APS March Meeting

Oxides related to CdTe solar cells

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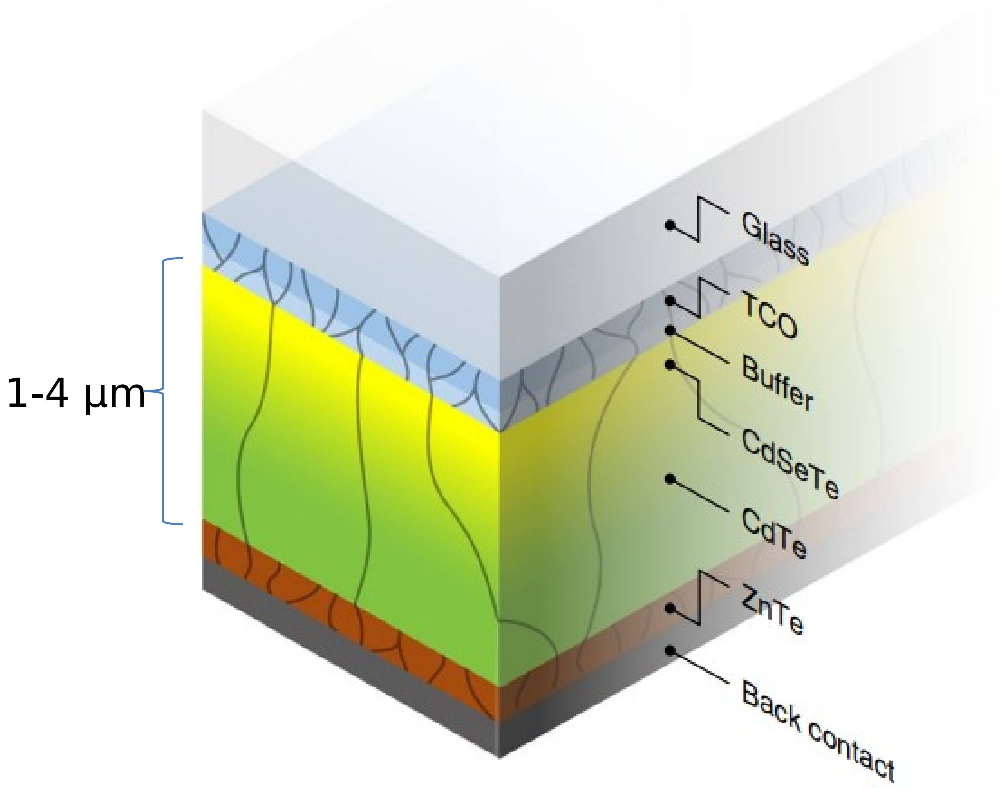
ACCESS Advancing Innovation

CdTe solar cells

- One of the most important thin-film photovoltaic (PV) technology, commercially available
- Direct band gap of 1.5 eV → absorption coefficient 10 times that of Si
  - low production cost
  - record efficiency in the lab > 22%
  - record efficiency is 19% in modules (First Solar)

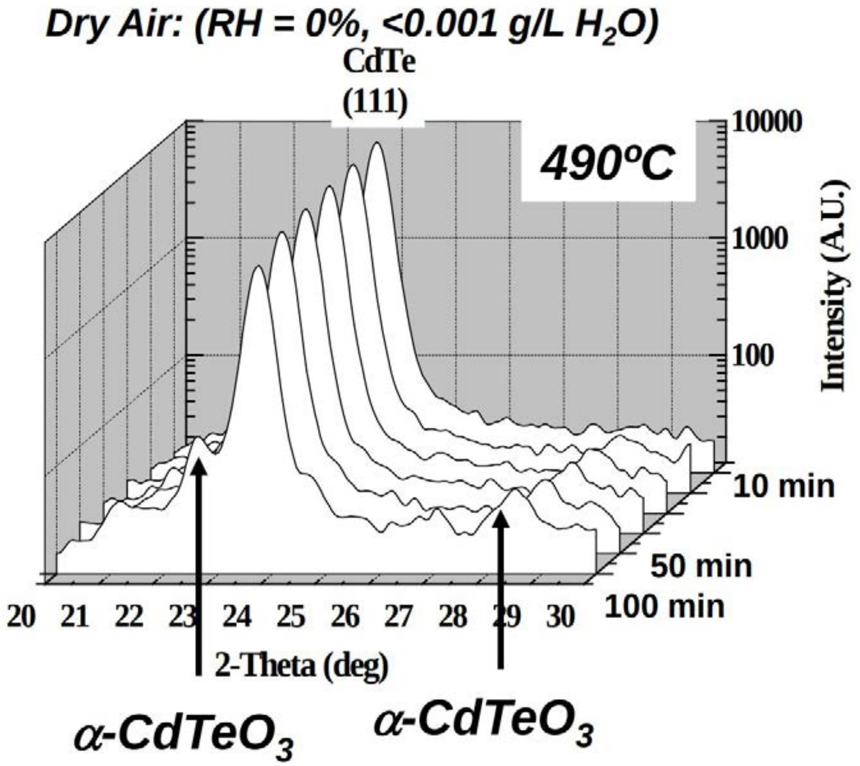
- Current limitations:
  - low V_{oc}, << E_g
  - low hole concentrations ~10^{14} cm^{-3}
  - As-doped layers show low doping efficiency
  - short carrier lifetimes
  - Polycrystalline films
    - → recombination at grain boundaries
    - → role of possible oxide formation



