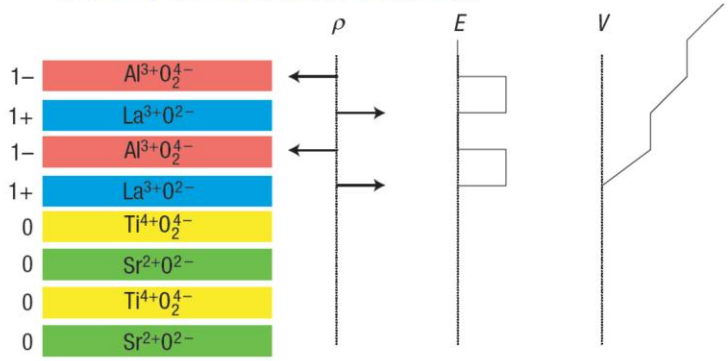


Origin of the metallic phase?

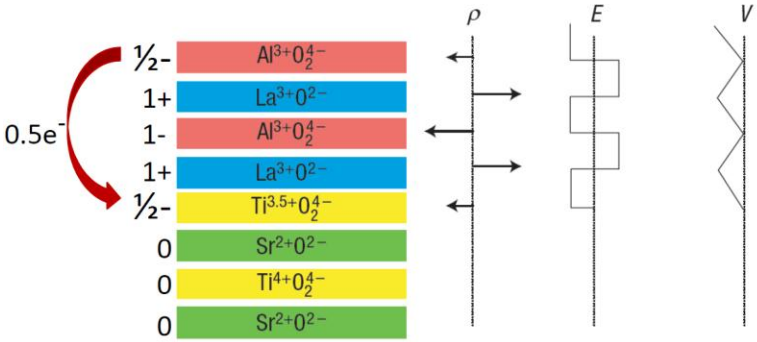
intrinsic

electronic reconstruction

before reconstruction:



after reconstruction:



$0.5e^- \rightarrow n_{2D} \approx 3.4 \cdot 10^{14} cm^{-2}$

extrinsic

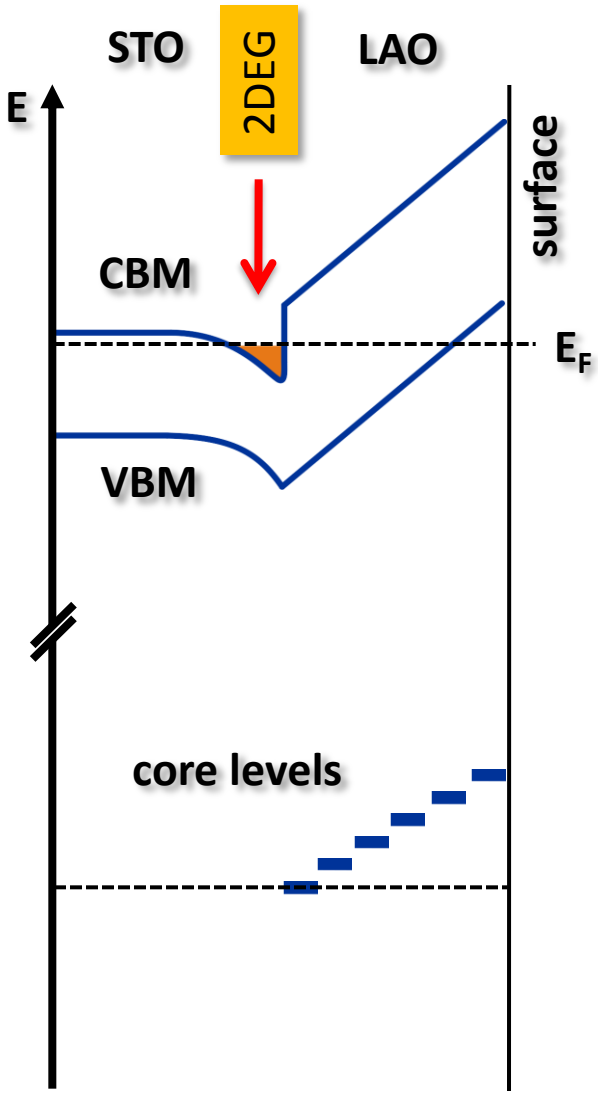
oxygen vacancies / preparation properties

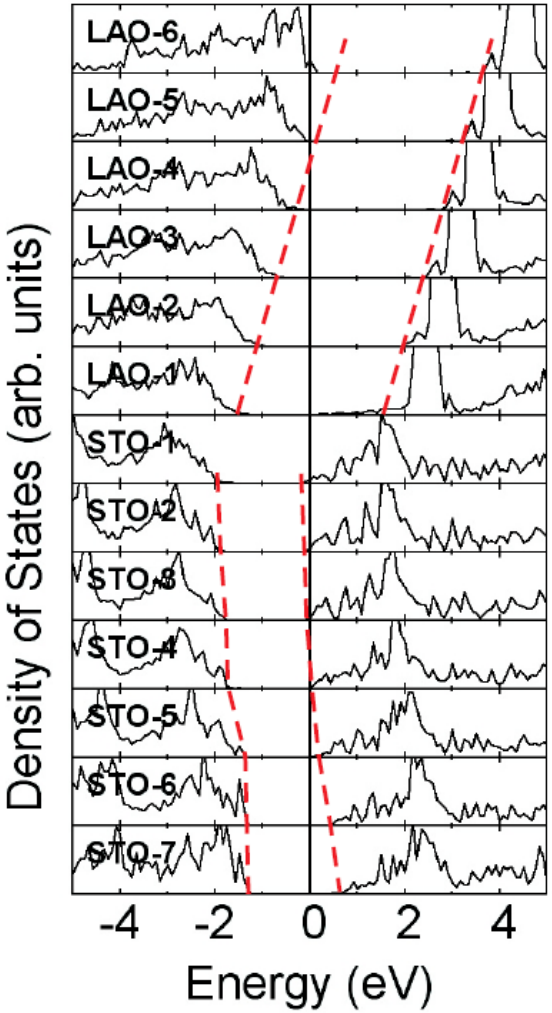
La/Sr intermixing

in experiments:

- carrier density much **smaller** ($n_{2D} \approx 5 \cdot 10^{13} cm^{-2}$)
- 2DEG confined to only a **few unit cells (uc)** in STO

