# Oxide Heterostructures for Solar Cells

Elias Assmann

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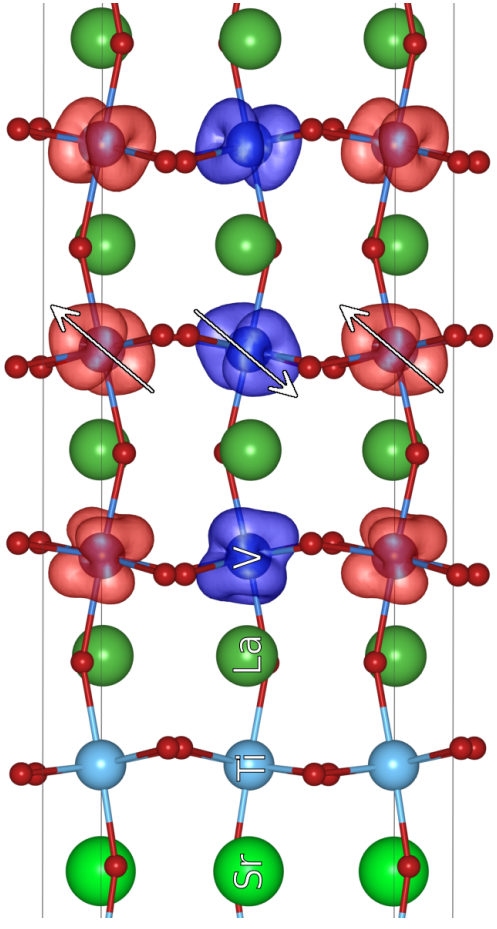


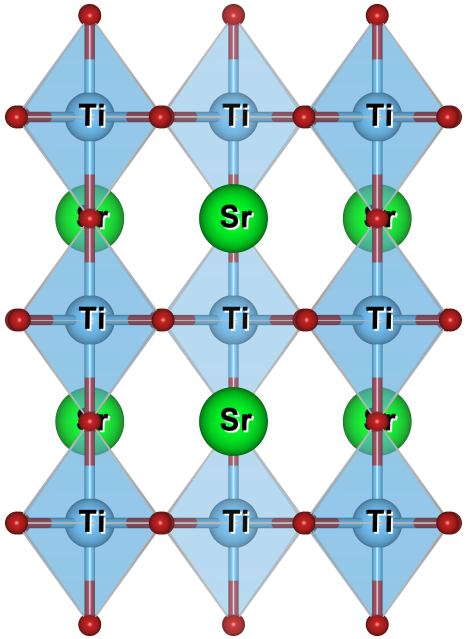

E.A., Peter Blaha, Robert Laskowski, Karsten Held, Satoshi Okamoto, and Giorgio Sangiovanni:

- Phys. Rev. Lett. 110, 078701 (2013)
- Synopsis in APS's *Physics*

$LaVO_3 | SrTiO_3$ proposed as solar cell absorber

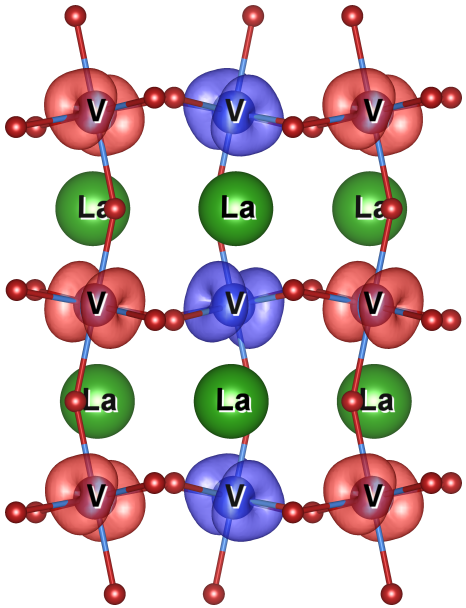
1. large intrinsic electric field
2. conducting interface(s)
3. direct gap 1.1 eV
4. flexible multijunction design

# Bulk $SrTiO_3$ and $LaVO_3$




## $SrTiO_3$

- (almost) cubic Perovskite [$ABO_3$]
- $TiO_6$ octahedra
- $d^0$ band insulator

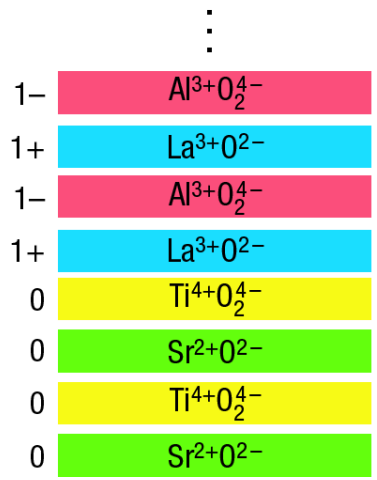



## $LaVO_3$

- distorted Perovskite ($VO_6$ octahedra)
- $d^2$ Mott insulator
- band gap: 1.1 eV
- AF-C spin, AF-G orbital order

# Polarized layers in $LaVO_3|SrTiO_3$ [001]

- $SrTiO_3$: $(SrO)^0$, $(TiO_2)^0$
- $LaVO_3$: $(LaO)^+$, $(VO_2)^-$




adapted from N. Nakagawa et al., Nature Mat. 5, 204 (2006)

[Ohtomo and Hwang, Nature 427, 423 (2004), Okamoto and Millis, Nature 428, 630 (2004)]

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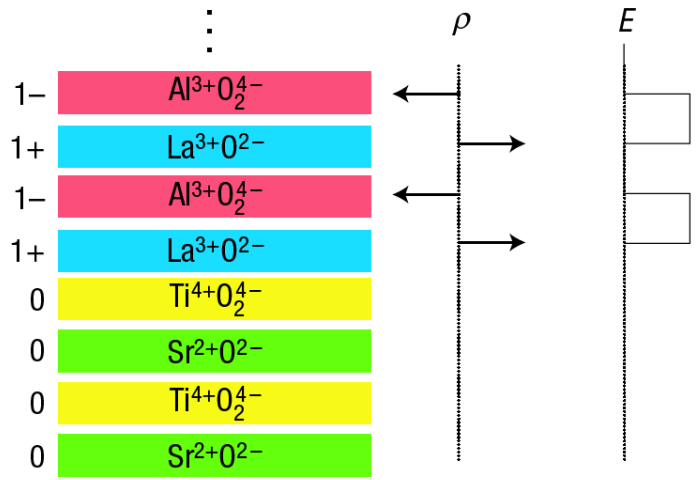
⇝ large internal electric field