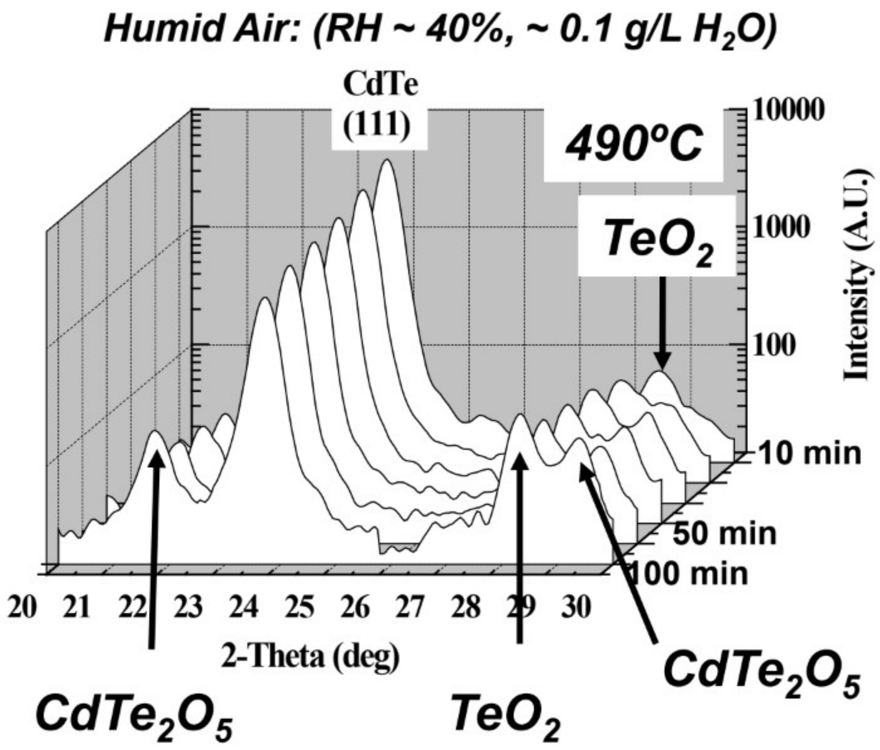
Metzger *et al.* Nat. Energy **4,** 837 (2019)

Signatures of oxide formation in CdTe thin-films

- $CdCl_2$ post-deposition treatment is needed for high-efficiency CdTe solar cells
- → Can produce surface oxidation if environment is not free of oxygen