View from band theory





Yu Lin et al., arXiv 0904.1636 (2009)
Pentcheva and Pickett, PRL 102, 107602 (2009)

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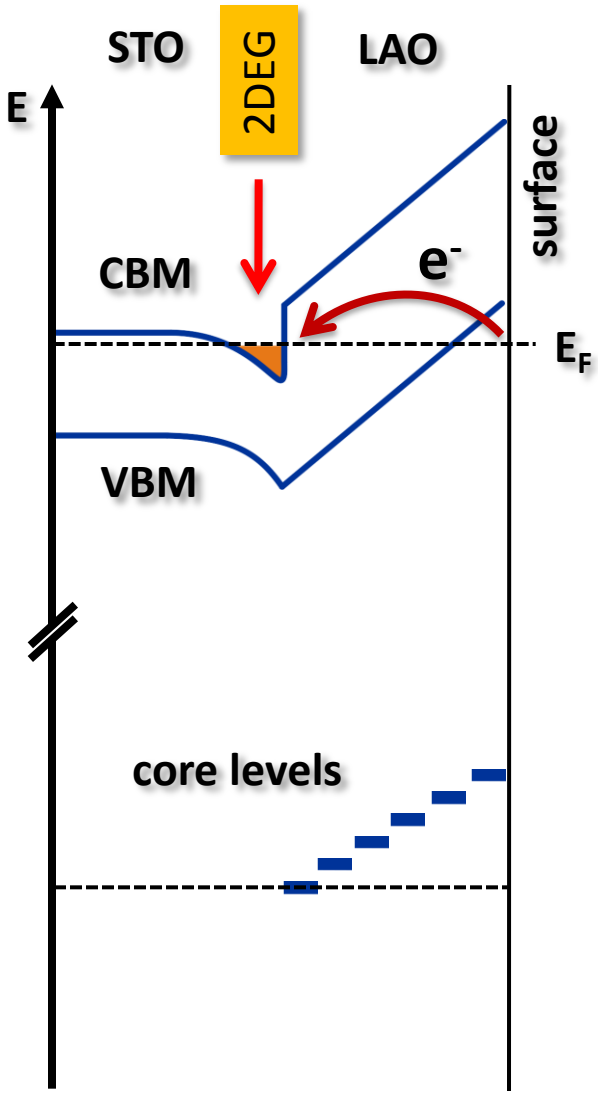