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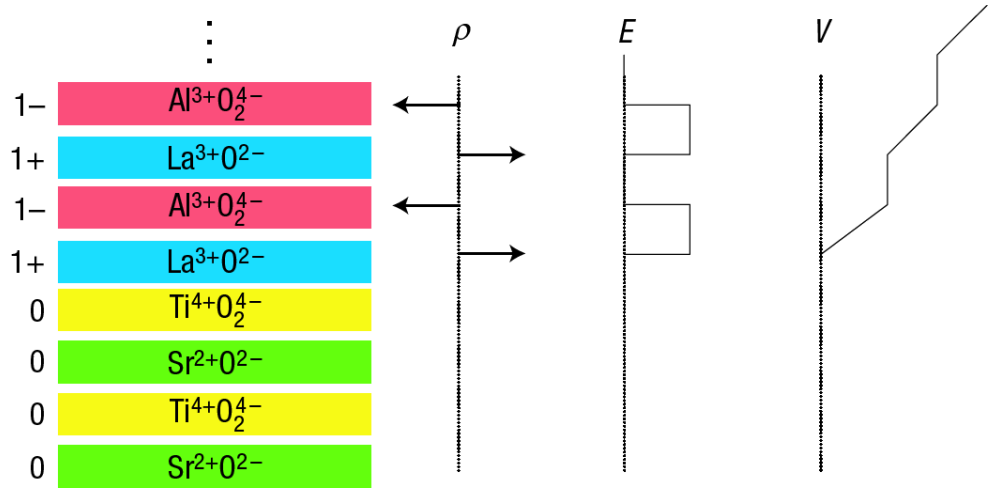


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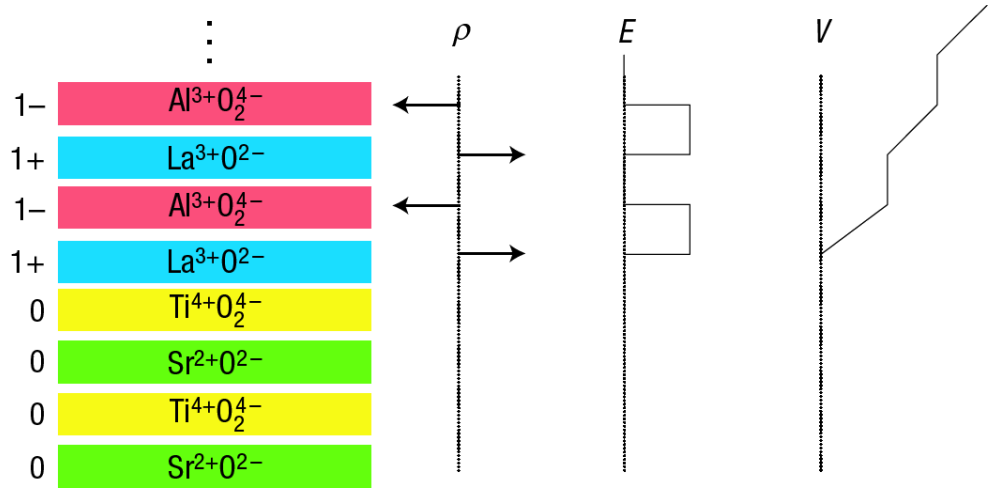


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- experimental finding: conducting "n-type" interface
  - insulator + insulator = metal !

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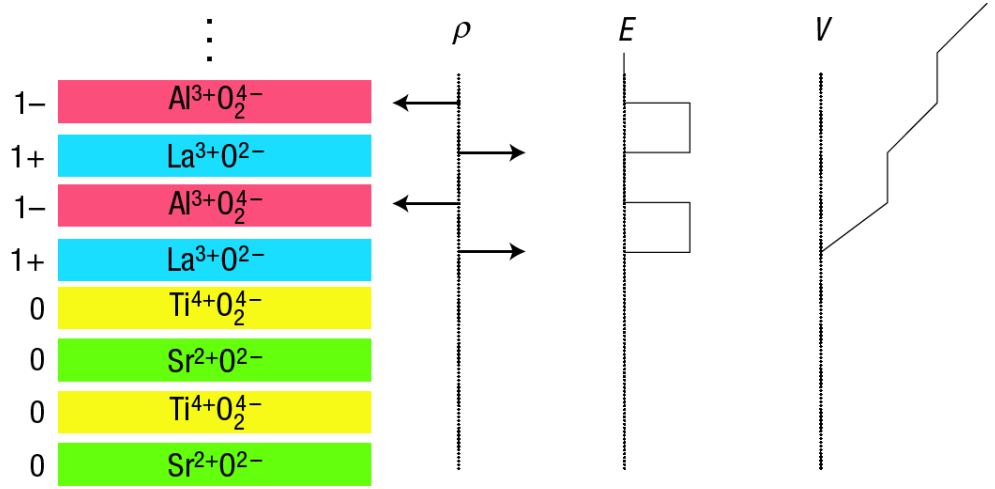


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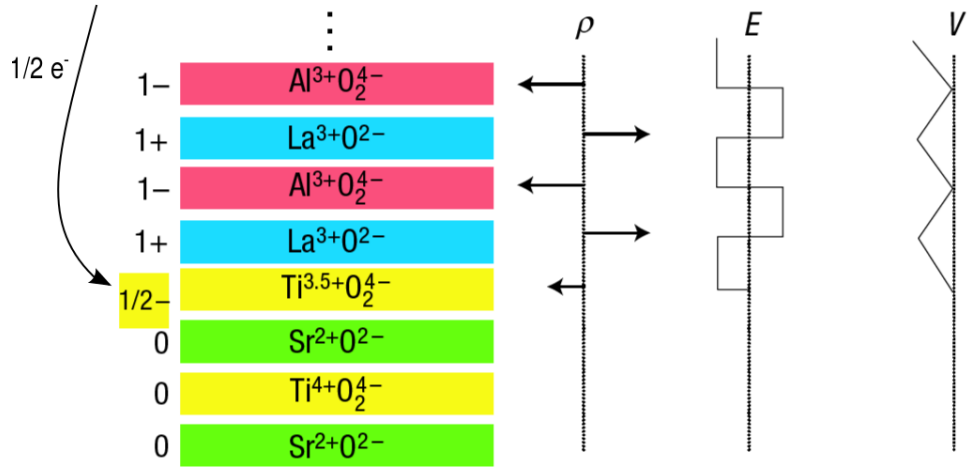
- experimental finding: conducting "n-type" interface
  - insulator + insulator = metal !