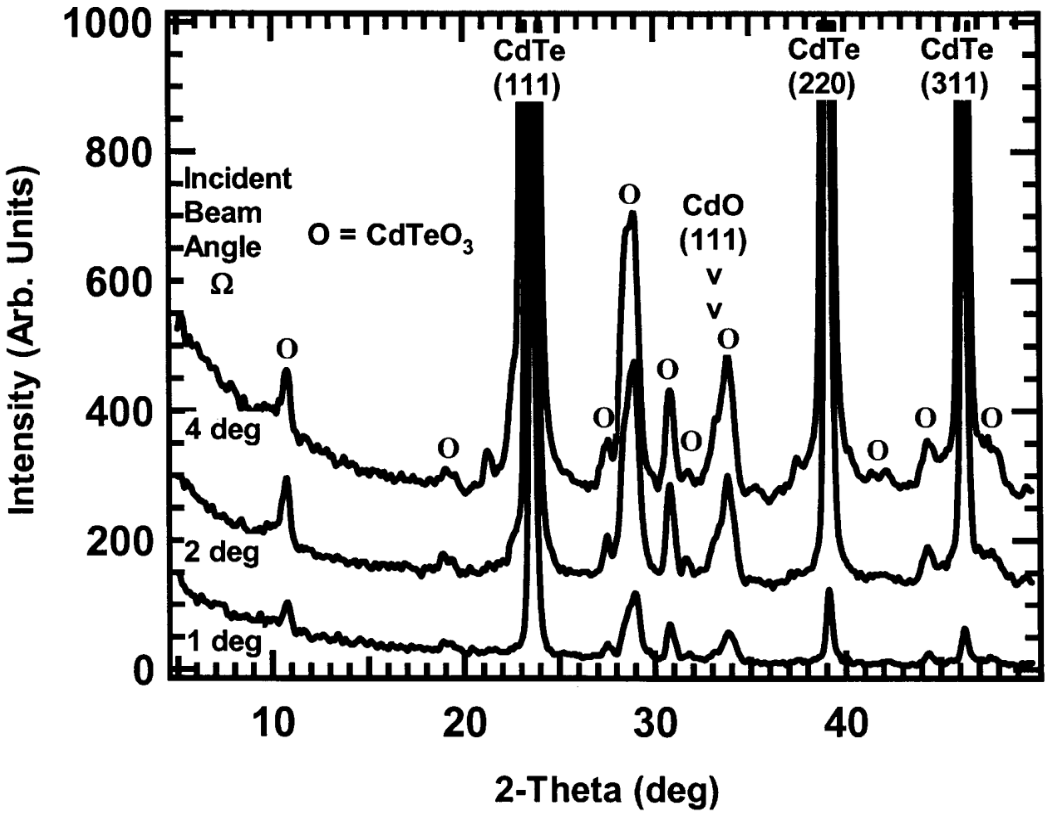


- Dry environment
- Formation of α-$CdTeO_3$ is observed
- CdTe intensity increases as oxide intensity decreases with time



- Humid environment
- Formation of TeO_2 and then $CdTe_2O_5$
- CdTe intensity increases as oxide intensity decreases

Signatures of oxide formation in CdTe thin-films



McCandless *et al*. Thin Solid Films **431**,249 (2003)

- CdO with $CdTeO_3$ were also observed after $CdCl_2$ air treatment

Benefits/problems of oxide formation

- Surface/defects passivation

  → oxides can passivate surface defects and reduce recombination

  → reduce density of surface states to improve electronic properties
- Reduced carrier collection

  → reduce the carrier concentration by acting as a barrier to carrier transport
- Corrosion

  → high oxide concentration can lead to corrosion of the metallic contacts, descreaed performance and lifetime
- Contact resistance

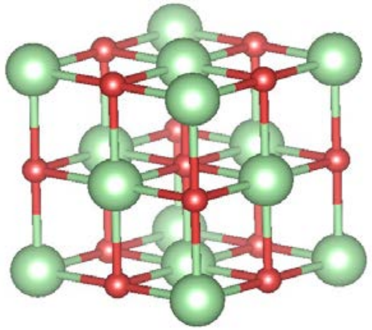
  → increase the contact resistance between the CdTe and the other layers, decreased efficiency

Effects of oxygen can be complex and depend on oxygen concentration and material processing

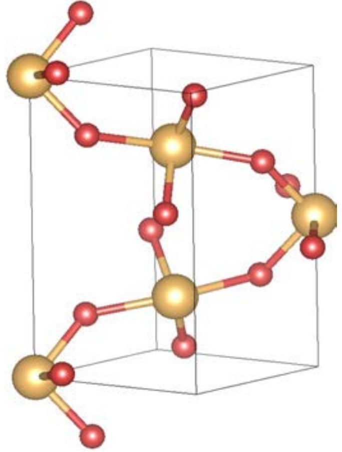
Possible oxides that form in CdTe thin-films