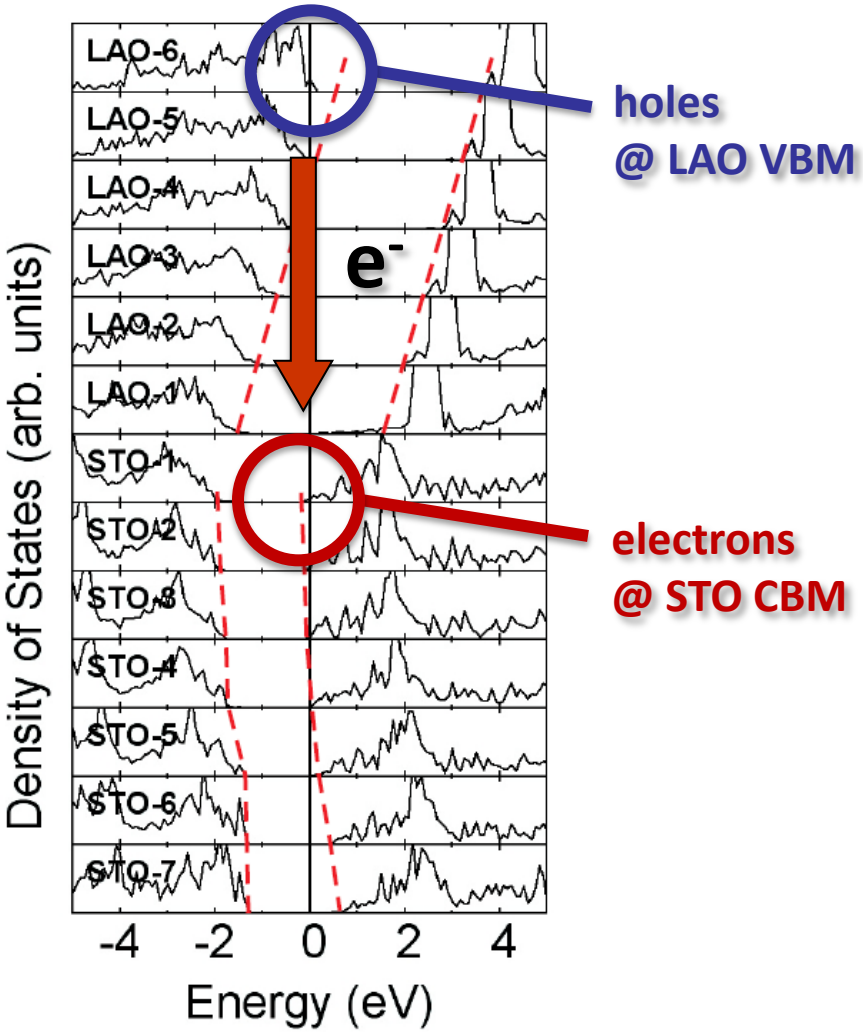

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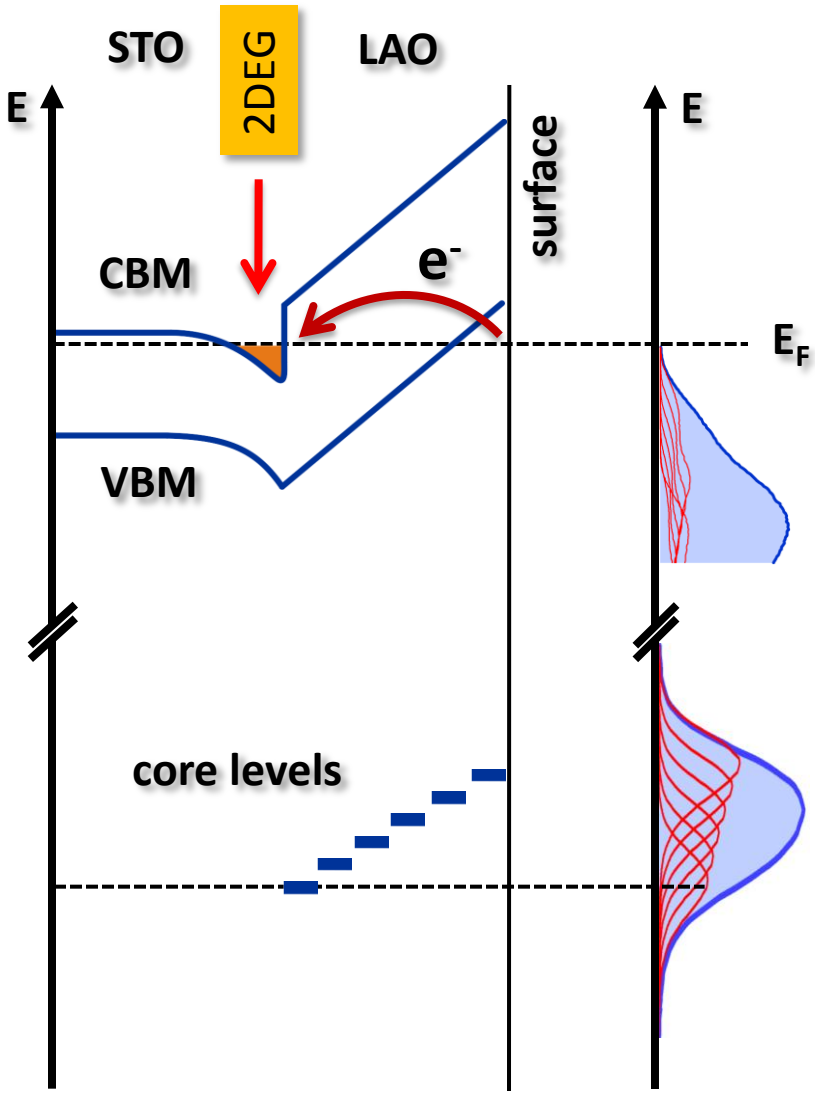
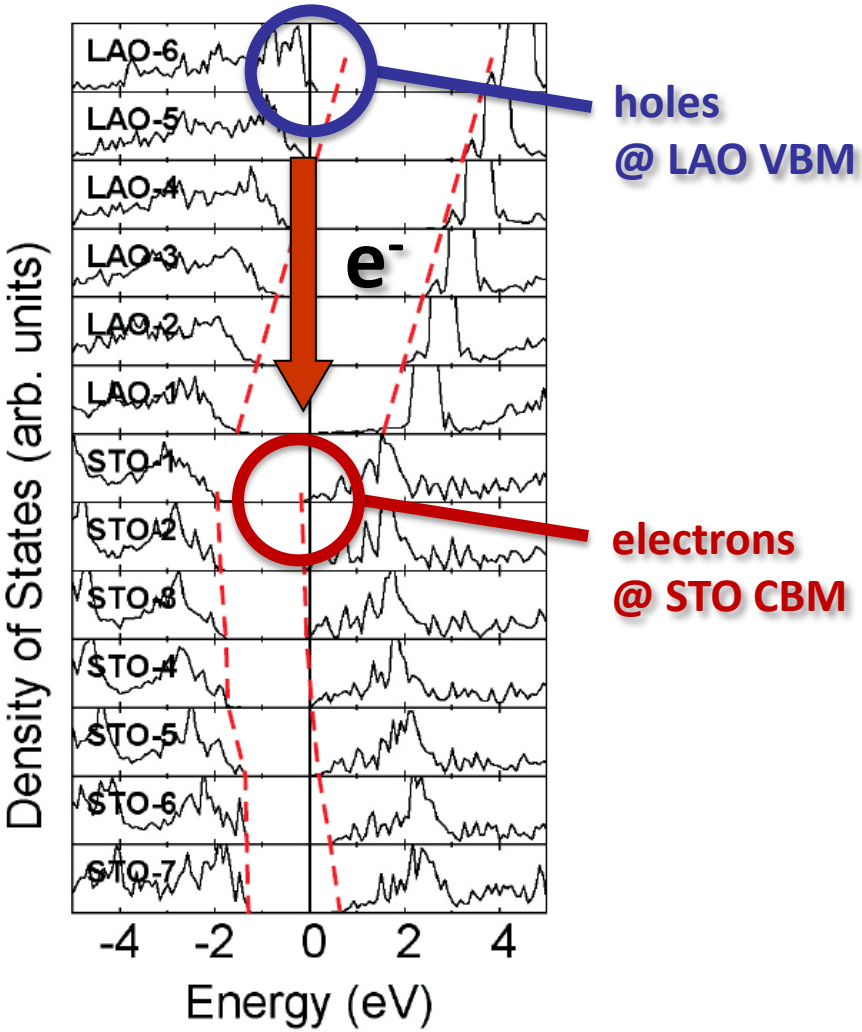
Expectations from XPS





