NATIONAL RENEWABLE ENERGY LABORATORY

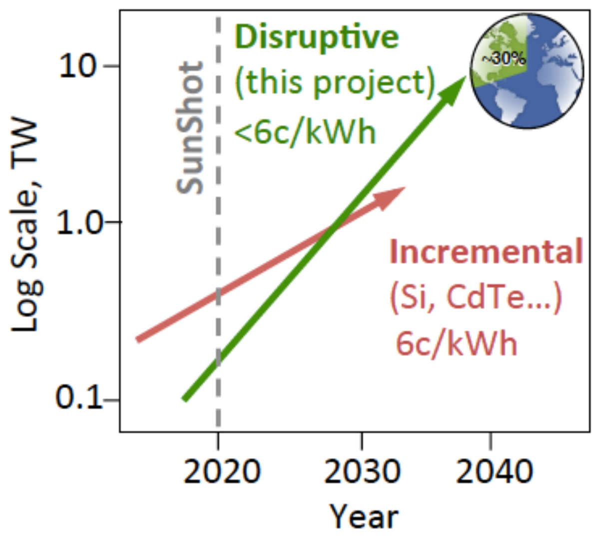
NREL is a national laboratory of the U. S. Department of Energy, Office of Energy Efficiency and Renewable Energy, operated by the Alliance for Sustainable Energy, LLC.

Rapid Development of Nitride- and Oxide- Based Disruptive PV Technologies

E. Arca, A. N. Fioretti, S. Lany, A. C. Tamboli, G. Teeter, C. Melamed, H. Peng, A. Bikowski, J. Pan, K. Wood, E. S. Toberer and A. Zakutayev - National Renewable Energy Laboratory

"Rapid Development" project

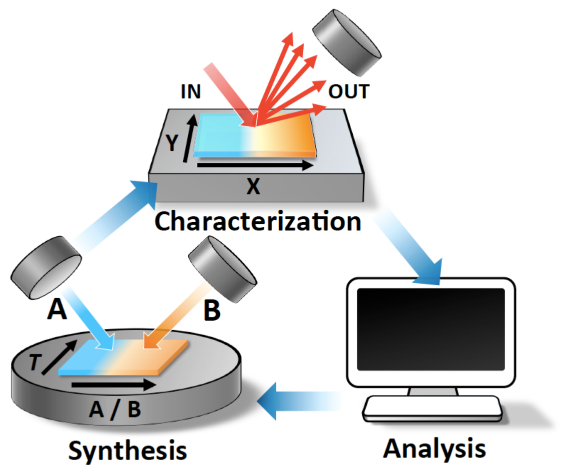
Project summary



Remarkable progress has been achieved in incremental cost reduction of Si and CdTe solar cells towards 1TW level of deployment. However disruptive PV technologies that can be scaled more easily are needed to reach ~10TW level. This project aims to establish disruptive PV technology based on defect-tolerant oxide- and nitride absorbers.

S. Lany, T. Gershon, A. Zakutayev, Journ. Opt., 18, 073004 (2016)
A. Zakutayev, Curr. Opinion. Green. Sust. Chem. 4, 8, (2017)

Project Approach



Combinatorial synthesis:

- Composition/Temperature gradients
- Not only materials, also devices

Spatially-resolved characterization:

- Composition, structure/phase
- Optoelectronic properties

Semi-automated data analysis:

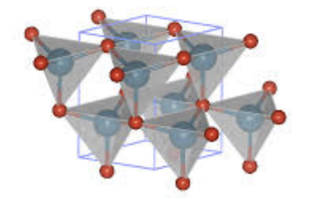
- Close comparison with theory
- Database development in progress

First-principles computations

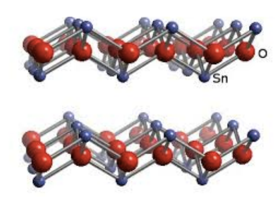
- Leveraging "Center for Next Generation of Materials by Design" EFRC
- Accurate calculations results in database: materials.nrel.gov

Project Materials

Nitrides: $ZnSnN_2$



Oxides: (Sn,M)O



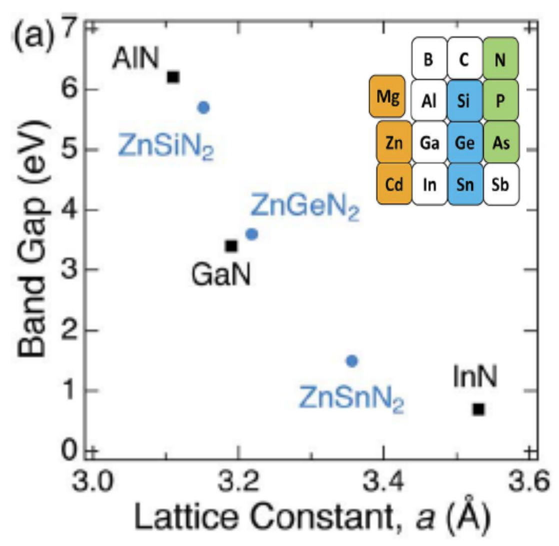
Oxide and Nitride absorbers:

- Suitable for large-scale manufacturing by commercial in-line sputtering:
- $ZnSnN_2$ – ionic materials tend to have defects than covalent materials
- (Sn,M)O – anti-bonding VBM may lead to additional defect tolerance

A. Zakutayev, S. Lany et al J. Phys. Chem. Lett. 5, 1117 (2014)
A. Zakutayev J. Mater. Chem. A 4, 6742 (2016)

Nitride absorber materials

II-IV-N_2 absorber motivation

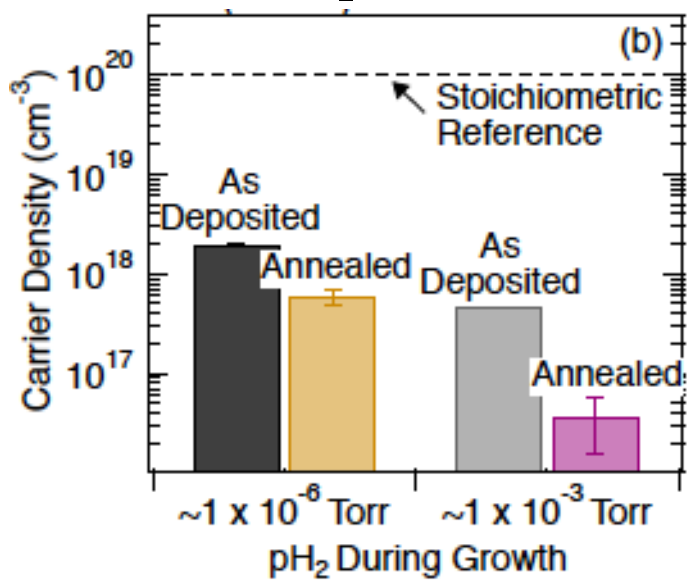


II-IV-N_2 absorber promise:

- Replace costly III-V absorber semiconductors and overcome the miscibility gap of III-V alloys
- Possibility of tunable band gap and constant lattice constant by cation disorder

A. D. Martinez, A. N. Fioretti, E. S. Toberer, A. C. Tamboli
B. J. Mater. Chem. A, 2017,5, 11418

$ZnSnN_2$ doping control

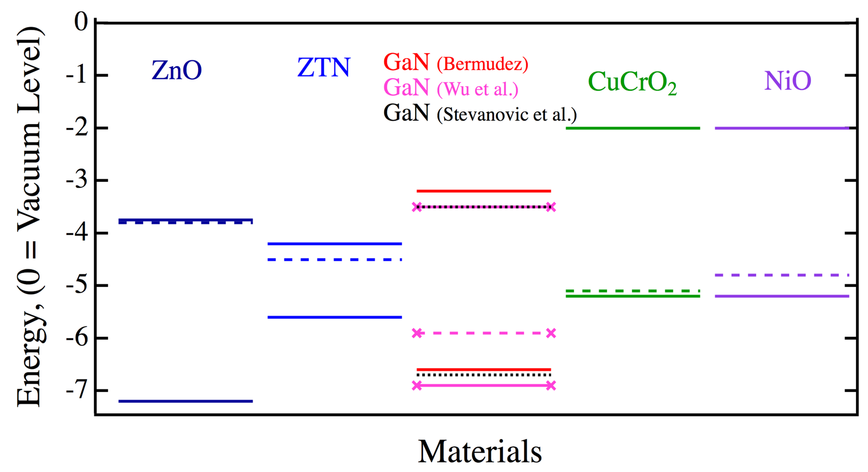


Doping in $ZnSnN_2$ can be controlled:

- By controlling Zn concentration at low temperature (10^{18} cm^{-3})
- By growing Zn-rich samples in H_2 and then annealing (10^{17} cm^{-3})

A. A. N. Fioretti, E. S. Toberer, A. C. Tamboli, A. Zakutayev et al
J. Mater. Chem. C, 3, 11017 (2015); Adv. Electron. Mat. 3, 1600544, (2017)

$ZnSnN_2$ band edge positions



E. Arca, A. N. Fioretti, S. Lany, A. C. Tamboli, G. Teeter, C. Melamed, J. Pan, K. Wood, E. S. Toberer and A. Zakutayev, , IEEE PVSC 2017

