Modeling of CdSeTe device properties and operatio

Dmitry Krasikov
First Solar
Senior Member of ˉ
Dmitry.Krasikov@first

First Solar

LEADING THE WORLD'S
SUSTAINABLE ENERGY FUTURE

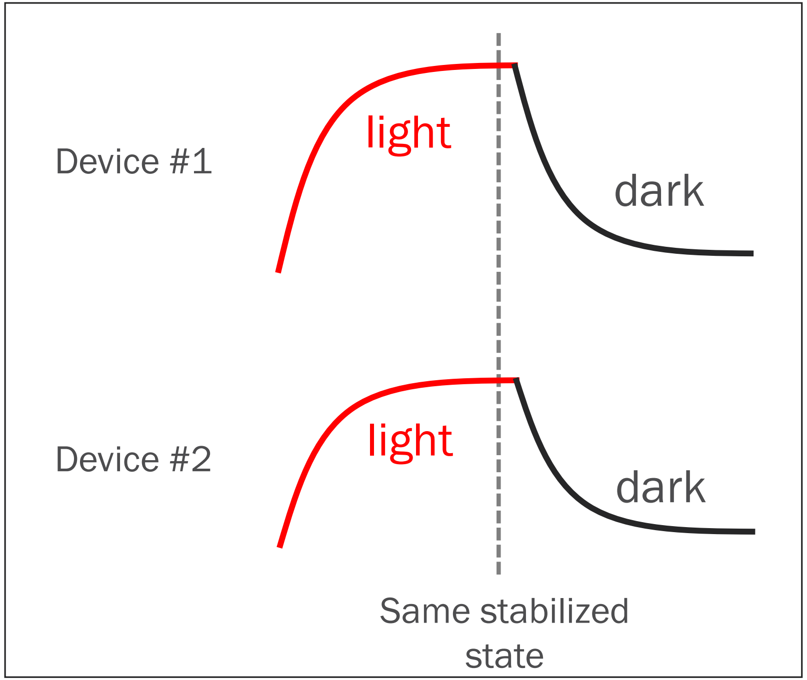
Outline

- What do we model? (snapshots of stabilized device)
- 1D model features
- Losses of V_{oc} and P_{mp} at contacts
- Some signatures of $V_{oc}(T)$, FF(T)
- Prospects of thin absorber

Mind the device state

Stress (T, light, V) ⟶ <u>device state</u> ⟶ V_{oc}(T), FF(T)

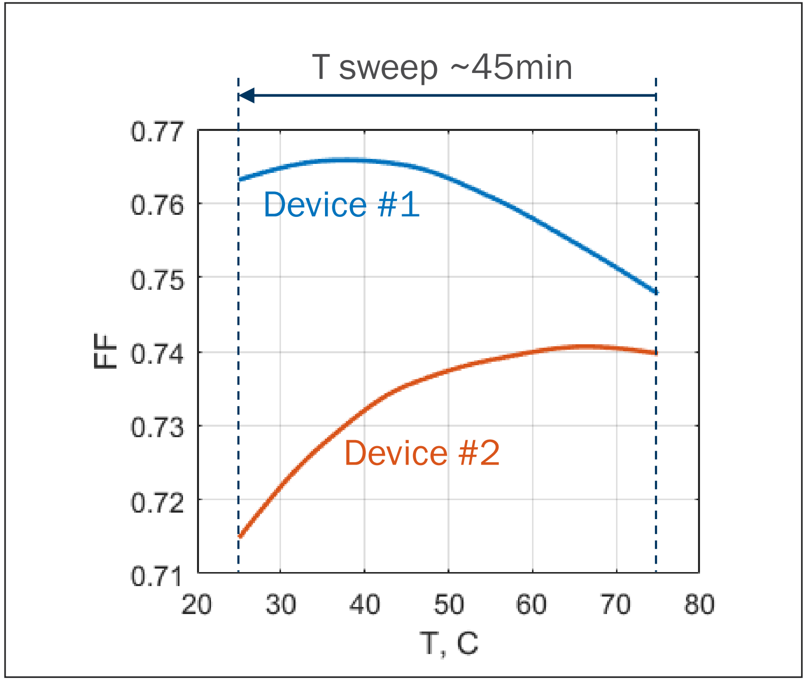
- Stabilize device state
  (SC ≠ MPP ≠ OC)
- Beware of dark soak
- Do not compare different devices in different states