● Cd
● Te
● O

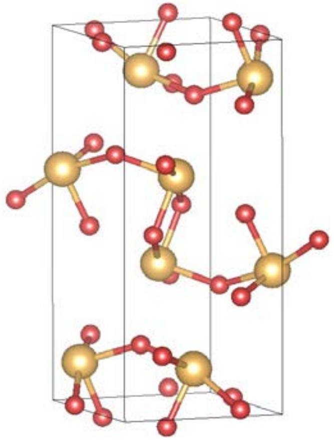
CdO
Fm-3m



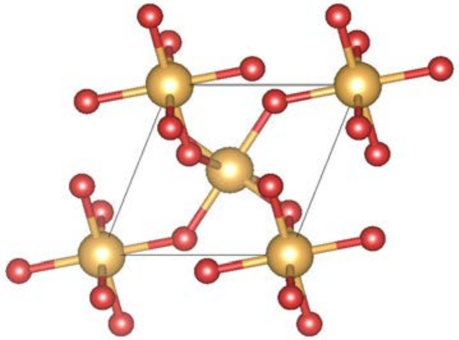
α-TeO_2
$P4_12_12$



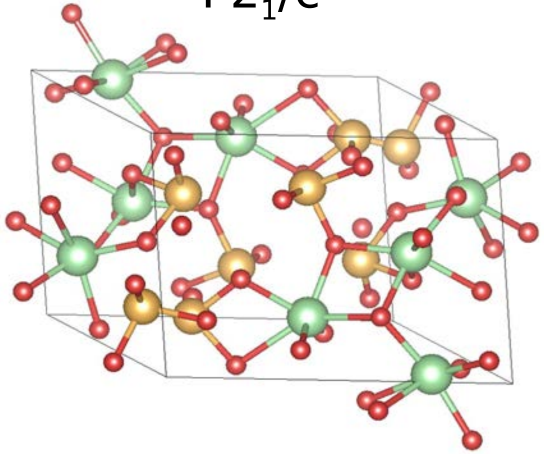
β-TeO_2
Pbca



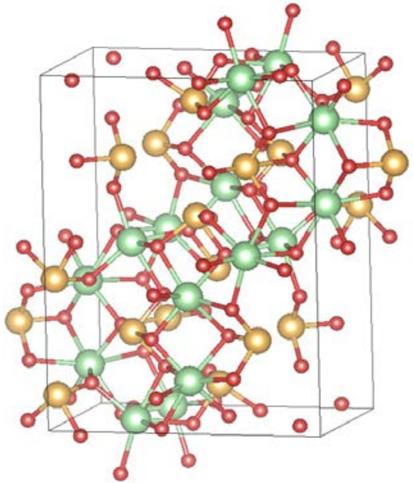
β-TeO_3
R-3c



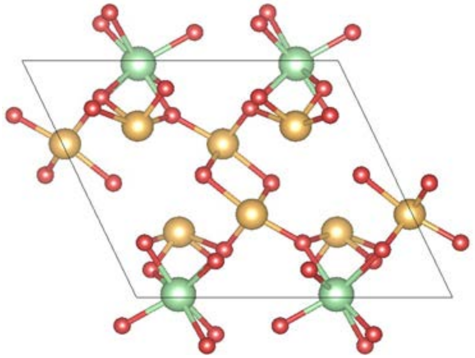
α-$CdTeO_3$
$P2_1/c$



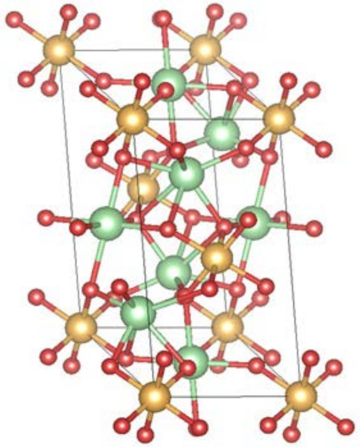
β-$CdTeO_3$
Pnma



β-$CdTe_2O_5$
$P2_1/c$



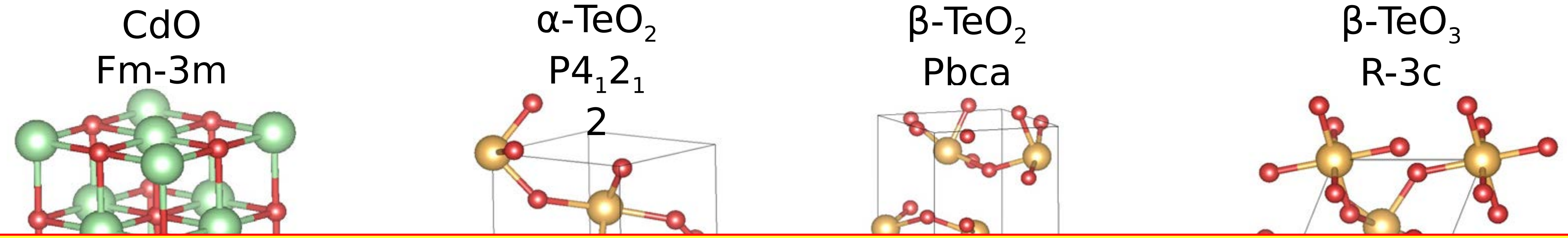
Cd_3TeO_6
$P2_1/c$



CdTe-associated oxides

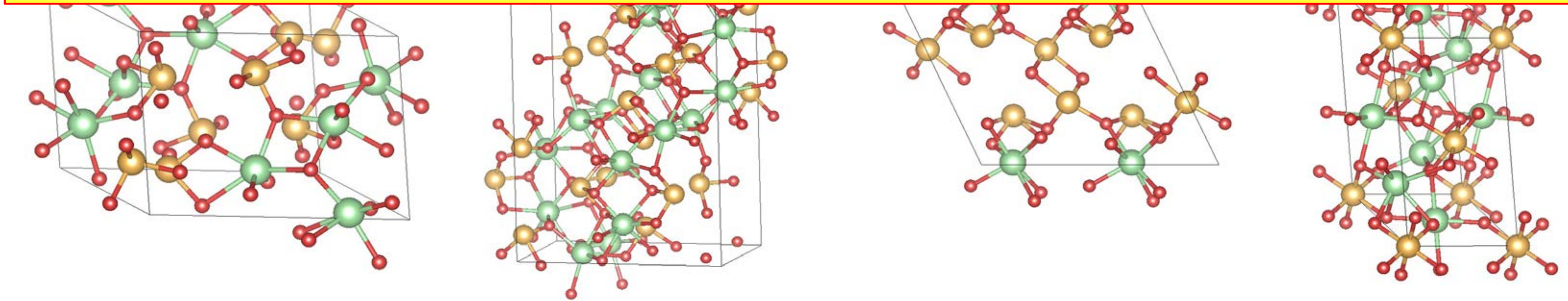
	Lattice parameters (Å) [DFT-GGA]	Lattice parameters (Å) [Exp.]	Band gap (eV) [HSE]	Bandgap (eV) [Exp.]
CdO	a= 4.66	4.674	0.86 (I) 2.34 (D)	0.84 (I) 2.28 (D)
β-$CdTeO_3$	a=7.37, b=14.48, c=11.03	7.458, 14.522, 11.046	3.55 (I)	3.55 (I)
α-$CdTeO_3$	a=7.82, b=11.17, c=7.36	7.79, 11.253, 7.418	3.98 (I)	3.91 (I)
Cd_3TeO_6	a=5.52, b=5.66, c=9.77	---	2.12 (D)	2.80 (D)
β-$CdTe_2O_5$	a=9.41, b=5.59, c=10.90	9.45, 5.58, 10.86	3.99 (I)	3.63 (I)
α-TeO_2	a=4.82, b=7.44	4.808, 7.612	4.00 (I)	3.75 (I)
β-TeO_2	a=5.34, b=5 .70, c=11.82	5.464, 5.607, 12.035	3.07 (D)	2.26 (D)
β-TeO_3	a=4.97, b=13.14	4.901, 13.03	2.54 (I)	3.25 (I)

Possible oxides that form in CdTe thin films



Except for CdO, they all have complicated crystal structures