- Position of VB and CB determined by a combination of XPS, UPS, Kelvin Probe
- GaN has a band alignment unfavorable for minority carrier (holes) extraction
- $CuCrO_2$/NiO are more favorably aligned – improvement possible by tuning the metal/oxygen ratio or Cu/Cr ratio

Towards $ZnSnN_2$ PV devices

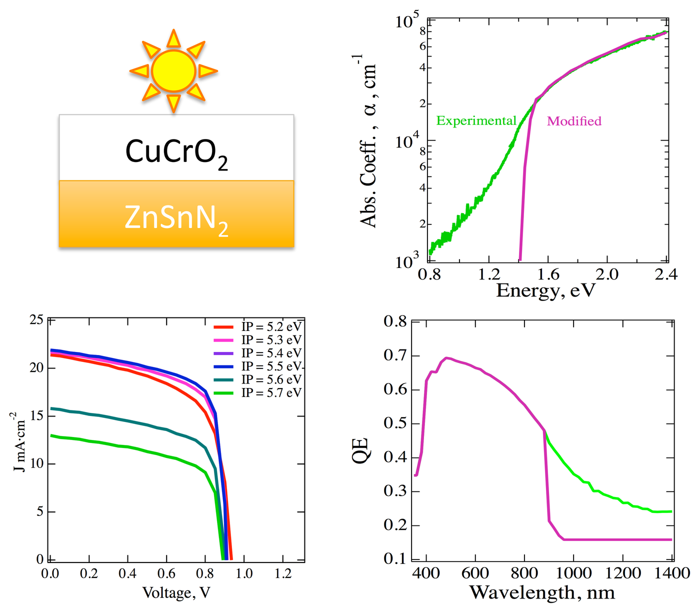
Device simulations parameters

Input parameters (no defect model)		
	ZTN	Mg:$CuCrO_2$
e_0	15	7.5
EA eV	4.2	2
E_g eV	1.4	3.2
N_C cm^{-3}	1.2×10^{18}	2.8×10^{20}
N_V cm^{-3}	7.8×10^{19}	8×10^{20}
μ_e $cm^2V^{-1}s^{-1}$	0.5	0.1
μ_h $cm^2V^{-1}s^{-1}$	0.05	0.1
N_d cm^{-3}	1.005×10^{19}	0
N_a cm^{-3}	1.001×10^{19}	5×10^{21}
d nm	1000	50
Abs. Coef.	Modified (no tails)	Experimental

Cell's Output parameters	
V_{OC}, V	1.08
J_{SC}, $mAcm^{-2}$	26.1
FF %	80.9
η , %	22.9

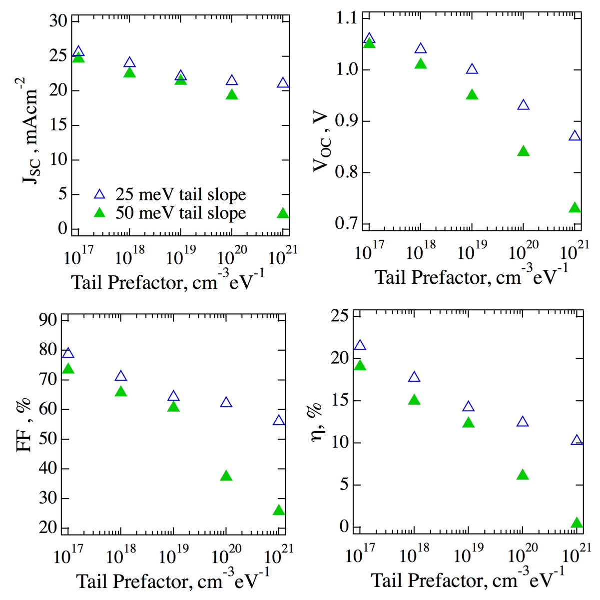
- Device simulations in absence of defects show that ZTN has potential for highly performing single junctions devices
- Defects models was built to account for:
  - Effect of tail state
  - Effect of recombination
  - Role of minority carrier mobility

Device simulations results



- Experimental absorption coefficient shows Urbach Tail
- A modified absorption is needed to avoid artifacts in the simulation results
- JV curves as a function of IP of Mg:$CuCrO_2$: 0.3eV increase of its IP will improve extraction of minority carrier

