Oxide heterostructures for efficient solar cells

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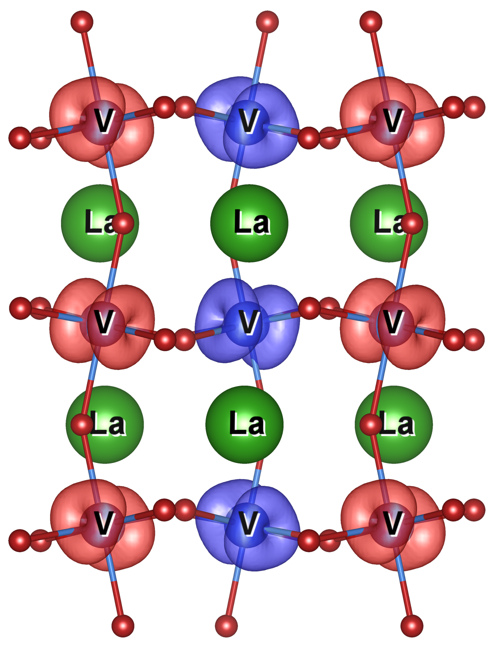
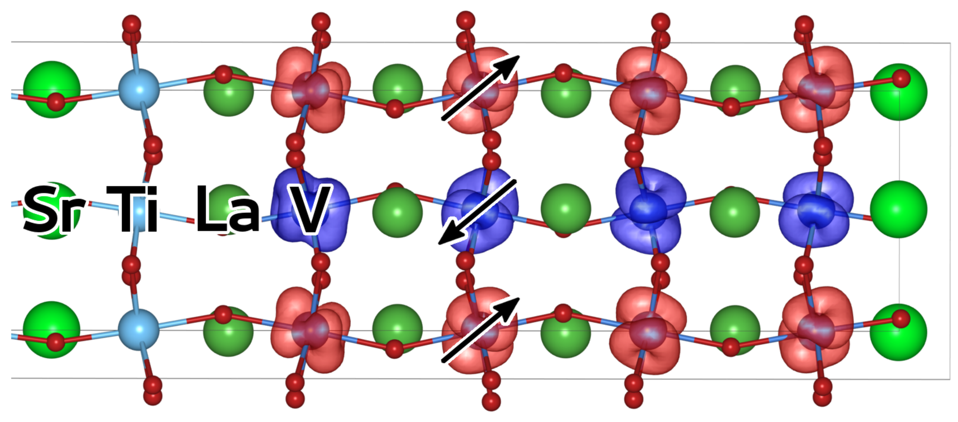
Bulk $LaVO_3$

- distorted perovskite
- d^2 Mott insulator
- direct band gap $\Delta = 1.1$ eV
- antiferromagnetic below 140 K
- strong optical absorption throughout solar spectrum