- Electronic reconstruction:
  - ⇝ $e^-$ doped n-type interface, $h^+$ doped p-type interface
  - critical thickness

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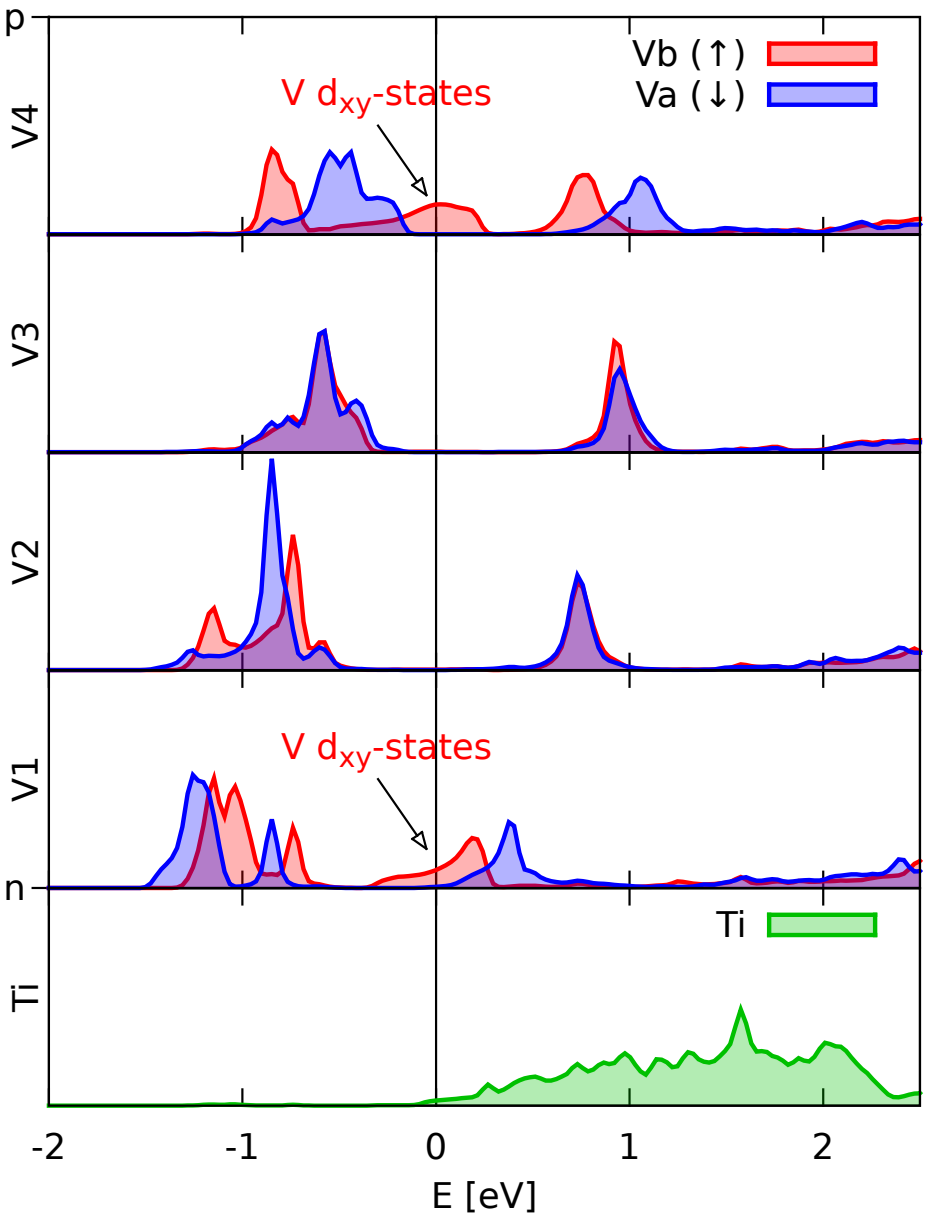
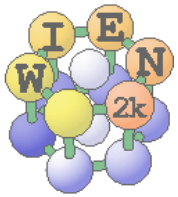
# 1: Potential gradient