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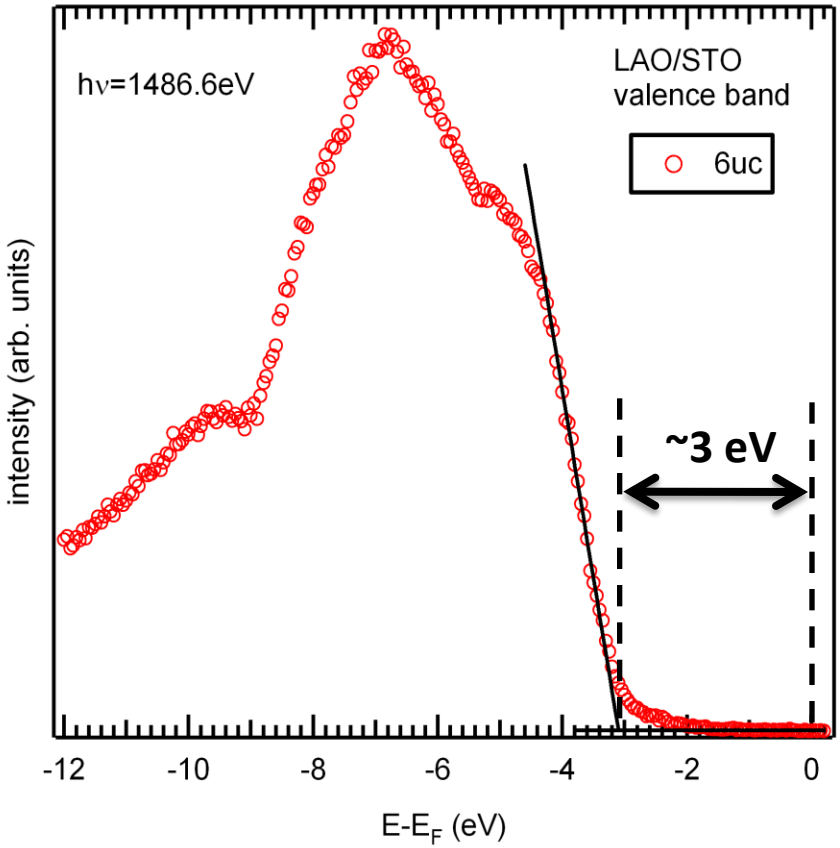
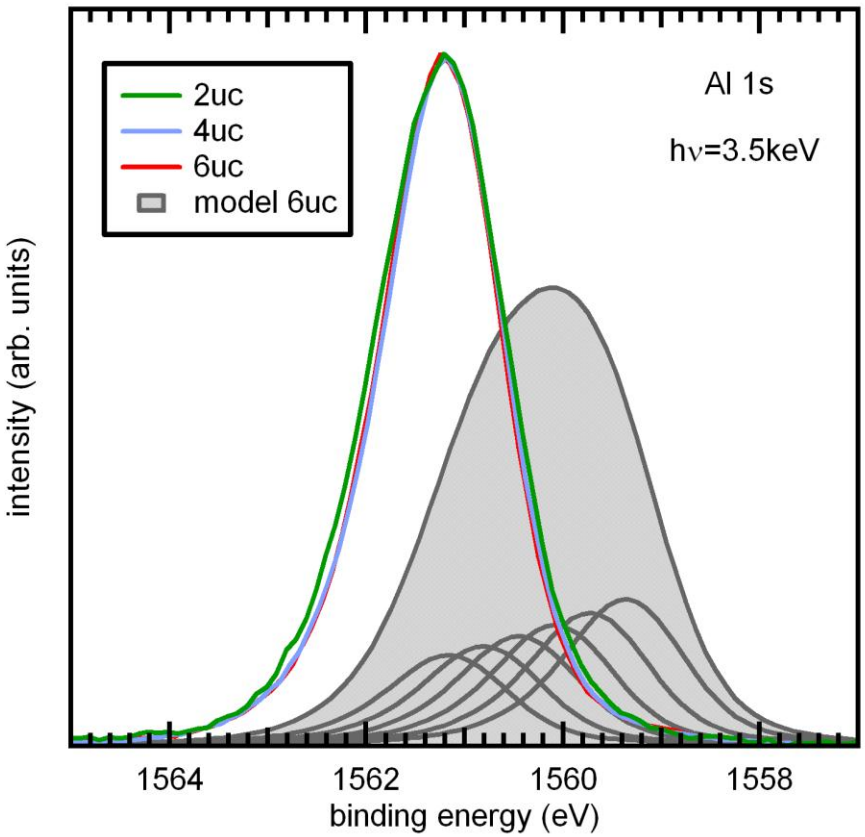
Results from XPS

valence band



Al 1s core level

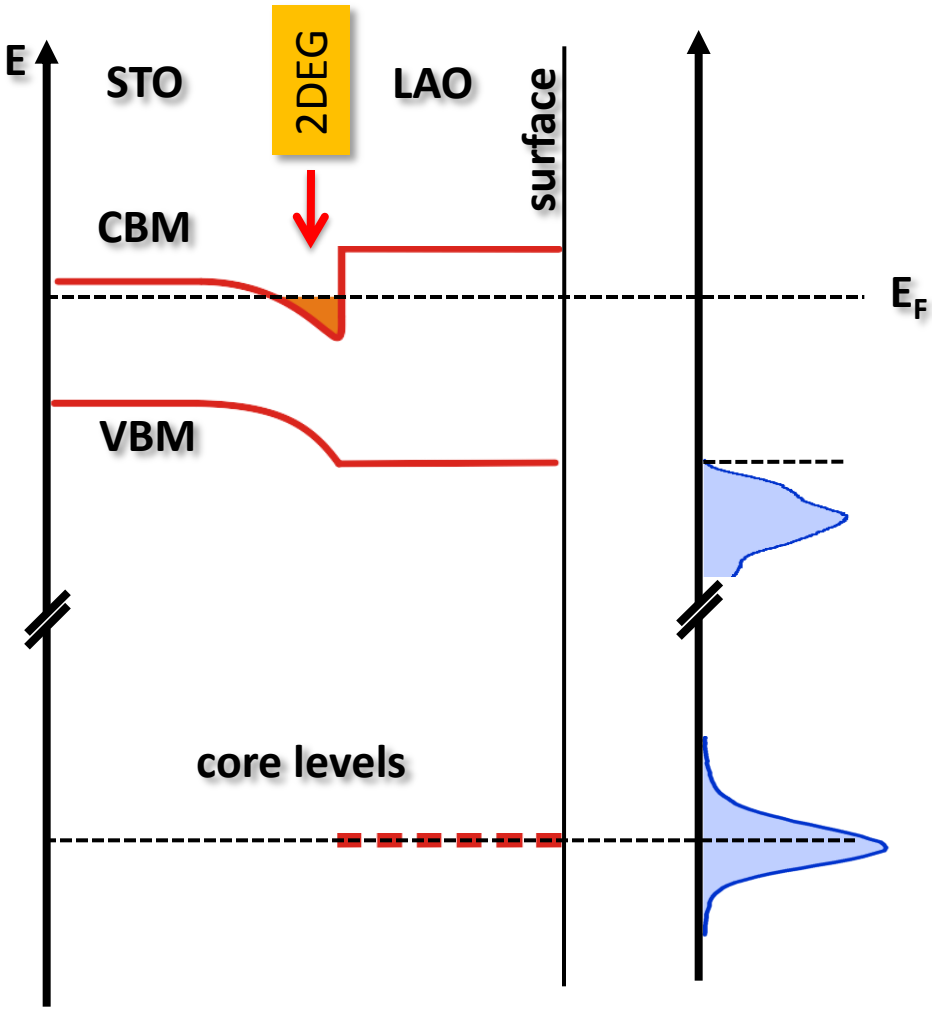


VBM: ~ **3 eV** below E_F

same width for **all** samples!