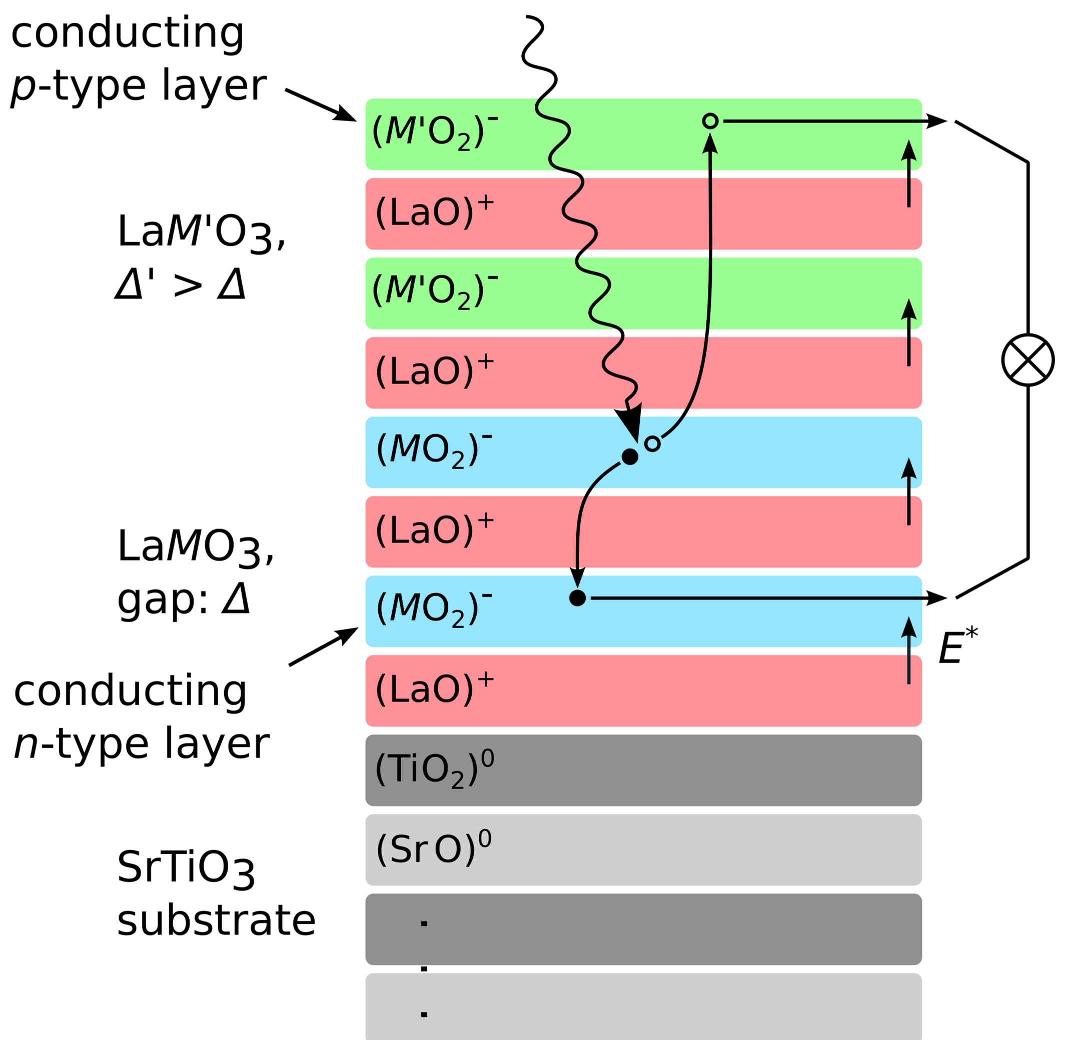


$LaVO_3|SrTiO_3$ heterostructure

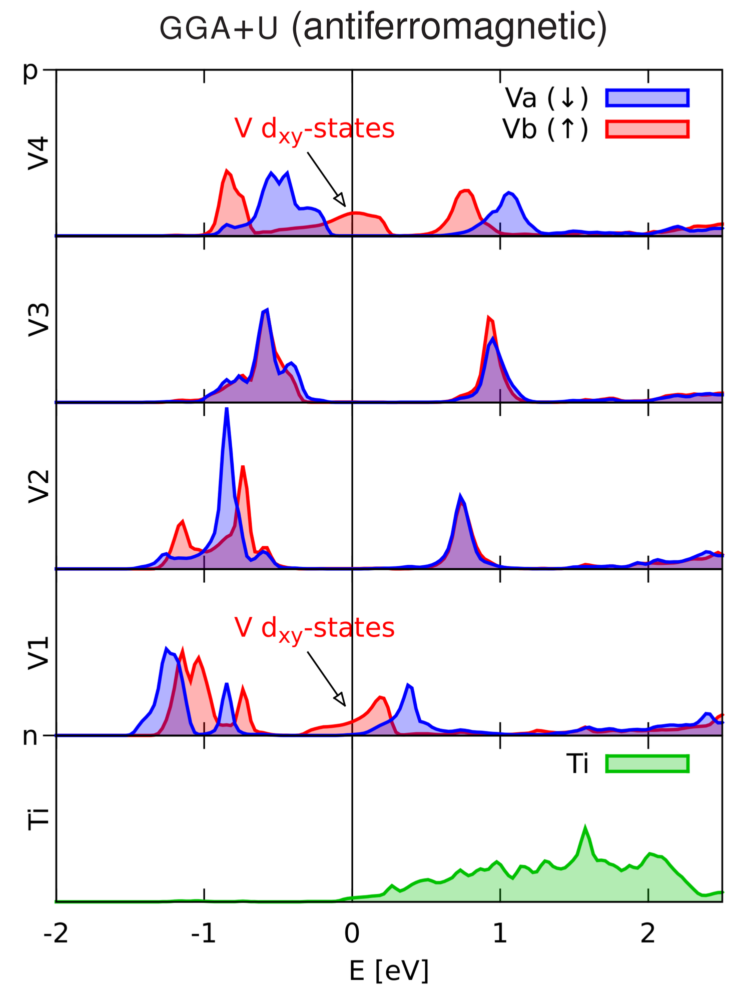


- polar|non-polar interface
  - potential gradient
  - conducting interface above critical thickness ~ 4 atomic layers
  - 2d electron gas