Device simulations analysis

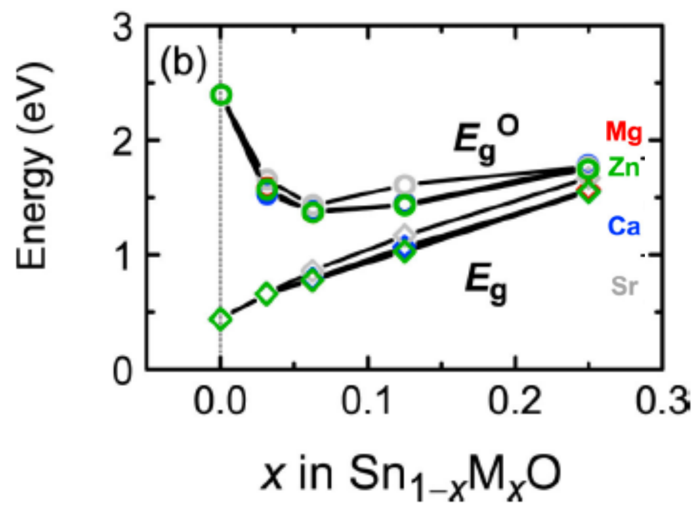


- Band tails could severely hinder device performances especially for low mobility minority carriers
- Recombination centers have a severe effect only at concentration comparable to the net carrier densities.

"Band edge positions of $ZnSnN_2$ and their impact on the simulated performance of the solar cells", E. Arca, A. N. Fioretti, S. Lany, A. C. Tamboli, G. Teeter, C. Melamed, J. Pan, K. Wood, E. S. Toberer and A. Zakutayev, *IEEE PVSC 2017*

Oxide absorber materials

(Sn,M)O alloy motivation

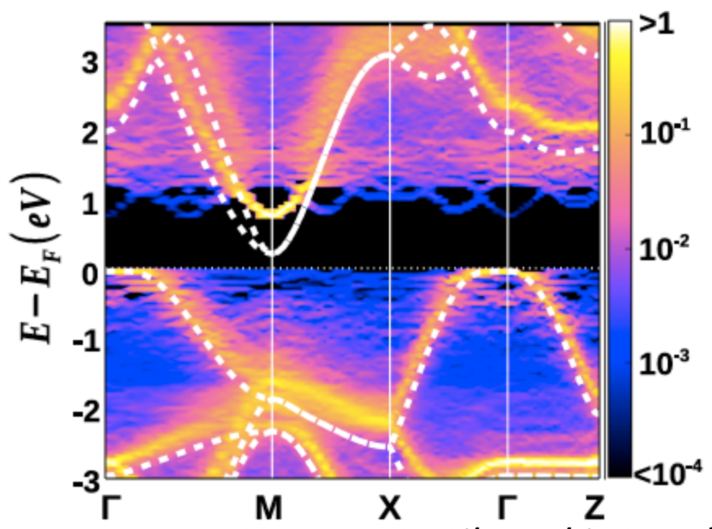


SnO is an interesting oxide:

- SnO has very low hole mass, 0.6 m_0 along (001)
- SnO has indirect band gap (0.7eV vs 2.7 eV)
- Alloying with Mg, Zn, Ca, Sr improves the band gap

H.Peng, A. Bikowski, A. Zakutayev, and S. Lany
APL Mater. 4 , 106103 (2016)

(Sn,Zn)O alloy theory

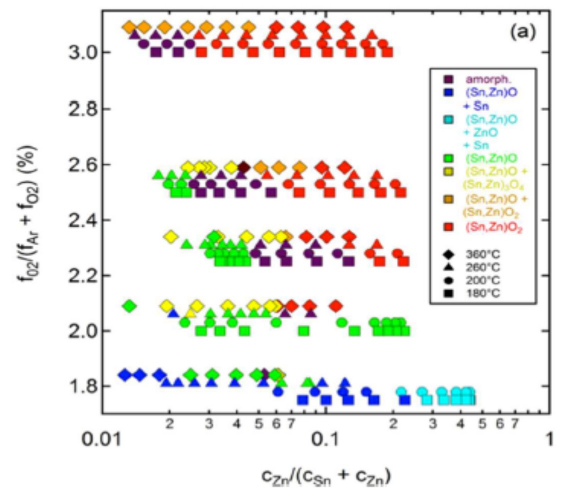


Compared to SnO, the (Sn,Zn)O alloys have:

- Wider electronic band gap (0.7 eV for SnO, 1.0 for 12% alloys)
- Lower optical band gap (2.5 eV for SnO, 1.5 eV for 12% alloys)

H.Peng, A. Bikowski, A. Zakutayev, and S. Lany
APL Mater. 4 , 106103 (2016)

(Sn,Zn)O alloy experiments



Combinatorial synthesis of (Sn,Zn)O indicates that:

- Increasing Zn concentration requires decreasing oxygen flow
- Metastable SnO alloys with up to 10-20% of Zn were synthesized

A. Bikowski, H.Peng, S. Lany, A. Zakutayev et al
Chem. Mat. 28, 7765 (2016)

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