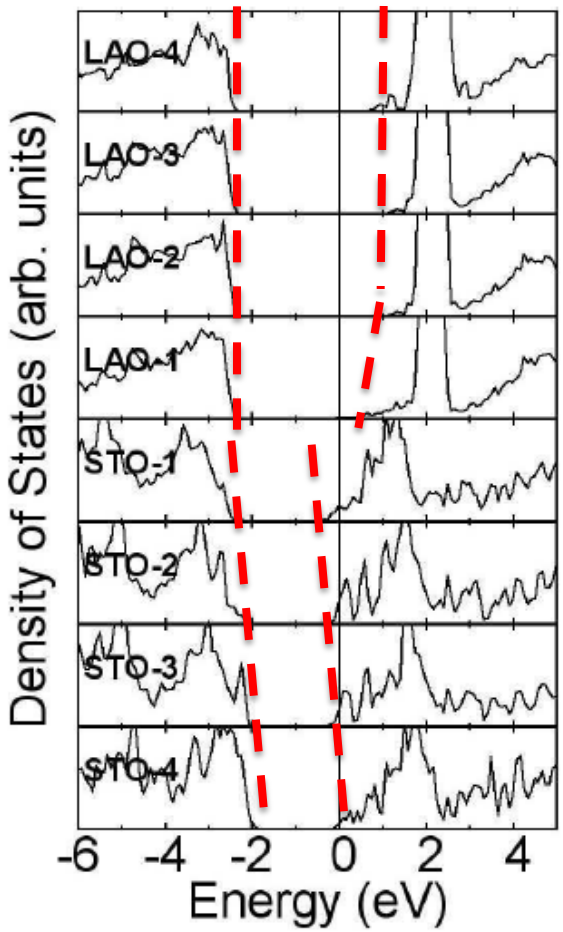
Results from XPS

picture from XPS



also observed by Segal et al., PRB 80, 241107(R) (2009)

band theory
oxygen vacancies at **LAO surface**



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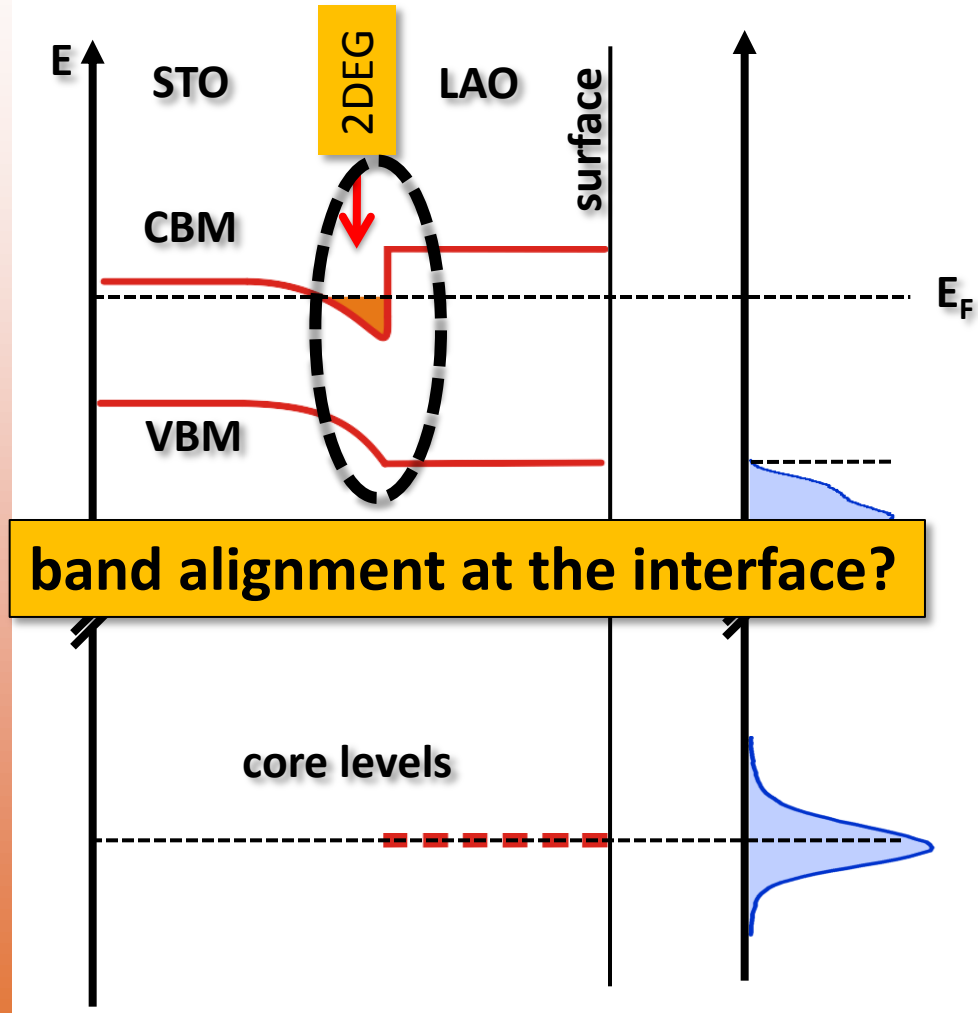

band alignment at the interface?