Measure IVT

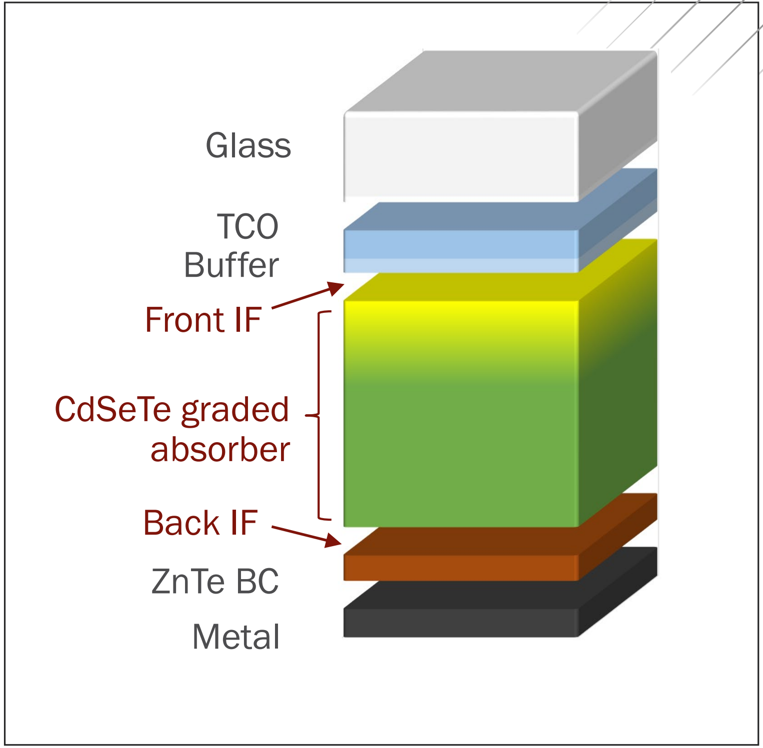
Stress (T, light, V) → device state → $V_{oc}(T)$, FF(T)

- IVT bears lots of physics
- IVT preceeded by stabilization
- IVT is fast (snapshot of state)

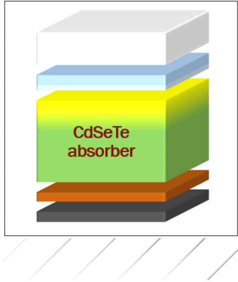


Model of a stack

- Mapping problem to 1D
- Lots of unmeasurable parameters
- Most critical parts:
  - Front IF
  - Absorber
  - Back IF

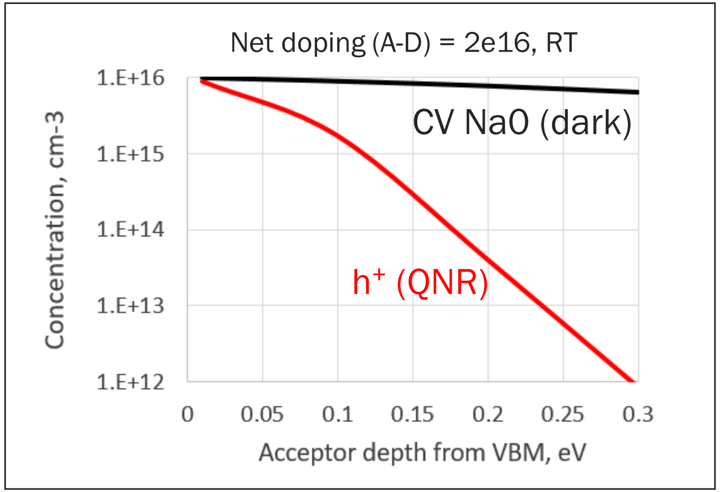


CdSeTe absorber with graded Se

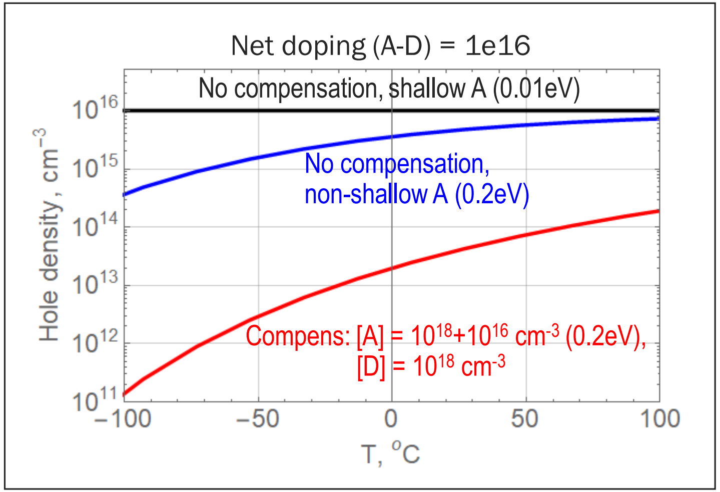


1. Compensated doping: net doping = [A]−[D]
2. Non-shallow acceptors: h^+ << net doping
3. Temperature-dependent hole density
4. Higher Se%: Affinity↑, E_g↓, VBM↓, deeper acceptors (p^+↓)