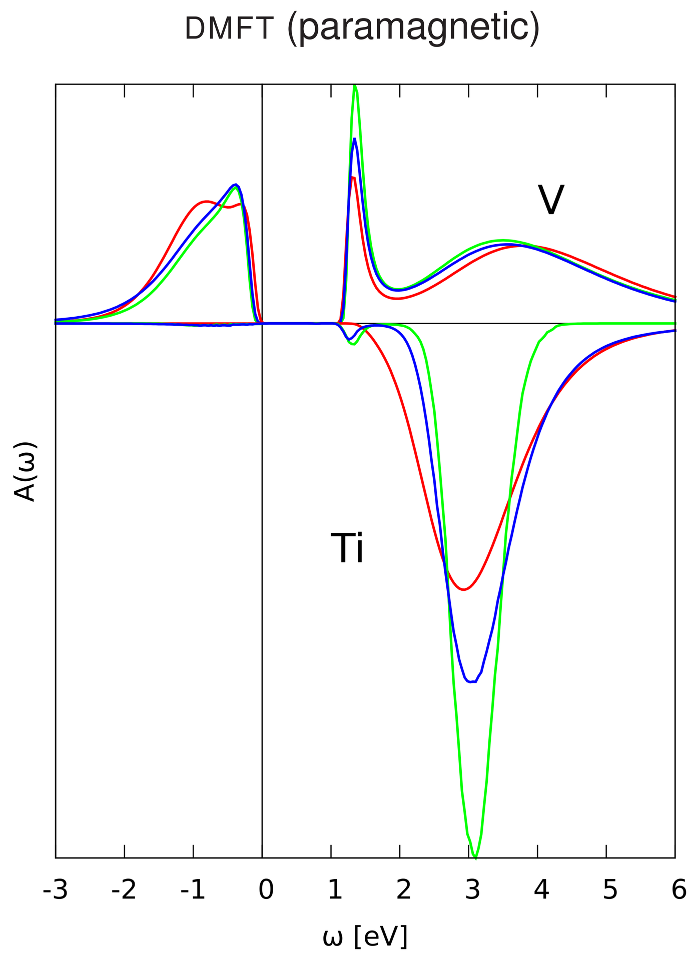
Proposal: $LaVO_3|SrTiO_3$ as absorbing material



- direct band gap ~ 1.1 eV in optimal range
- may be combined with other oxides for band-gap grading
- extraction of charge-carriers through conducting interface and possibly surface
- intrinsic electric field separates photo-excited charge carriers