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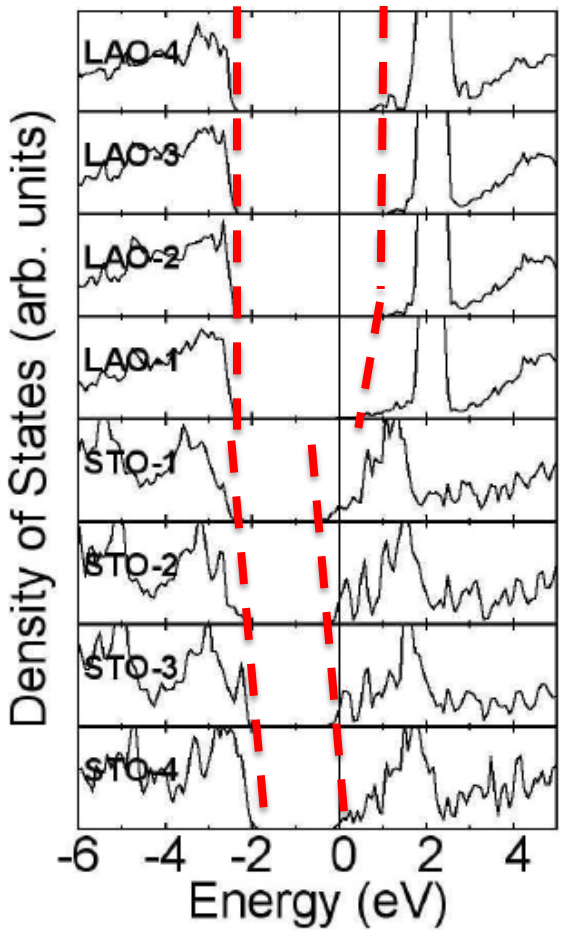

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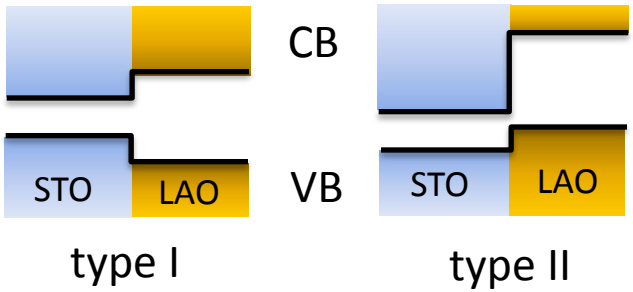
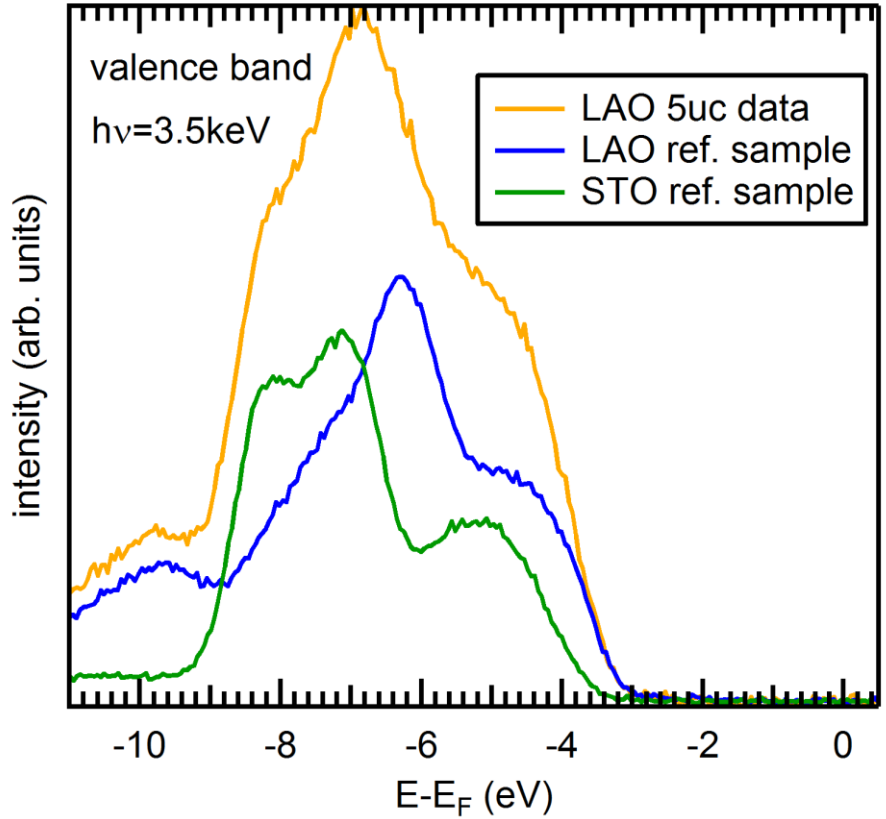
Valence band offsets

band alignment



valence band analysis



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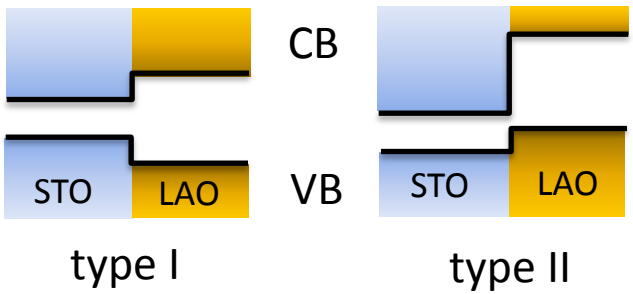
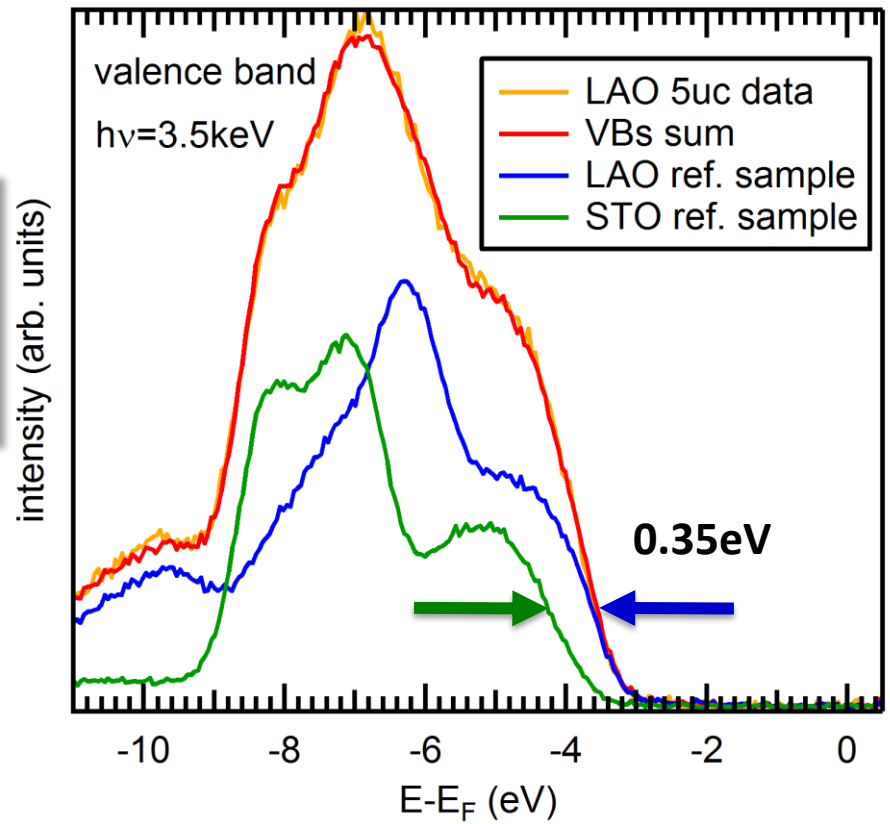