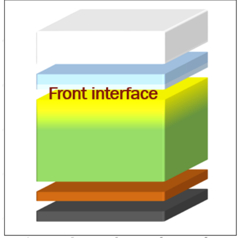
SCAPS model



0D charge-neutrality model

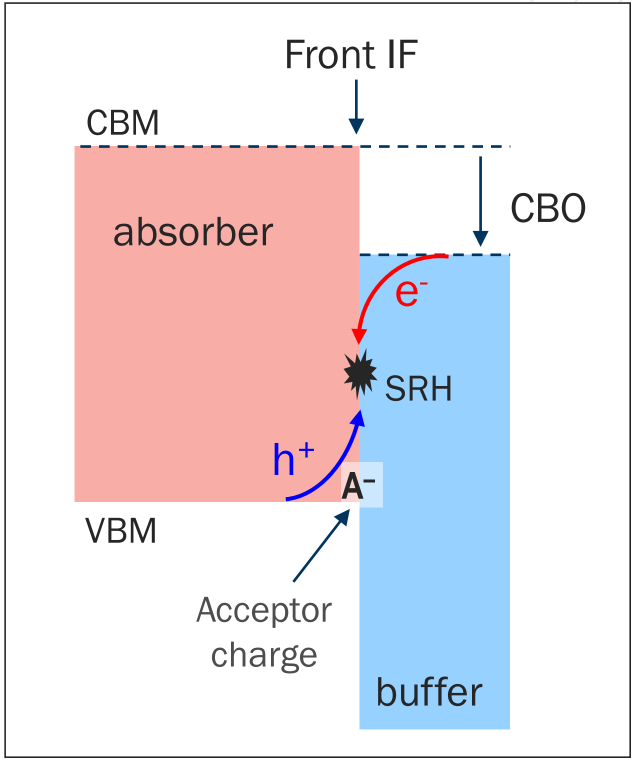


Effective 1D model of front interface

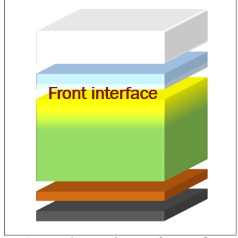


Main IF parameters:

1. **Conduction band offset (CBO)**
   - affected by orientation, termination, defects at IF
2. **Charged defects (acceptors at front IF)**
   - acceptors tend to accumulate where e^- density is high
3. **Recombination centers (SRH-like traps)**



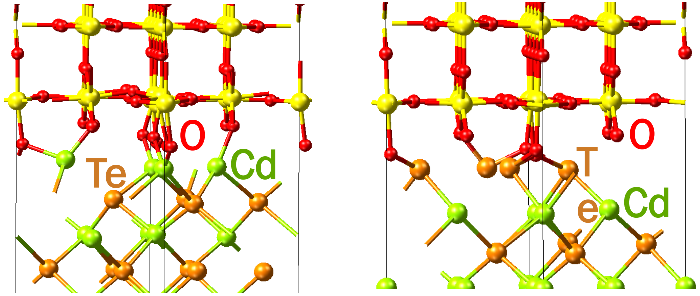
CBO from first principles



- Large negative CBOs predicted
- Worse IF with Te terminated CdTe (i.e. more negative CBO)

1) Build IF model

SnO_2(110) SnO_2(110)

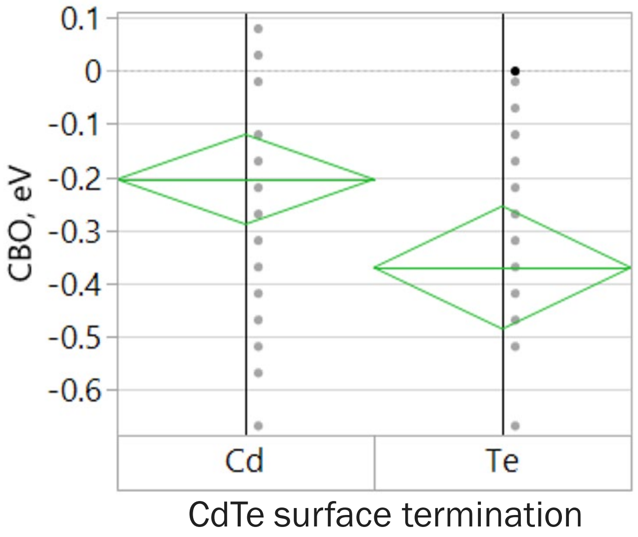


CdTe(001)Cd CdTe(001)Te

- SnO_2(110)/CdTe(001) interface
- 76 atomic configurations in total
- Variation in O coverage and $CdCl_2$ presence