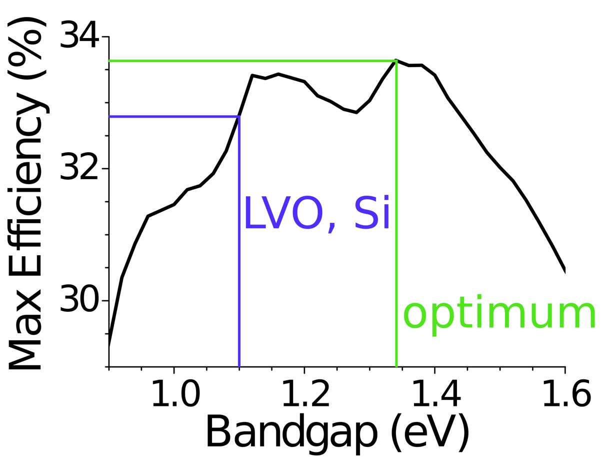


DOS for 4+6 layers $LaVO_3|SrTiO_3$



spectral function for 1+1 layers

Shockley-Queisser limit



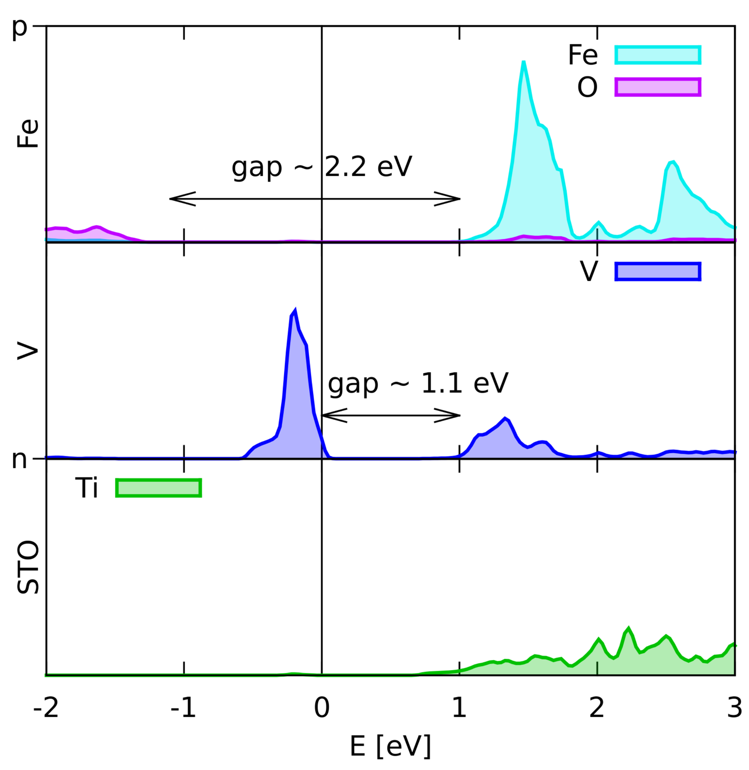
[from Wikipedia]

- 2 major sources of energy loss:
  - photons below gap are lost
  - excess energy above gap is lost

Band-gap grading with oxides

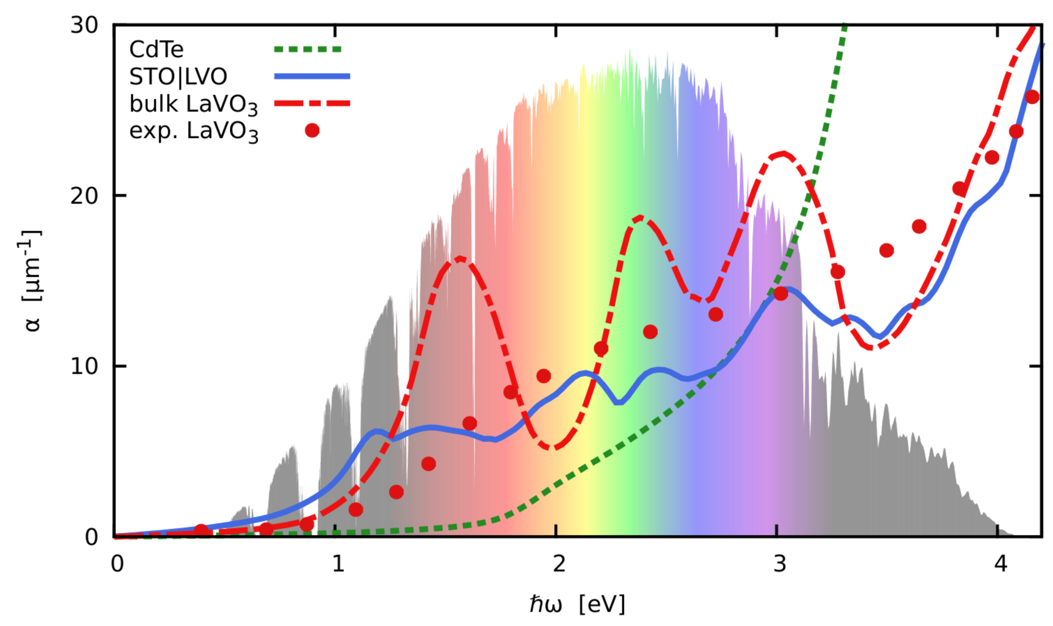
- "tandem" solar cells: smaller gap materials underneath
- $LaVO_3$ can be combined with $LaFeO_3$ (gap: 2.2 eV) or other oxides