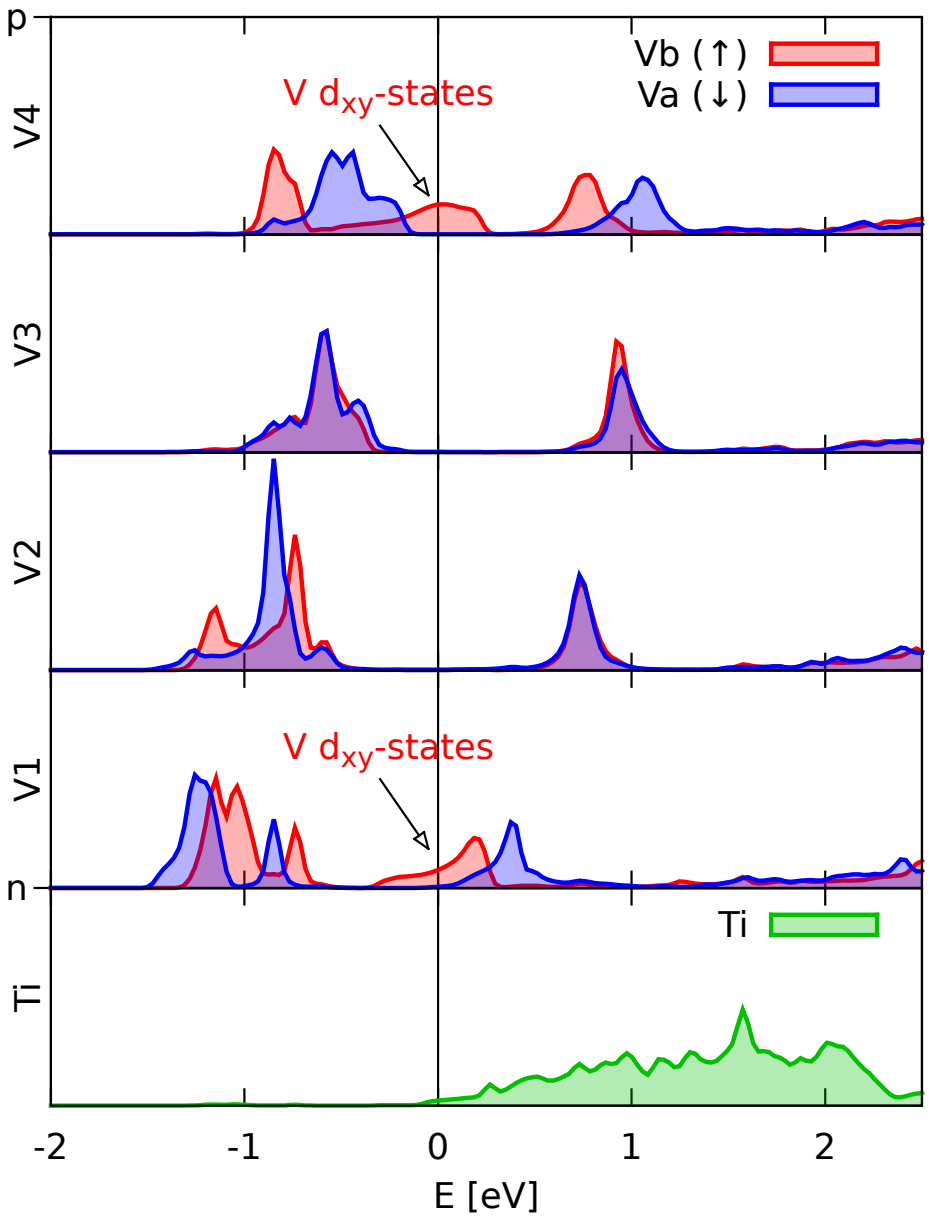



density-functional theory (GGA+U):




- layer-resolved density of states: band shift = potential gradient
- $\sim 0.3\,\text{eV/u.c.} = 0.08\,\text{eV/Å}$

# 1: Potential gradient & 2: Conducting interface(s)

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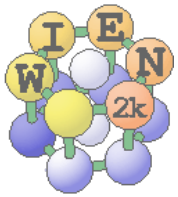
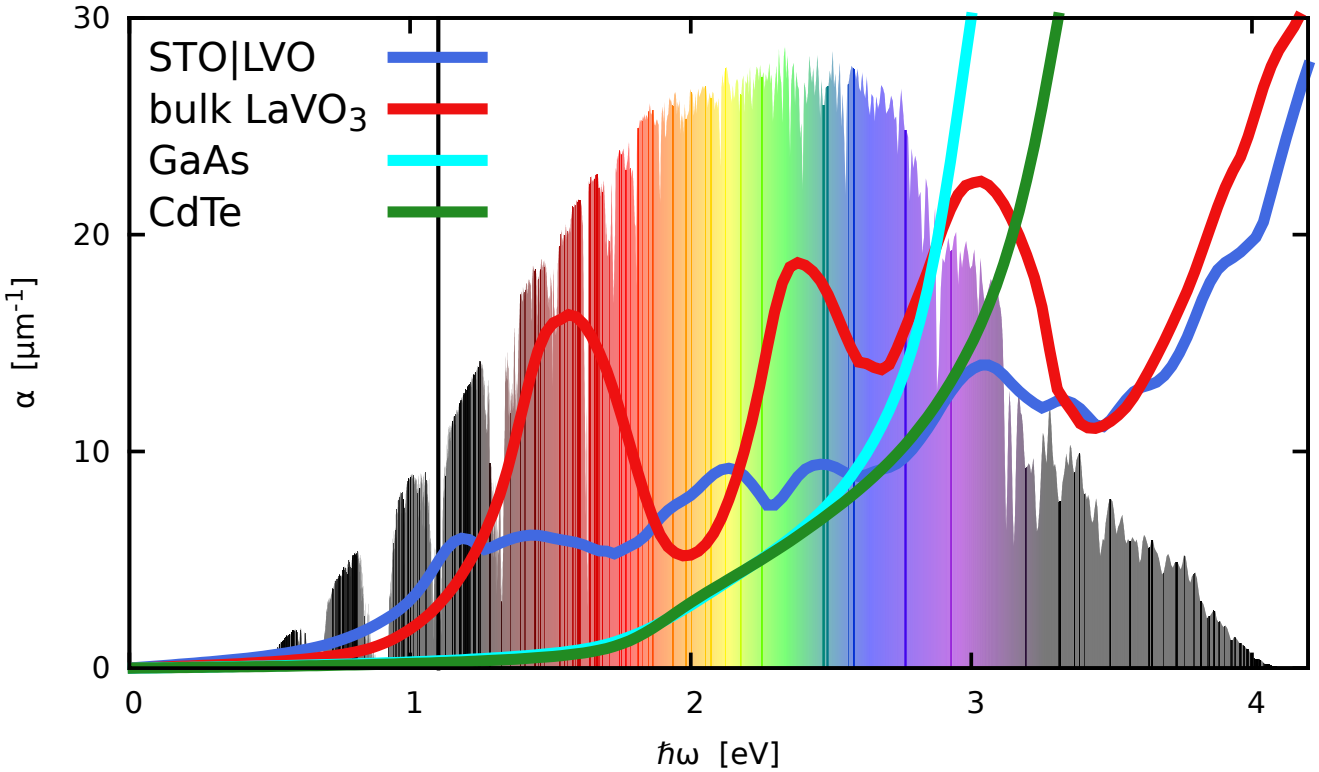