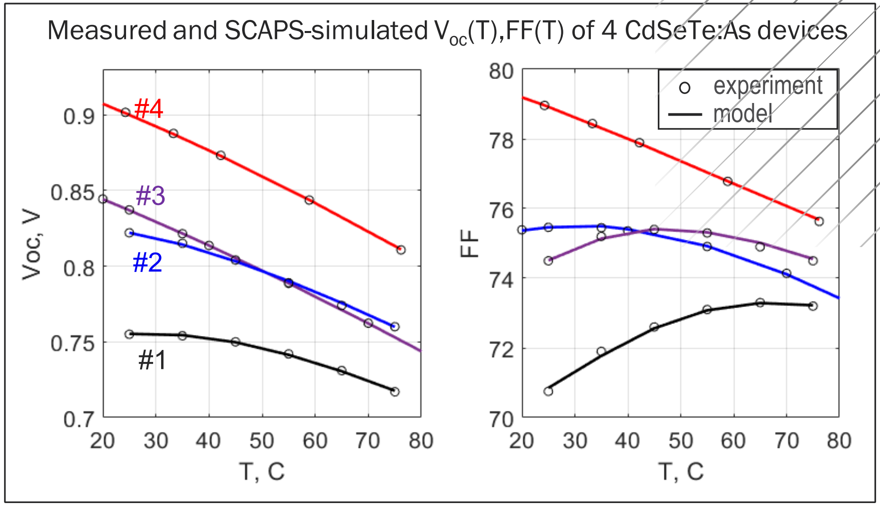
2) Structure relaxation

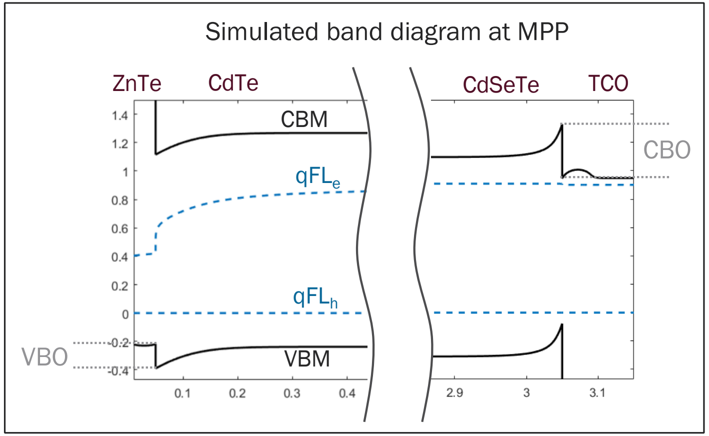
3) Calculate CBO



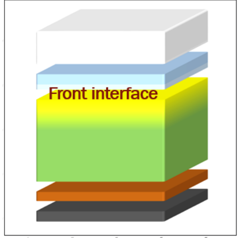
Fitted device model

- Device model fit to V_{oc}(T), FF(T) data
- 4 sifferent devices: qualit. similar models
- Large fitted CBO values: -0.38…-0.53eV