How are their bands aligned to those of CdTe?



Band alignment calculations

- Determine valence-band-maximum (VBM) and conduction-band-minimum (CBM) with respect to vacuum level using slab calculations

1) Calculate the VBM and CBM with respect to the average electrostatic potential in a bulk calculation

2) Use a slab calculations to determine the average electrostatic with respect to the vacuum level

3) Align VBM and CBM with respect to the vacuum level

Band alignment calculations

→ In the case of zinc blende CdTe, use slabs with non-polar (110) surfaces

→ In the case of rocksalt CdO, use slabs with non-polar (001) surfaces

What to do in the case of complicated crystal structures?

Transform the complicated structure into a more symmetric, manageable crystal structure with the same volume/formula unit

Use this more symmetric crystal structure to extract the average electrostatic potential in the bulk region with respect the vacuum region

But why we can do that?

Band alignment calculations

What to do in the case of complicated crystal structures?

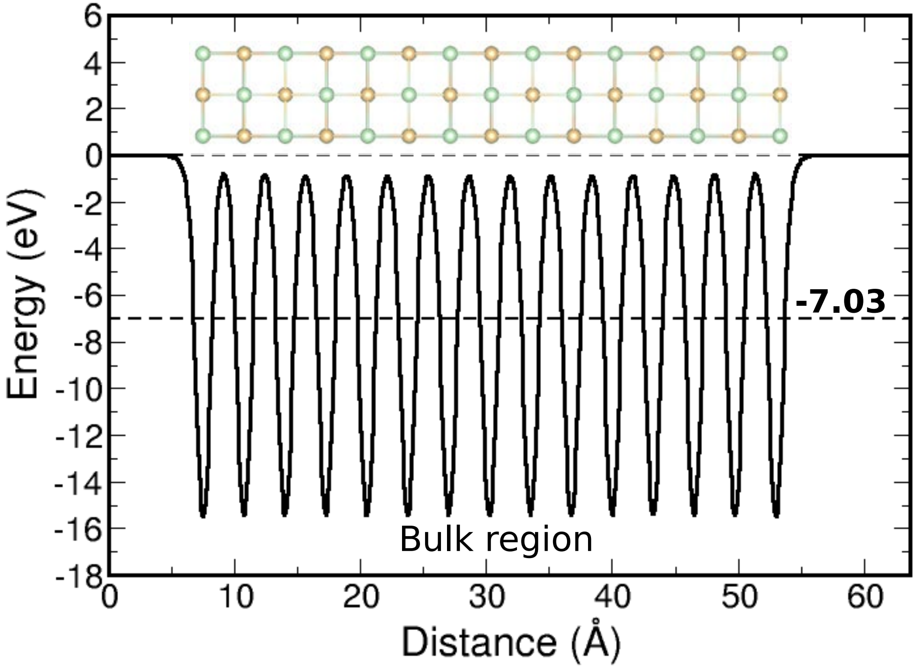
Transform the complicated structure into a more symmetric, manageable crystal structure with the same volume/formula unit