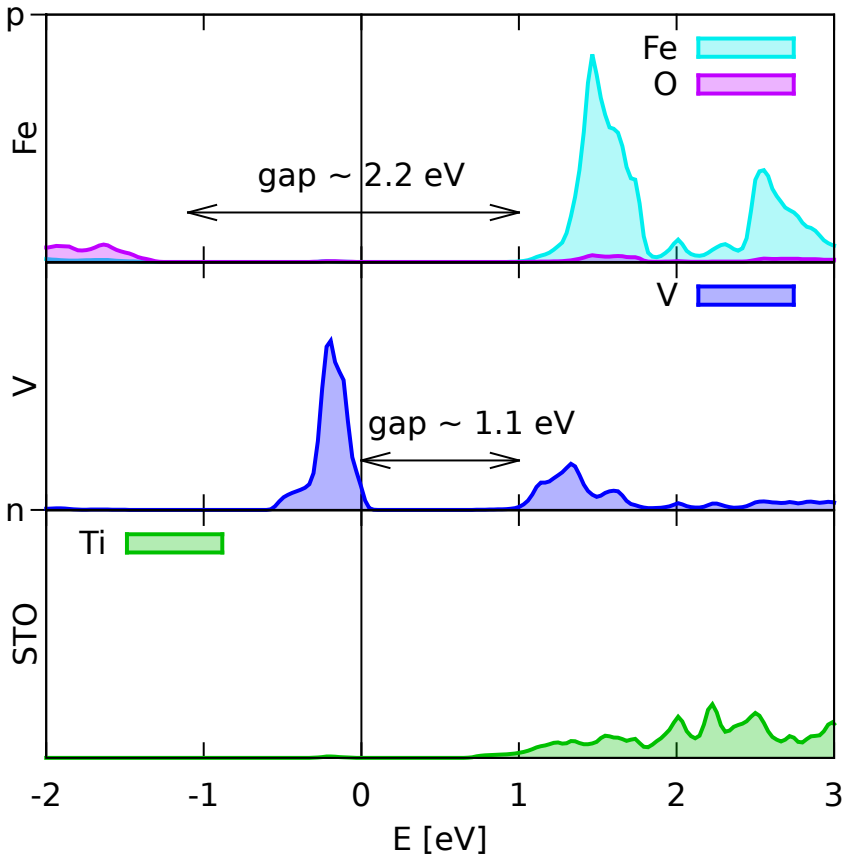

- layer-resolved density of states: band shift = potential gradient
- $\sim 0.3\,\text{eV/u.c.} = 0.08\,\text{eV/Å}$
- both interfaces conducting in DFT
- both interfaces occur by periodic boundary conditions

# 3: Strong absorption across solar spectrum




- optical absorption of $LaVO_3$ compares favorably to e.g. GaAs, CdTe
- band gap 1.1 eV is in the optimal range for efficiency

# 4: Flexible gap grading

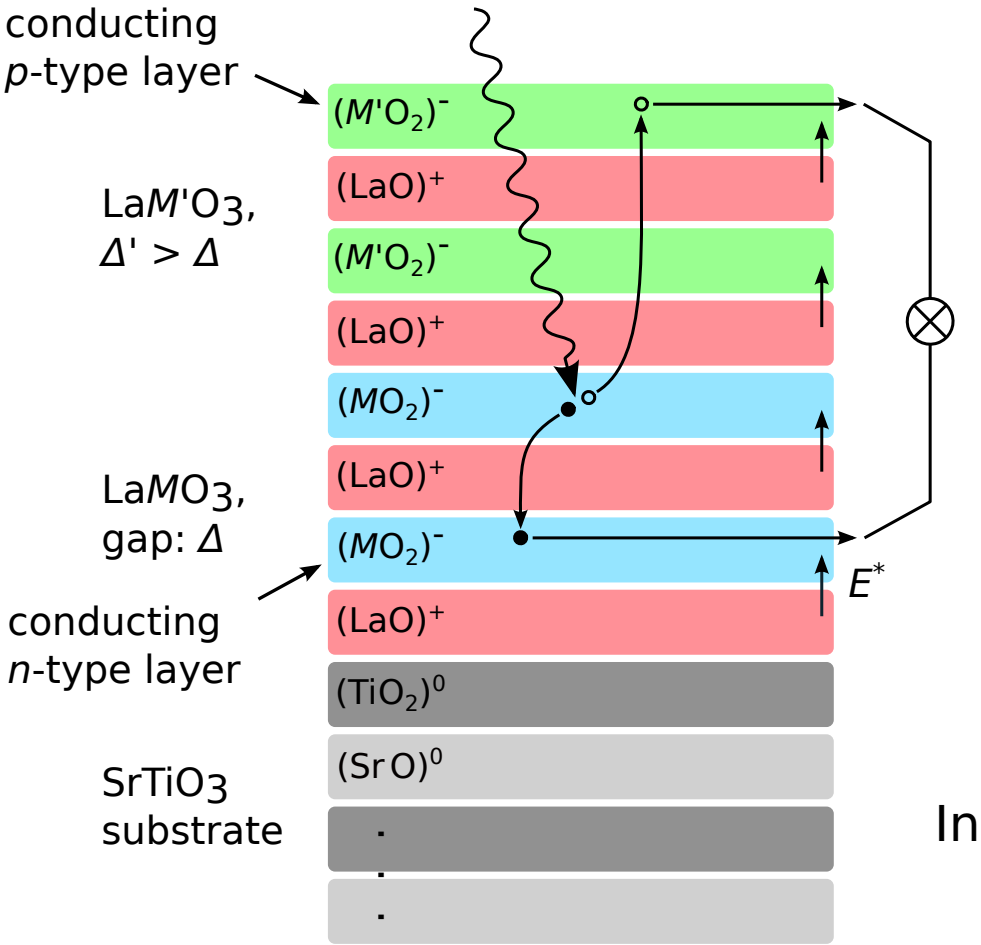



- heterostructures grown by pulsed laser deposition (PLD)

⇒ layer-by-layer band gap grading

- e.g., for a tandem cell, combine $LaVO_3$ and $LaFeO_3$ (gap: 2.2 eV)
- gradient, conducting interfaces persist

# Oxide heterostructures for efficient solar cells




1. large intrinsic electric field
2. conducting interface(s)
3. $LaVO_3$: direct gap 1.1 eV
4. combine oxides for gap grading

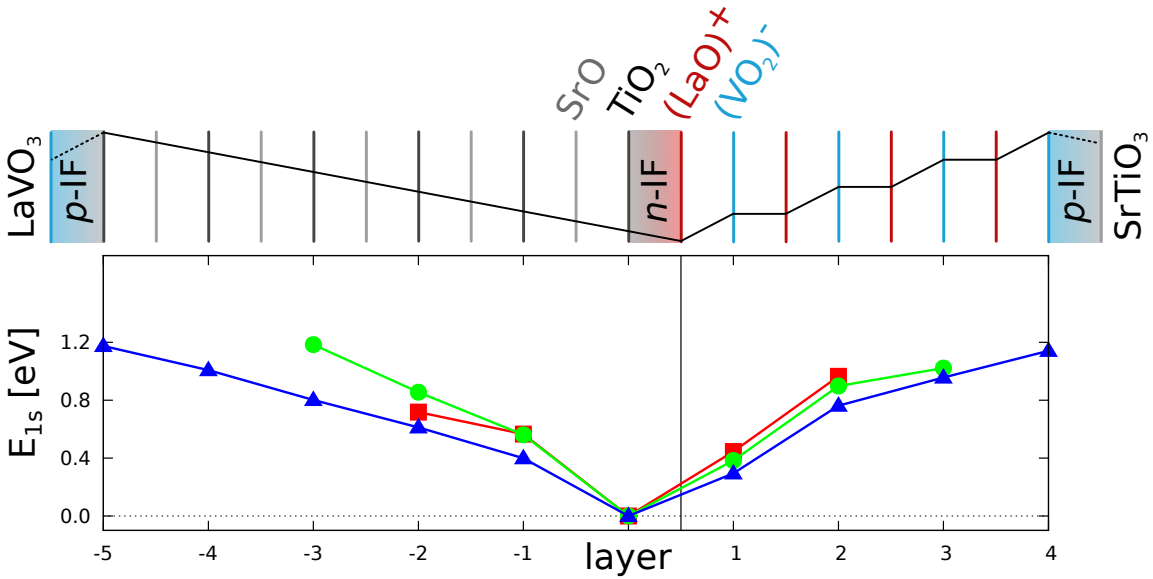
- experimental realization in work (R. Claessen & J. Pflaum)