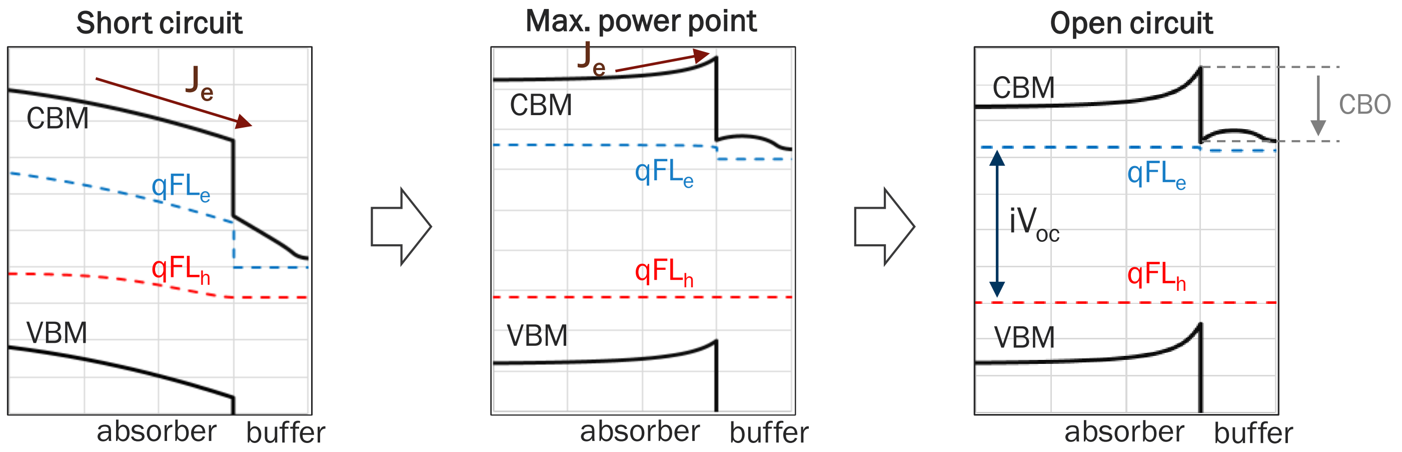




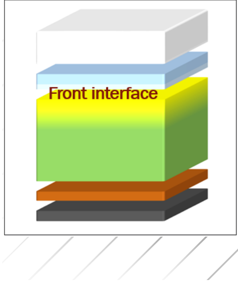
Front interface: strongest loss at OC



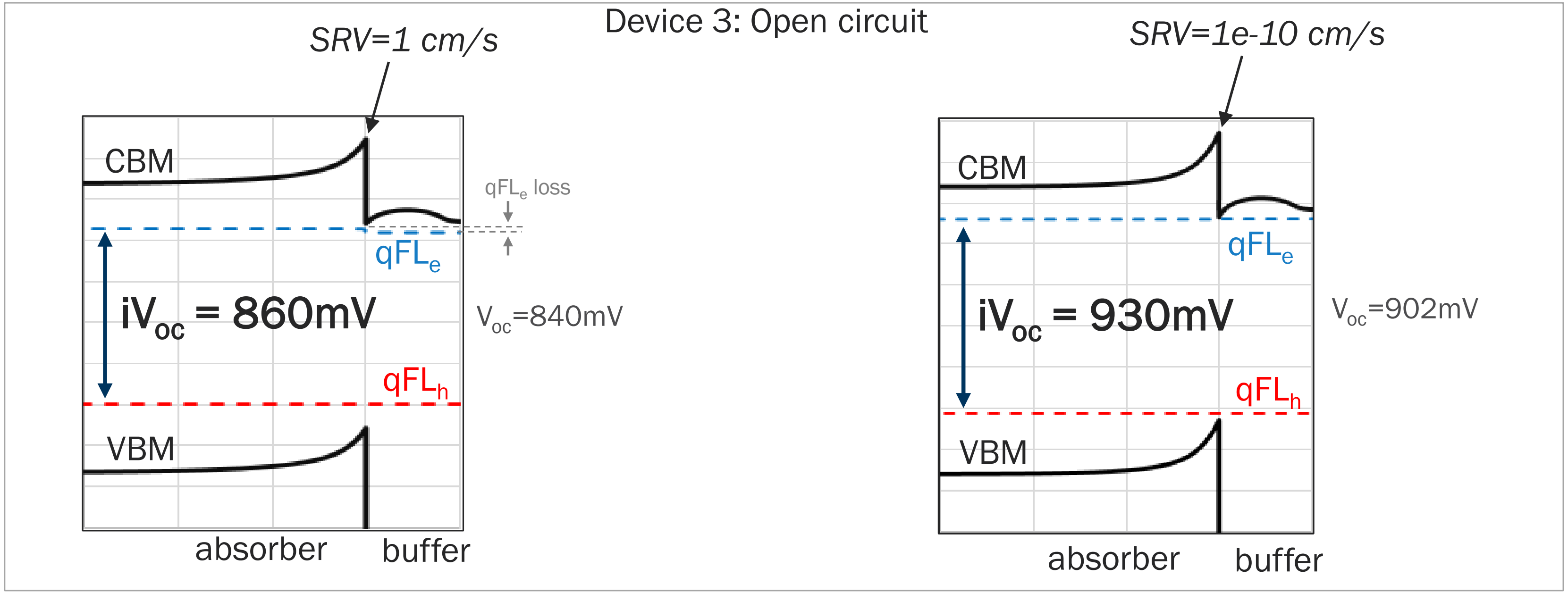
- CBM "spike" under forward bias
- Strong recombination and some e^- retainment under forw. bias
- J_e is against E-field at MPP