- VBM_{LAO} **above** VBM_{STO}
- **type II** interface
  (valence band offset: **0.35 ± 0.1eV)**
- **independent** of LAO thickness

confirmed by core level analysis!

valence band analysis



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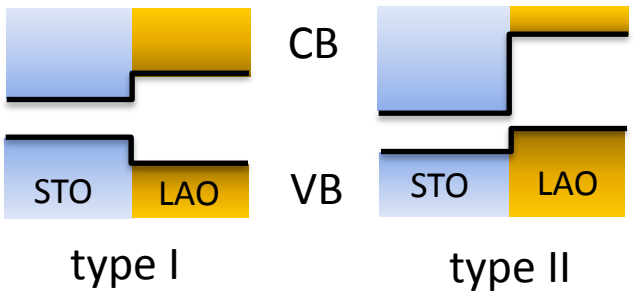

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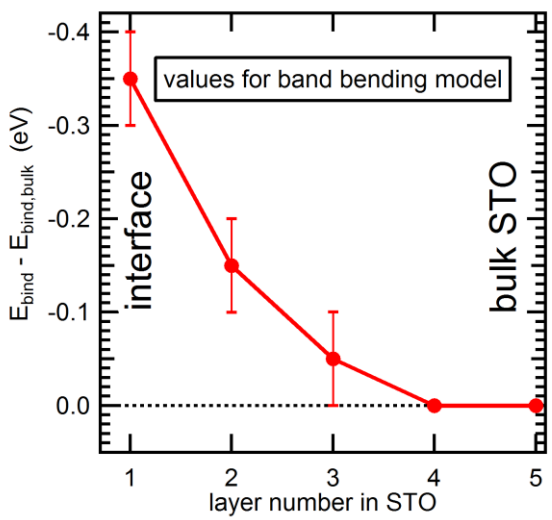
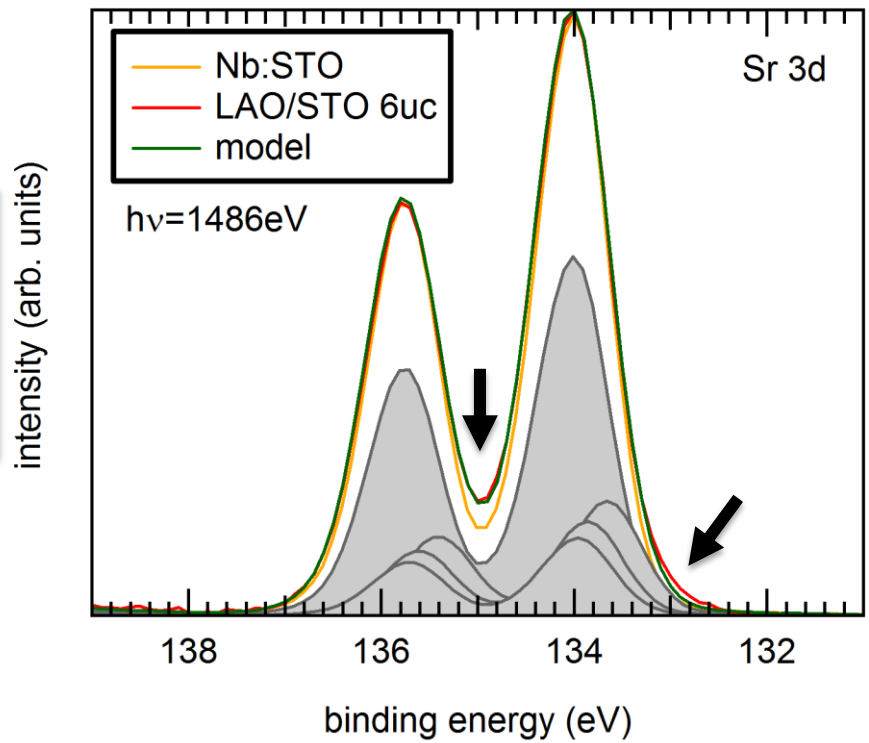


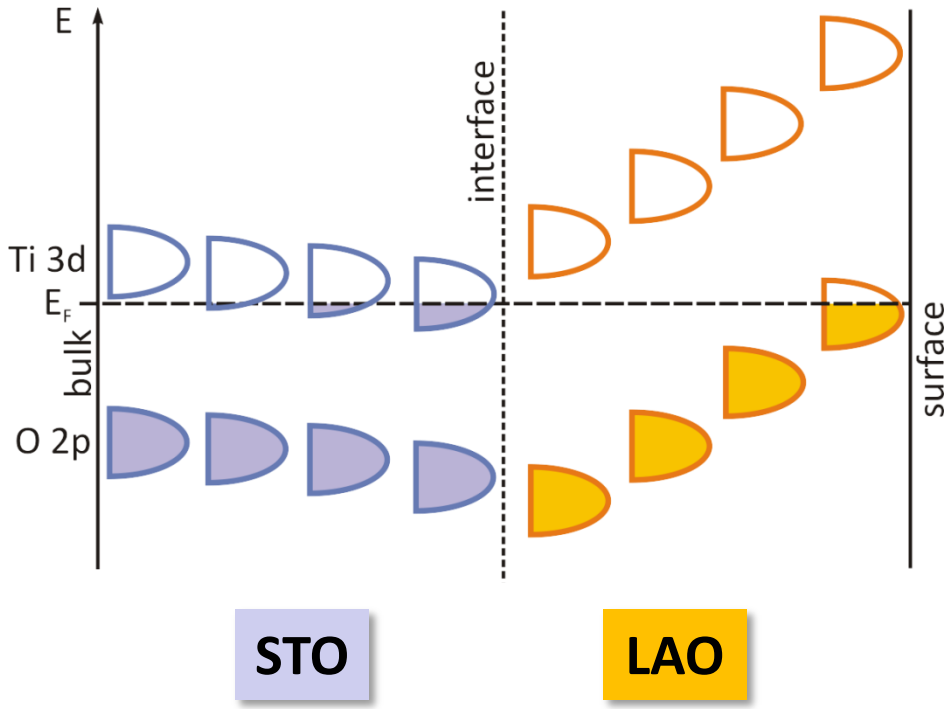
Sr 3d core level



upward band bending in first layers of STO!