⇒ gap-graded design in unprecedented flexibility



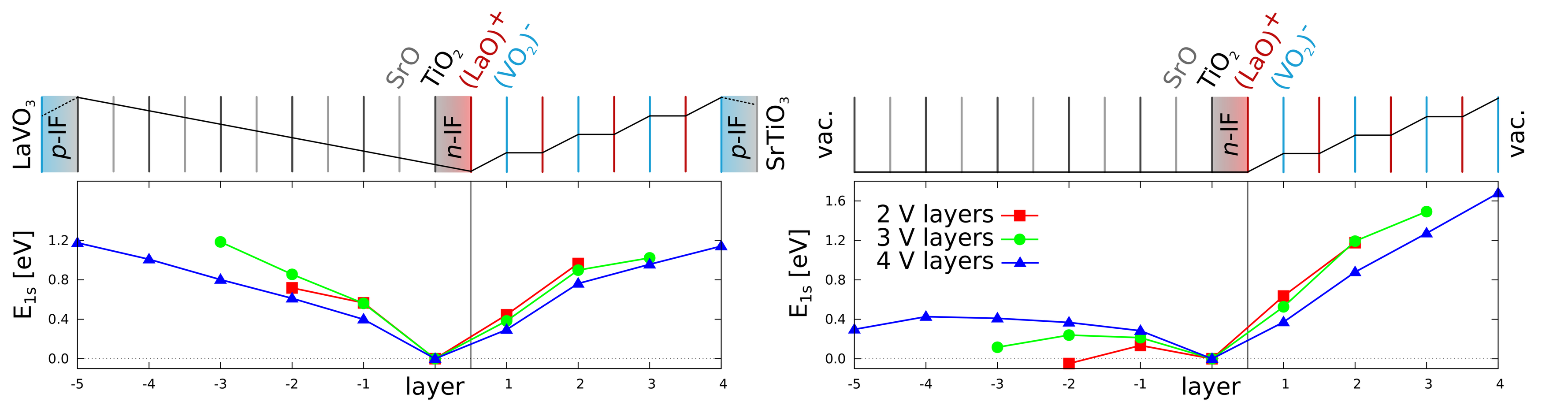
layer-resolved partial DOS in $LaFeO_3|SrTiO_3$

Optical absorption



$LaVO_3$ compares favorably with standard thin-film absorber CdTe

Polarization and potential gradient in $LaVO_3|SrTiO_3$



Schematic of expected layer polarization and internal electric field, compared with DFT results for a supercell (left) and thin film (right)

Experimental support

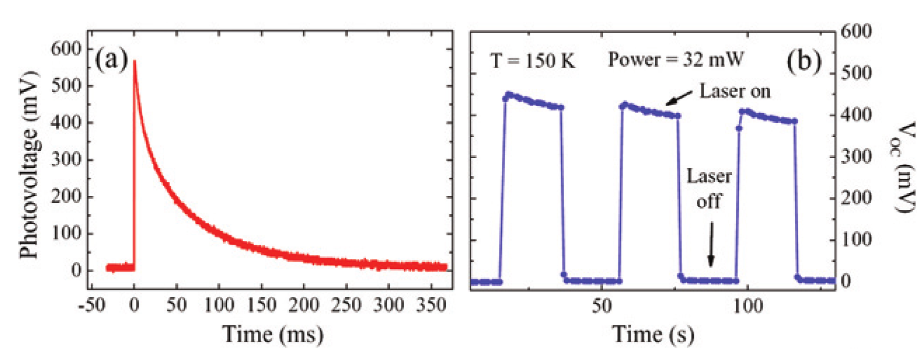
PV effect has been measured in

$LaAlO_3|SrTiO_3$ by Liang *et al.*

$Bi_2Sr_2Co_2O_y|Nb{:}SrTiO_3$ by Guo *et al.*

⇒ residual gradient exists

⇒ solar cell feasible in principle



BSCO|SNTO photovoltage under (a) pulsed (b) steady illumination. [From Guo *et al.*]

References

LAO|STO: A. Ohtomo and H.-Y. Hwang, Nature 427, 423 (2004); Z.S. Popović, S. Satpathy, and R.M. Martin, PRL 101, 256801 (2008)

LVO|STO: Y. Hotta, T. Susaki, and H.Y. Hwang, PRL 99, 236805 (2007)

Potential gradient: N. Nakagawa *et al.*, Nature Mater. 5, 204 (2006)

LAO|STO experiment: H. Liang *et al.*, Sci. Rep. 3, 1975 (2013)

BSCO|SNTO experiment: H.-Z. Guo *et al.*, EPL 103, 47006 (2013)

Schockley-Queisser: W. Shockley and H.J. Queisser, J. Appl. Phys. 32, 510 (1961)

this work: PRL 110, 078701 (2013)

Conclusions

We propose a **novel absorbing material** for efficient solar cells: heterostructures of insulating transition-metal oxides, specifically **$LaVO_3$** grown on **$SrTiO_3$** along the [0 0 1] direction.

- $LaVO_3$ has a **direct band gap in the optimal range**
- **Potential gradient** in $LaVO_3|SrTiO_3$ may **suppress recombination**
- **strong optical absorption** across solar spectrum
- can combine with e.g. **$LaFeO_3$** for **band-gap grading**
- above the "critical thickness" the interface becomes conducting; **conducting interfaces** may help to **extract charge carriers**