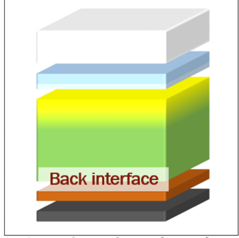
Front interface: strongest loss at OC



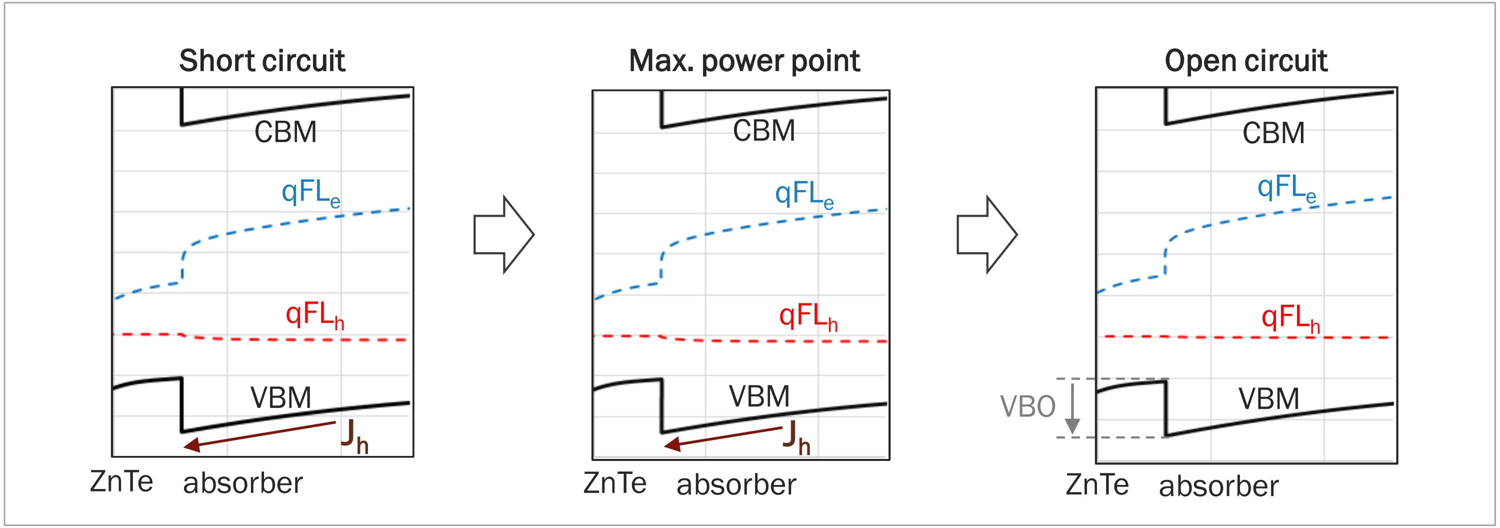
- iV_{oc} loss up to 70mV due to front IF recombination
  (iV_{oc} is not indicative of absorber quality only!)



Back interface: strongest loss at MPP

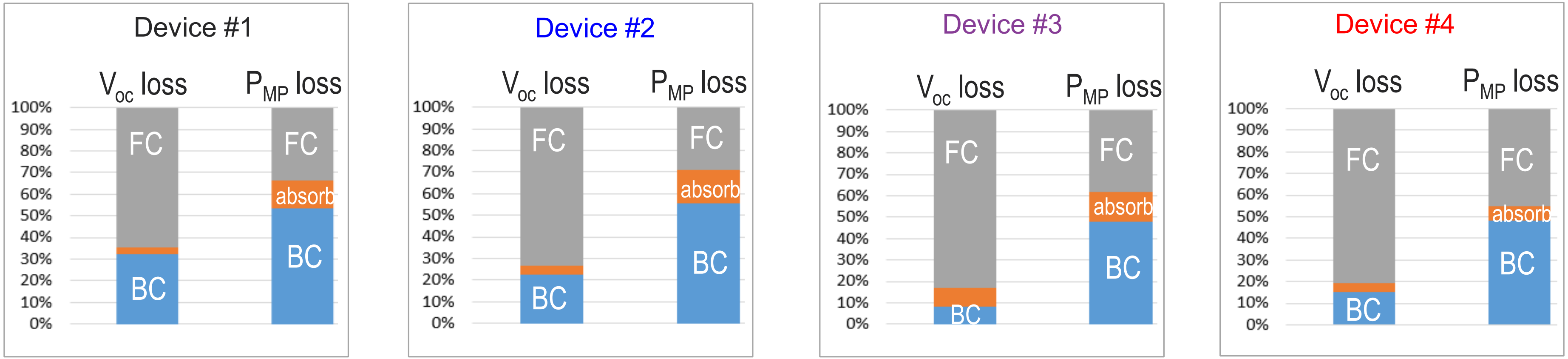


- Downwards band bending near BC
- J_h is against E-field at all conditions
- Some iV_{oc} loss at BC
- Slow h^+ extraction → qFL_h loss at MPP (FF loss)