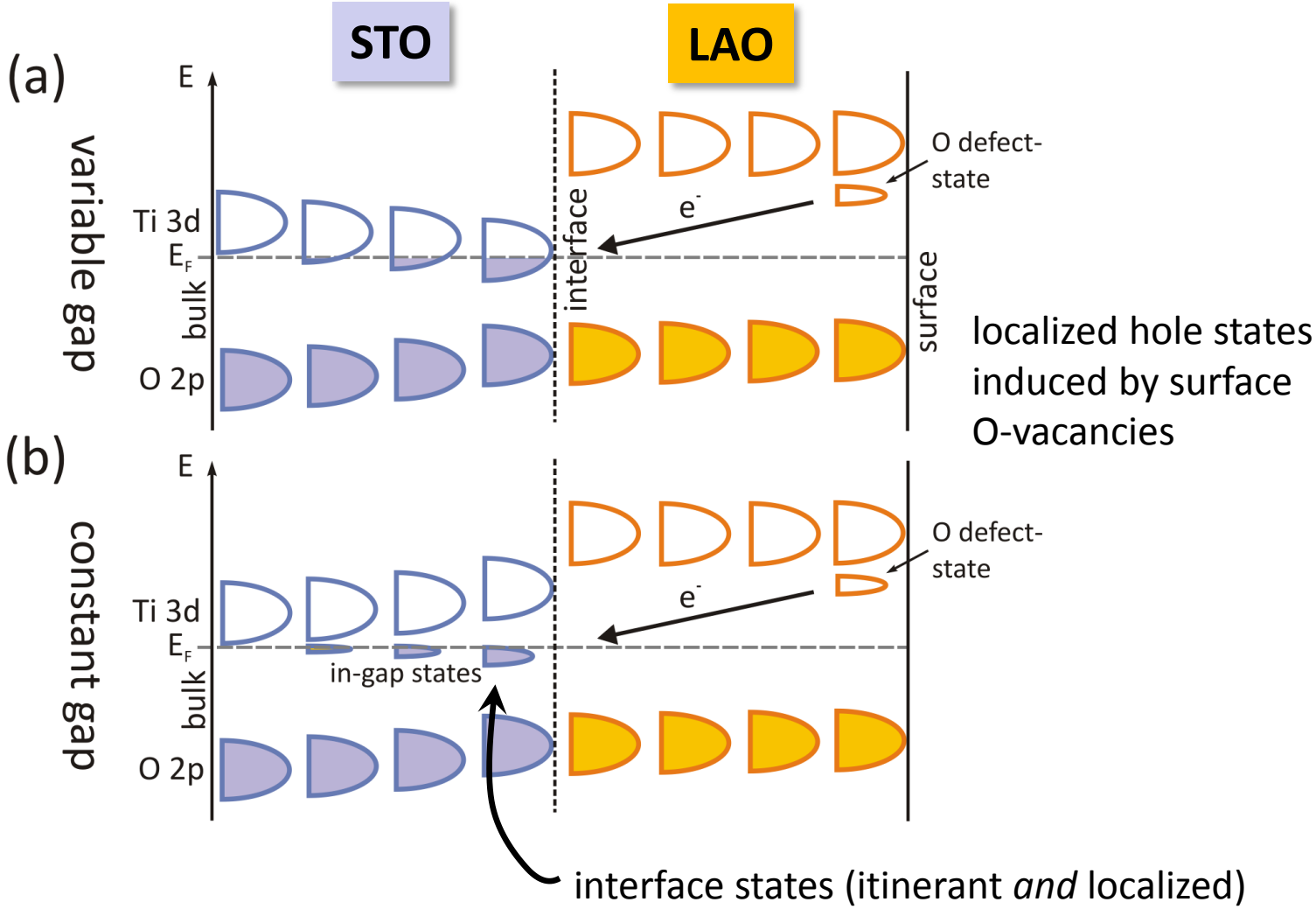
Band alignment: A possible scenario

DFT band theory:



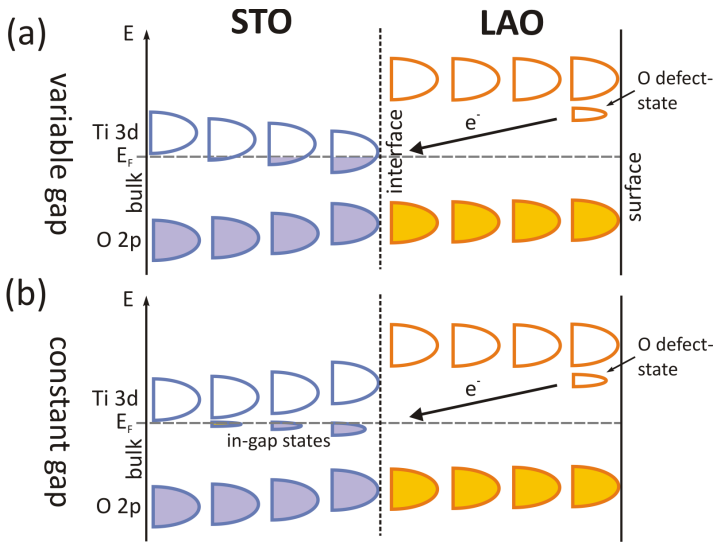
Band alignment: A possible scenario

Photoemission:



Conclusions

- **„flat band“** behavior in LAO overlayer
- **HAXPES vs. DFT**:
  qualtitative agreement if oxygen defects are included in calculations
- band alignment: **type II** interface
- two possible scenarios from HAXPES



open issues:

- **confirmation of interface states / band gap narrowing by theory?**
- **influence of photo-generated carriers?**
- **…**