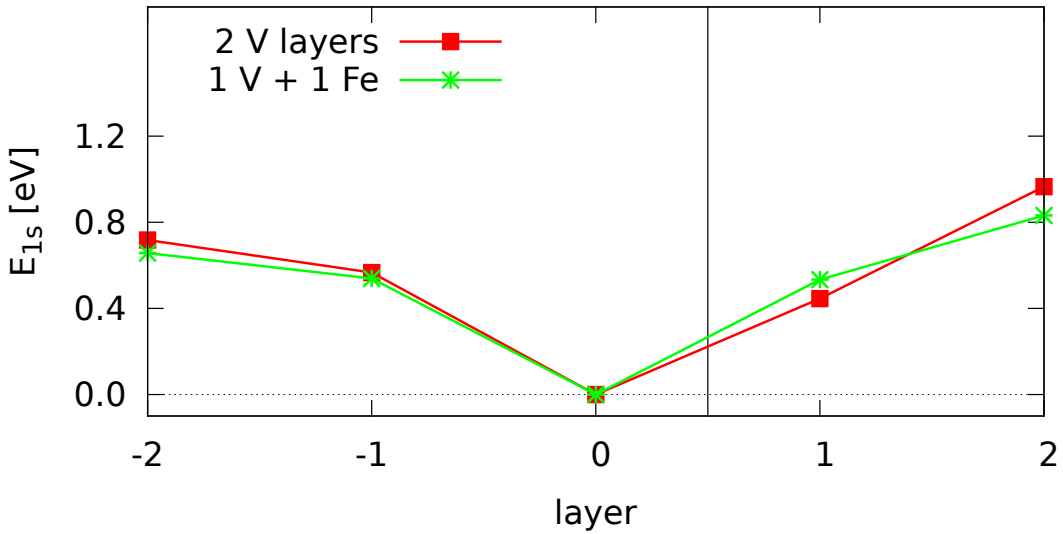
Interested? See PRL 110, 078701 (2013)


**Many thanks to:**

Peter Blaha, Ralph Claessen, Karsten Held, Robert Laskowski, Jens Pflaum, Satoshi Okamoto, Giorgio Sangiovanni, Zhicheng Zhong

# A closer look at the gradient




multi-layer:

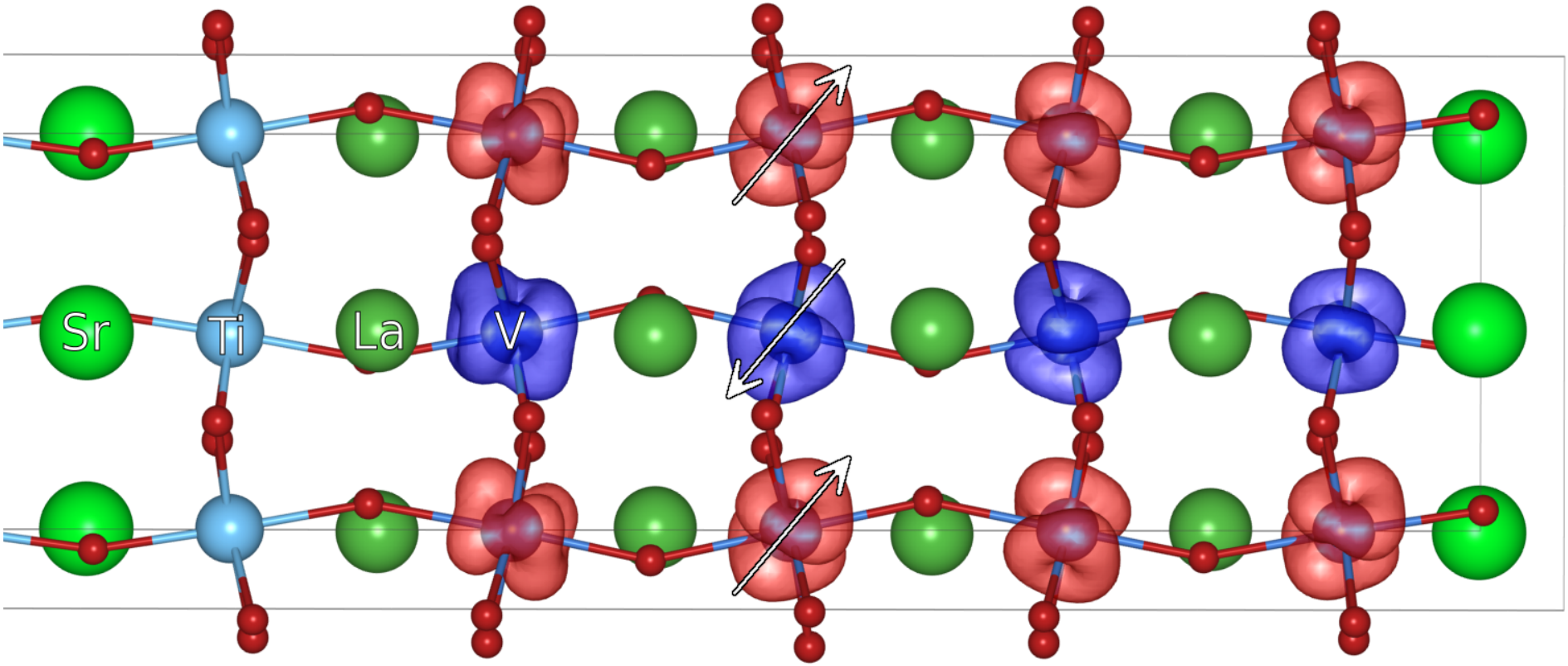
- potential gradient $\sim 0.3\,\mathrm{eV/u.c.}$
- repeated “V” due to PBC

tandem ($LaFeO_3|LaVO_3|SrTiO_3$):