Device operation and losses

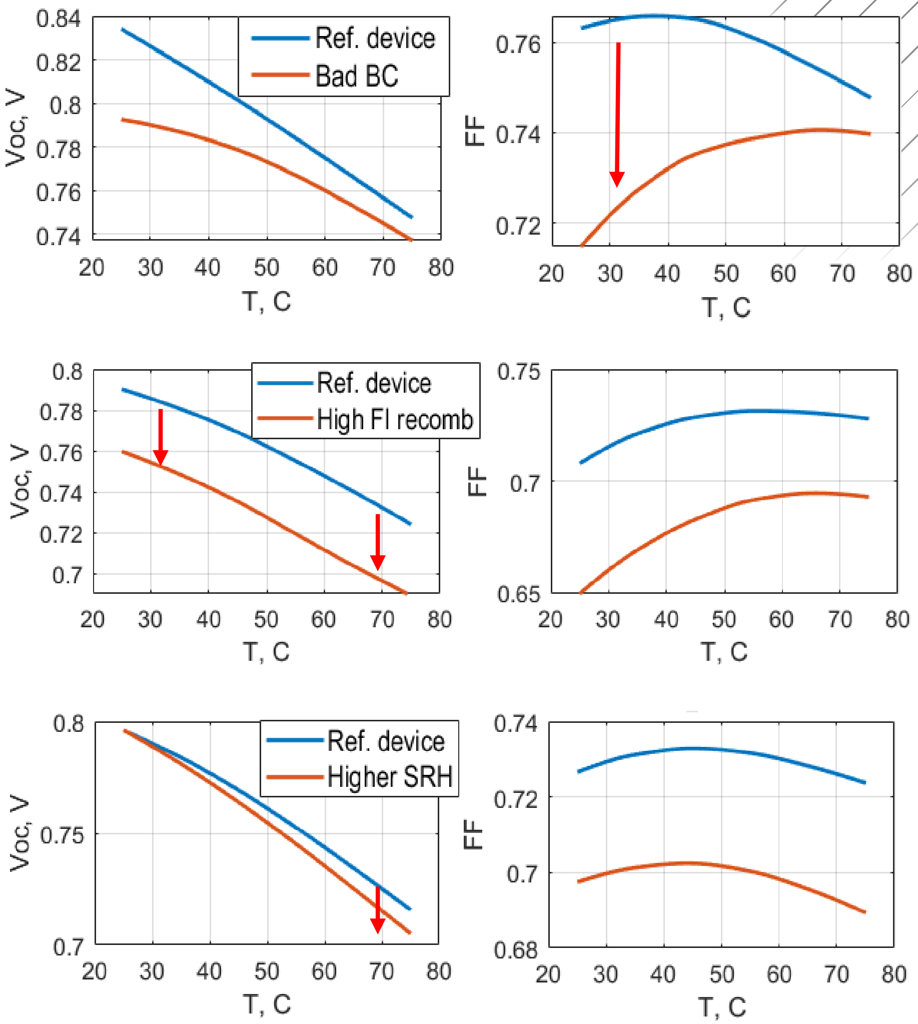
- Estim. of loss at contact: recomb. rate + qFL loss
- V_{oc} loss: mostly at front contact
  (more h^+ at FI under OC ⟶ higher recomb.)
- P_{mp} loss: strong loss at BC
  (due to slow h^+ extraction)