Use this more symmetric crystal structure to extract the average electrostatic potential in the bulk region with respect to that of the vacuum region

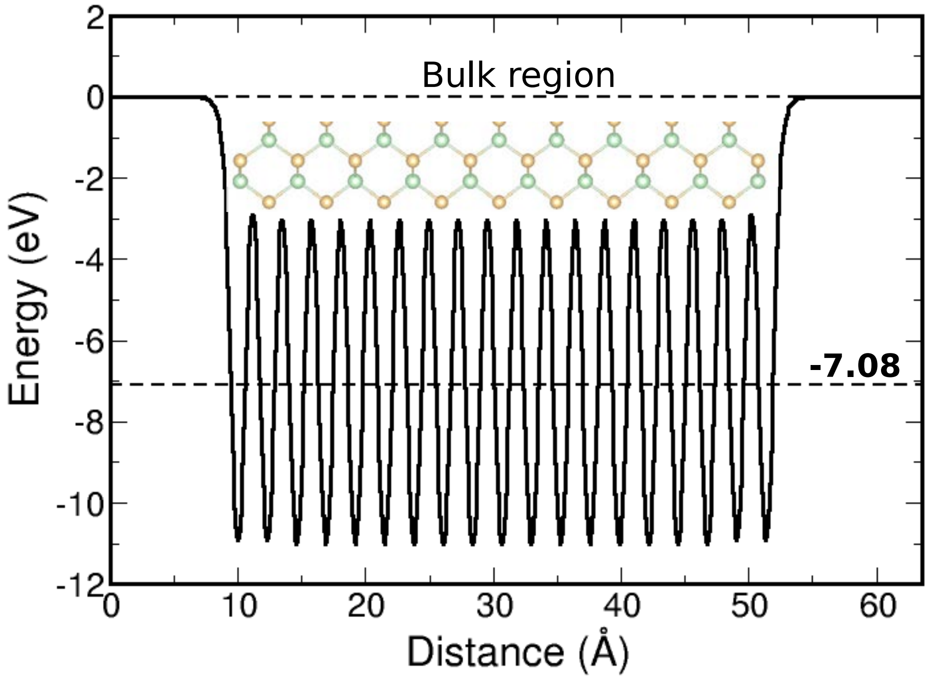
The average electrostatic potential does not depend on the crystal structure as long as they have the same volume!

Ex.: CdTe rs vs. zb

Rock salt slab



Zinc-Blende slab



Band alignment calculations

What at to do in the case of complicated crystal structures?

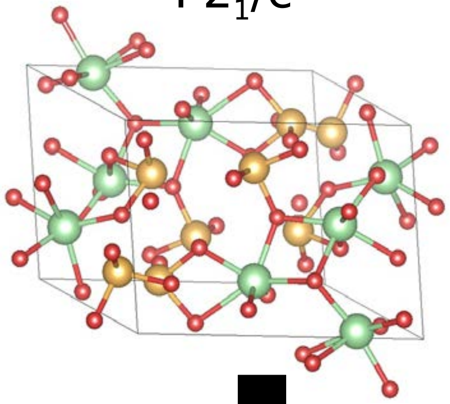
Transform the complicated structure into a more symmetric, manageable crystal structure with the same volume/formula unit

Use this more symmetric crystal structure to extract the average electrostatic potential in the bulk region with resect to that of the vacuum region

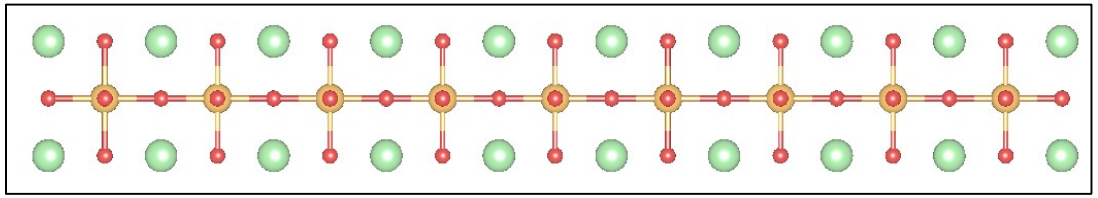
But one have to be careful with surface termination!