- gradient very similar to $LaVO_3|SrTiO_3$

# Computational method

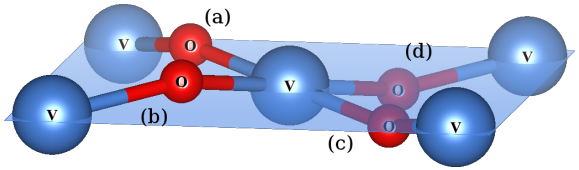
PBEsol GGA + $U_V = 3\,\text{eV}$, $U_{Ti} = 9.8\,\text{eV}$

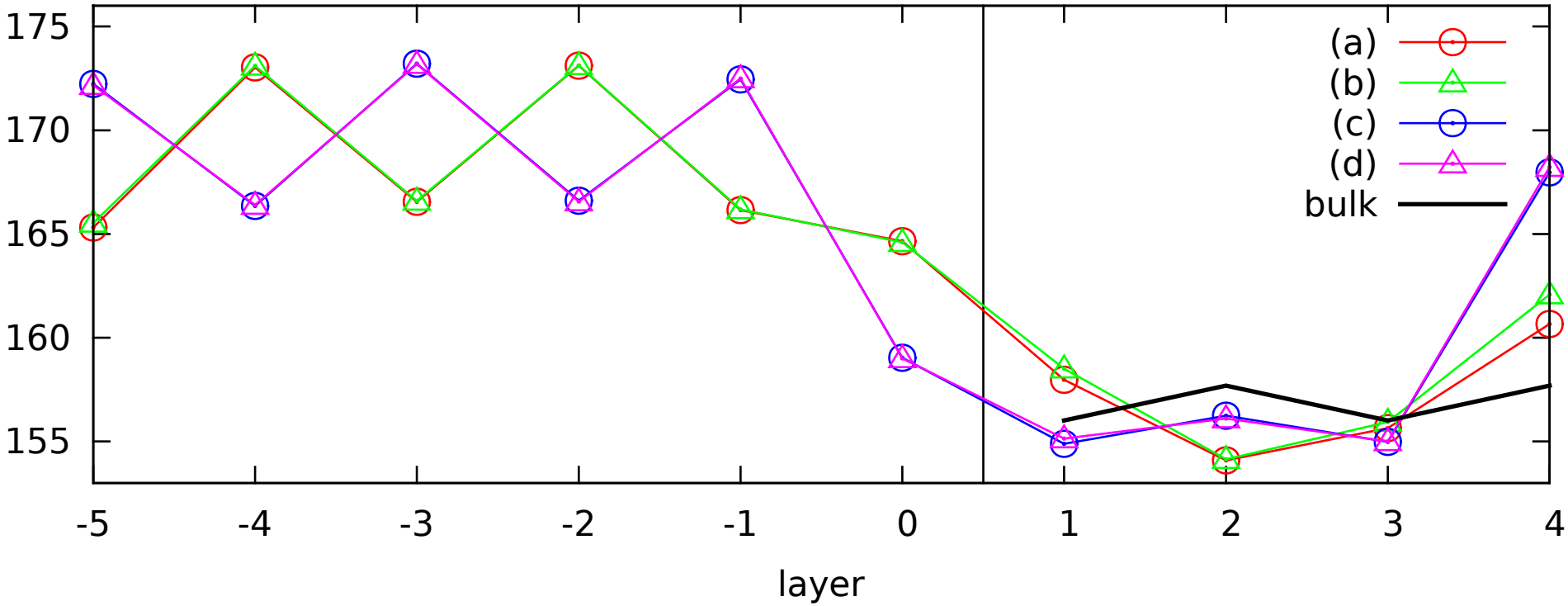


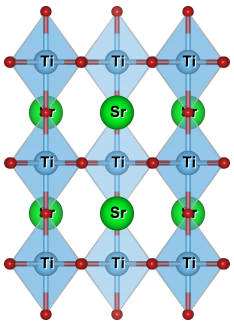

- spin order: AF-C
- orbital order: AF-G ($d_{xz}$ | $d_{yz}$)
- *multi-layer* vs. *thin-film*

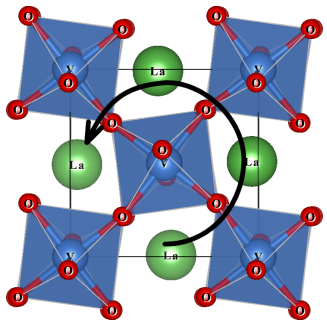
# *M*-O-*M* bond angle (*M* = V, Ti)

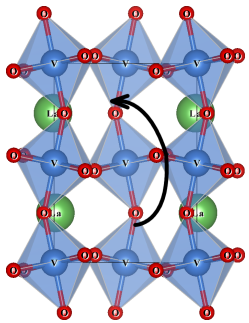
Lattice distortion in the heterostructure:



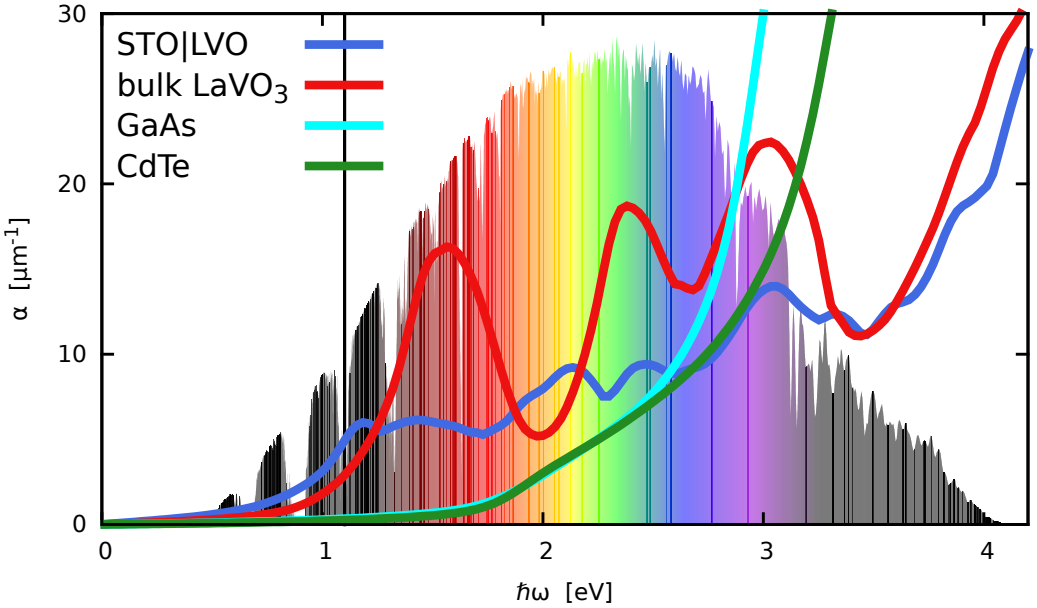



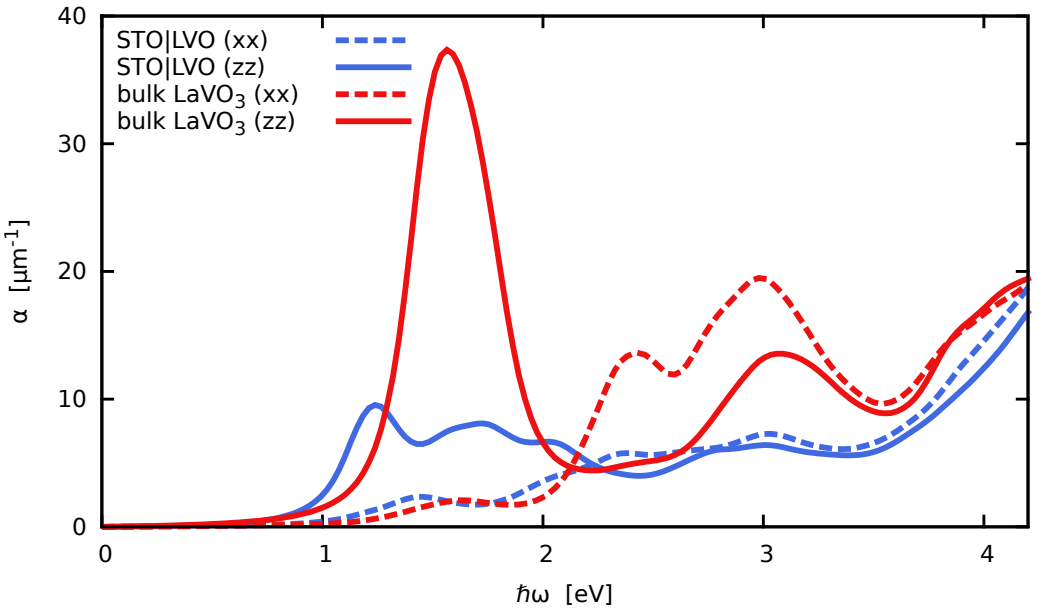



# $LaVO_3$ absorption: Details



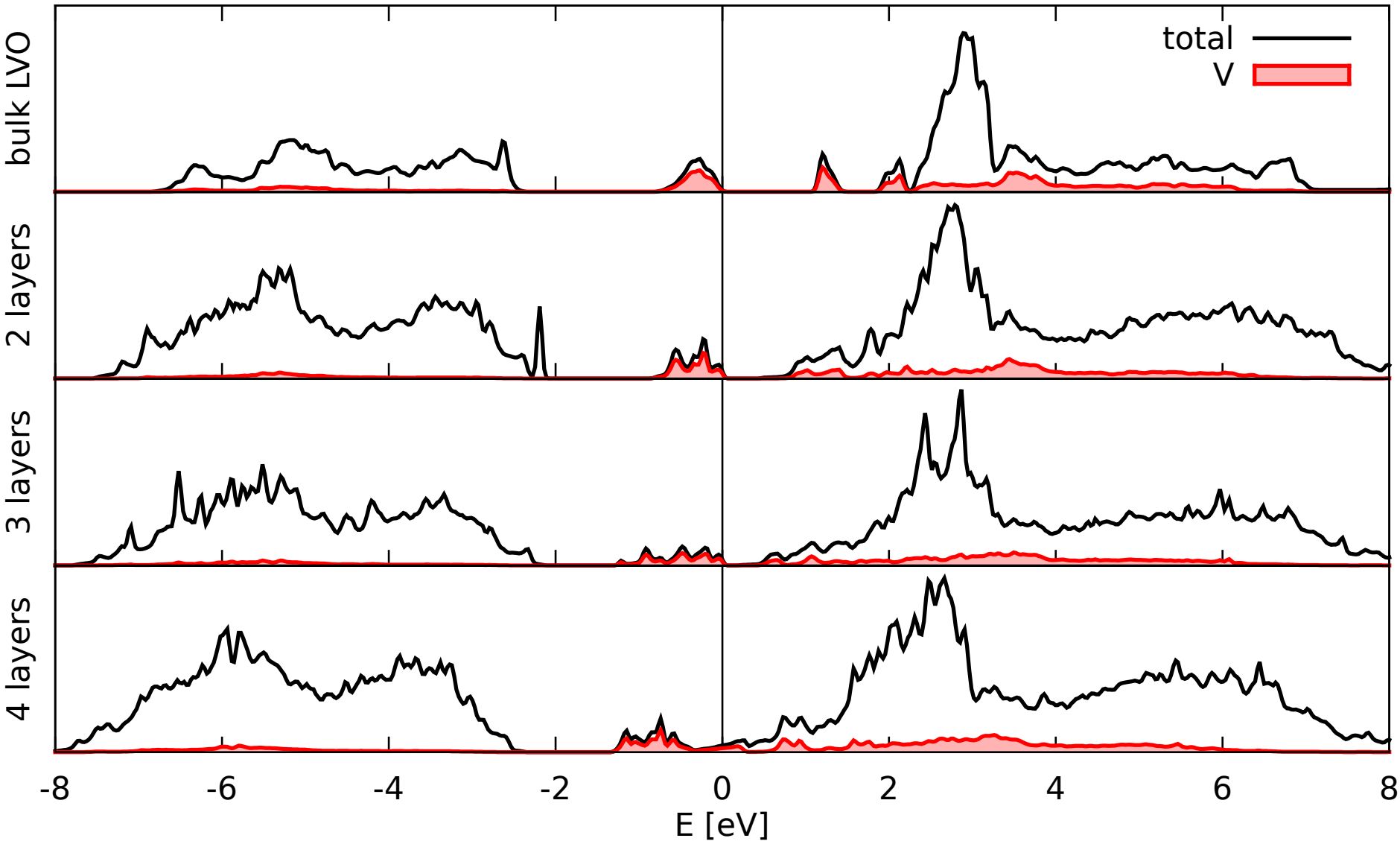




- Absorption: $I(x) \sim \mathrm{e}^{-\alpha x}$
- Lattice distortion: $\alpha(\omega) \rightsquigarrow \alpha_{ij}(\omega)$

$\rightsquigarrow$ for comparison, plot $\bar{\alpha} = \frac{1}{3}\sum_{ij} \alpha_{ij}$

back

# Total DOS for different heterostructure sizes




⇛ critical thickness: 4 layers $LaVO_3$