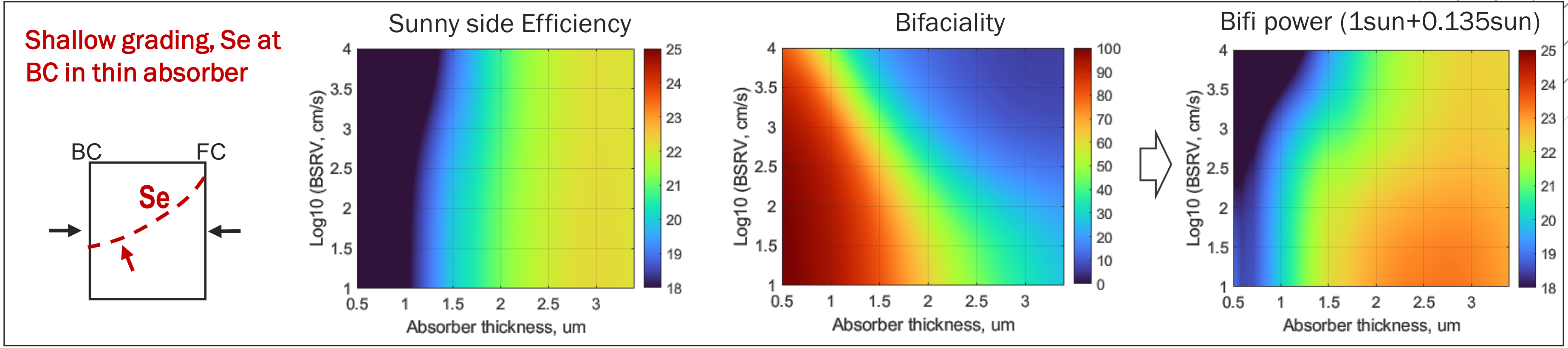
V_{oc}(T),FF(T) signatures

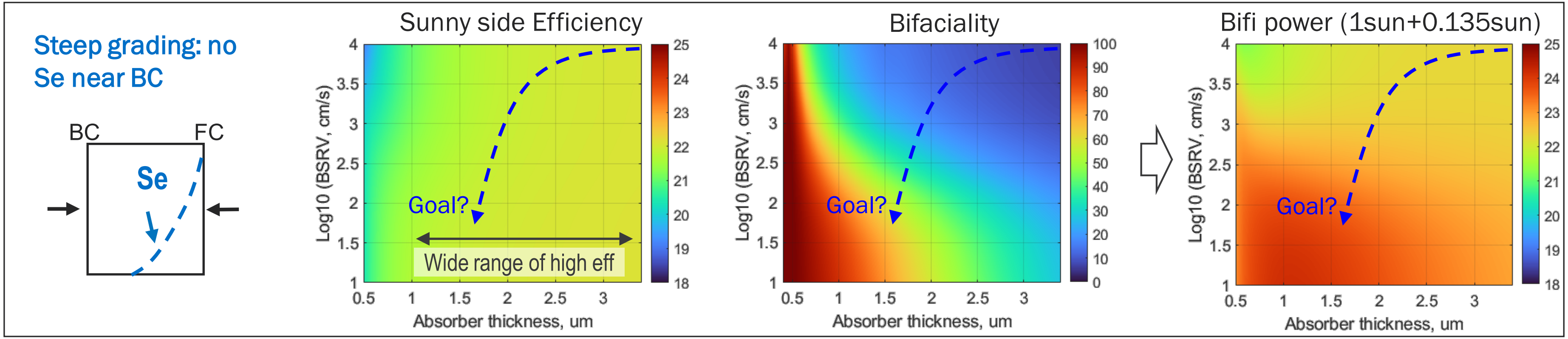
V_{oc}(T), FF(T):

- bear signatures of device operation
- restricts interpretation of IV data
- facilitate comparison of devices
- helps diagnose device failure



Model: thickness vs Se profile vs BSRV

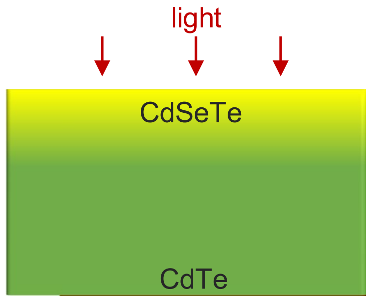




- 2μm is feasible with right Se profile even w/o BSRV↓
- Very high bifaciality with BSRV↓

Back up slides

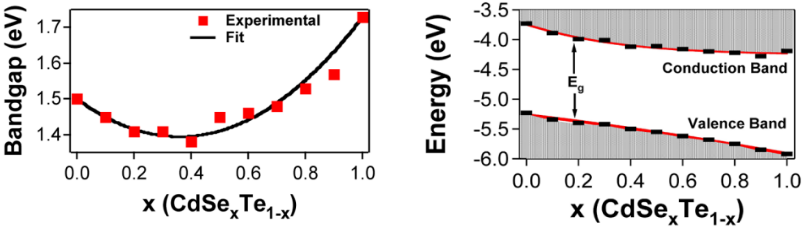
Graded CdSeTe absorber



In high-Se CdSeTe alloy:

1. ~0.1eV lower E_g (more light absorbtion)
2. ~0.2eV higher electron affinity[1] (smaller CBO with TCO, add-l grading for carrier separation)
3. Lower doping[2] (deeper acceptors, higher acceptor formation energy, both for Cu and As)
4. Seom evidences of lower recombination[3] despite lower E_g and deeper acceptors (not fully clear why)

Experimental [ACS Nano 2012, 6, 7, 5995–6004]



First-principles-calculated thermodynamic ionization levels

	Cu_{Cd} (0/-1) ioniz. level	As_{Te}^-/AX^+ ioniz. level
CdTe	0.18 eV	0.14 eV
$CdSe_{25\%}Te_{75\%}$	0.20-0.22* eV	0.16-0.23* eV

*Depending on local Te/Se surrounding

[1] Yang, Wei, Chinese Physics B 28 (2019) 086106
[2] Sankin, Krasikov, Phys. Status Solidi 216 (2019), 1800887
[3] Fiducia et al., Nature Energy 4 (2019) 504

LEADING THE WORLD'S
SUSTAINABLE ENERGY FUTURE