- average electrostatic potential in $CdTeO_3$ slab depends surface termination,

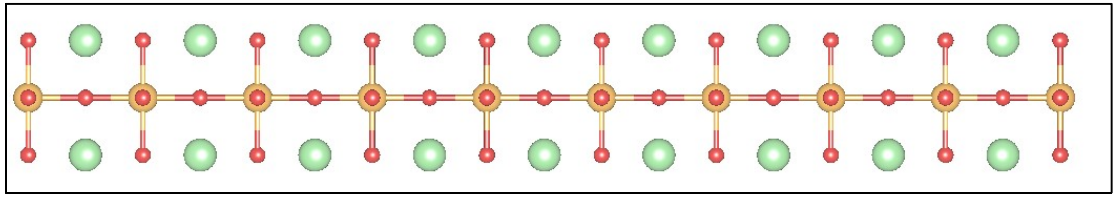
  i.e., TeO2 vs. CdO in the case of (001) orientation



α-$CdTeO_3$
$P2_1/c$

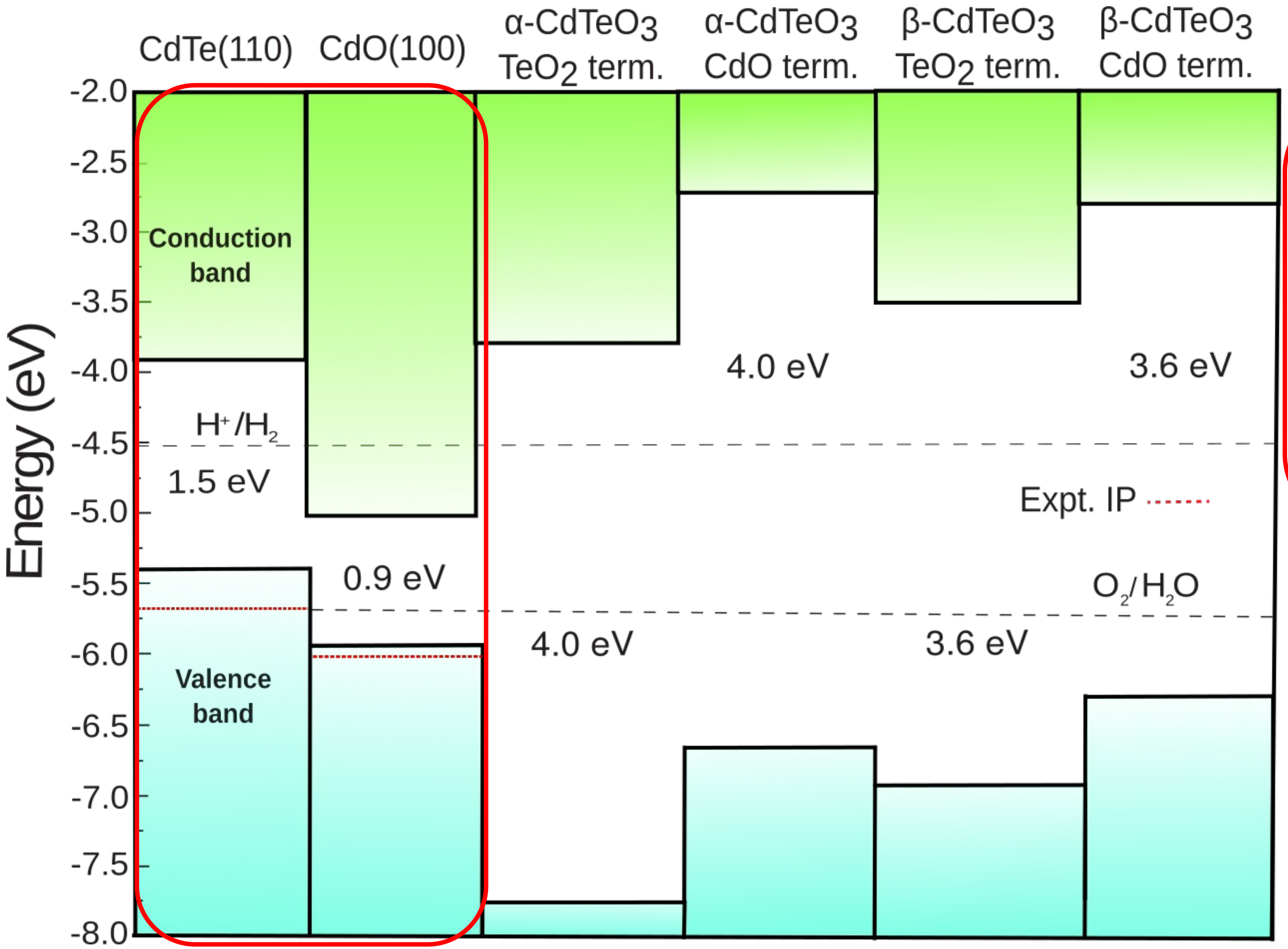


CdO termination



TeO_2 termination

Band alignments between CdTe and its oxides



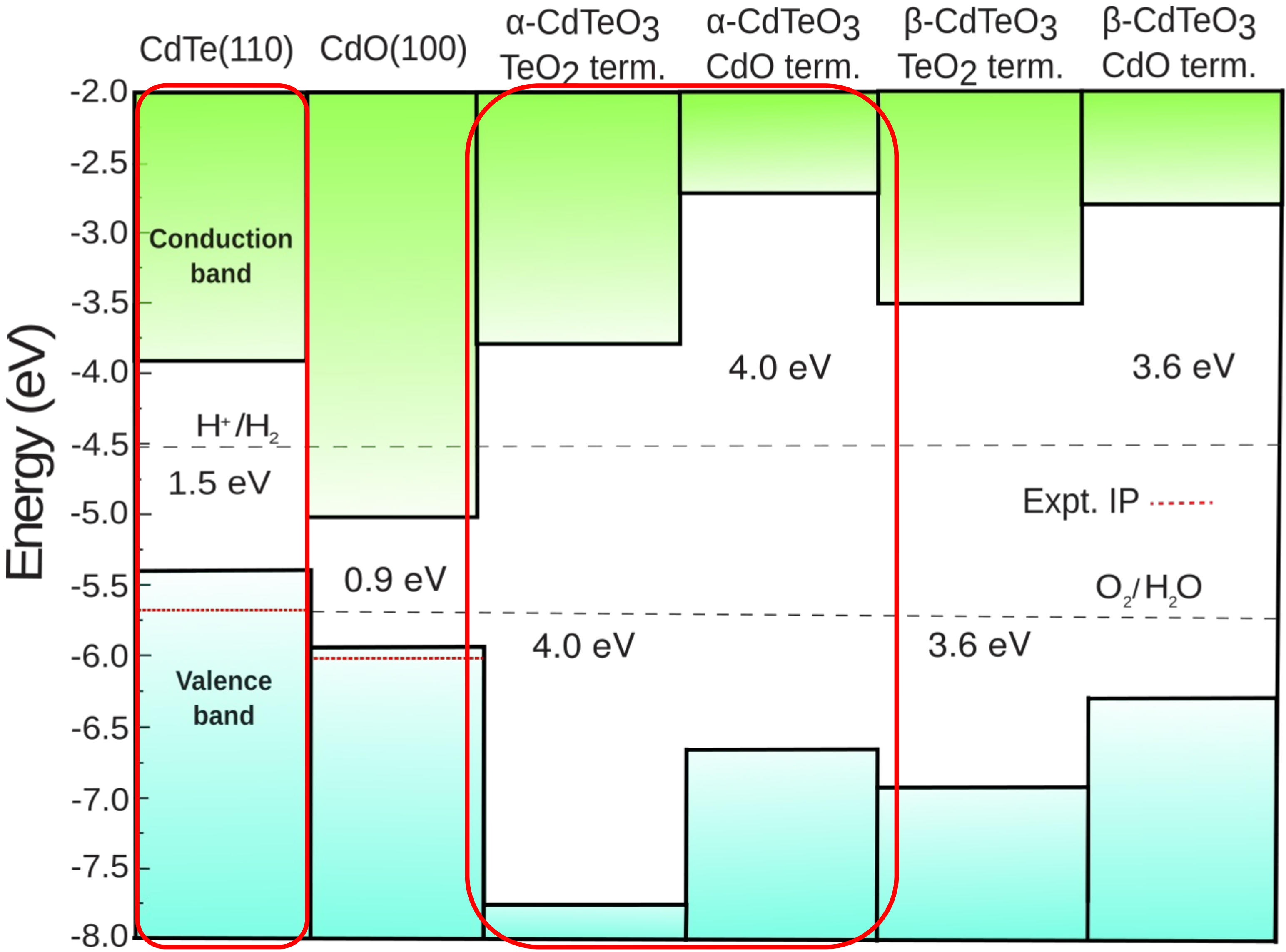
CdO/CdTe

- VBM of CdO is 0.6 eV lower than in CdTe
- CBM of CdO falls inside the gap of CdTe
  → potentially a problem for solar cells

$CdTeO_3$/CdTe

- No states inside the band gap of CdTe
  → passivation effects?
  need to consider details of the interface, such possible dangling bond states

Band alignments between CdTe and its oxides



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need to consider details of the interface, such possible dangling bond states

Summary and conclusions

- Most Cd-Te-related oxides have large band gap, except CdO (~1 eV) and Cd_3TeO_6 (~2 eV)
- Formation of CdO at grain boundary can be problematic: conduction band lies in the gap of CdTe
- $CdTeO_3$ may passivate grain boundaries, since there are no states in the gap of CdTe
- Next step: need to consider details of the interface CdTe/oxide

Thank you for your attention!