NREL
NATIONAL RENEWABLE ENERGY LABORATORY

Opportunities in Novel Thin Films Inorganic PV Materials

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October 18, 2016

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Energy Efficiency and Renewable Energy
Solar Energy Technology Program

SunShot
U.S. Department of Energy

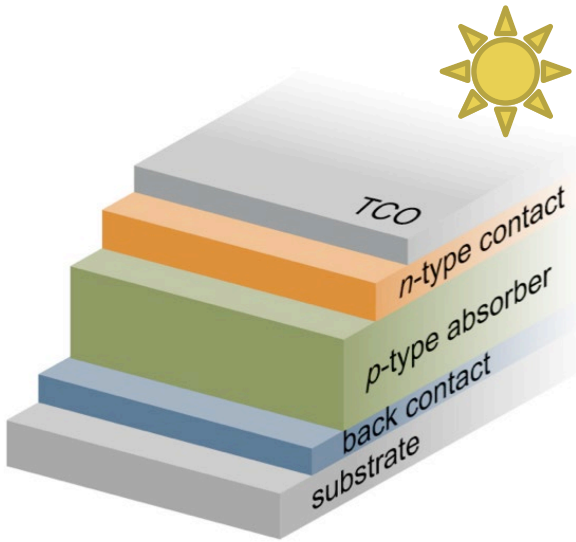
Why We Need Novel Thin Films Inorganic PV Materials?

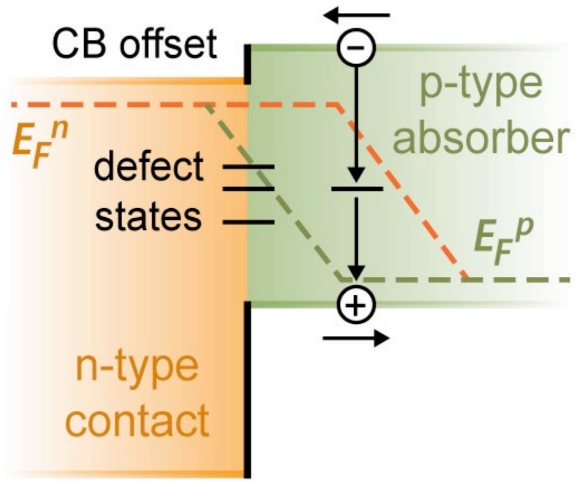
Technology	Cost, c/m^2	Effi. W/m^2	Lifetime, y.	Capital exp.	Abundance
Si	✔	✔	✔	?	✔
CdTe, CIGS	✔	✔	✔	✔	?
CZTS	✔	?	✔	✔	✔
Perovsk.	✔	✔	?	✔	✔
III-V	?	✔	✔	✔	✔
"Disruptive"	✔	✔	✔	✔	✔

- Si and CdTe made remarkable progress but may not be scalable to multi-TW level
- Perovskites and CZTS are scalable, but may have performance and reliability issues
- III-Vs meet all these criteria but the cost still remains relatively high

The search for **inexpensive** and **scalable** solar cell technology is still on

What materials does it take to make a photovoltaic solar cell?





<u>Solar cells are made of materials:</u>

1. ***n*-type transparent conductors**
Transmit light and conduct electrons

2. Solar absorbers
Absorb light and transports carriers

3. ***p*-type contacts**
Conduct holes, reflect electrons

<u>Requirements for each material:</u>

1. Intrinsic materials properties
- thermodynamic stability, absorption spectra

2. Extrinsic materials properties
- high-temperature processing, microstructure
- defects, electric doping, charge carrier transport

3. Device engineering
- band offsets, interface recombination, integration

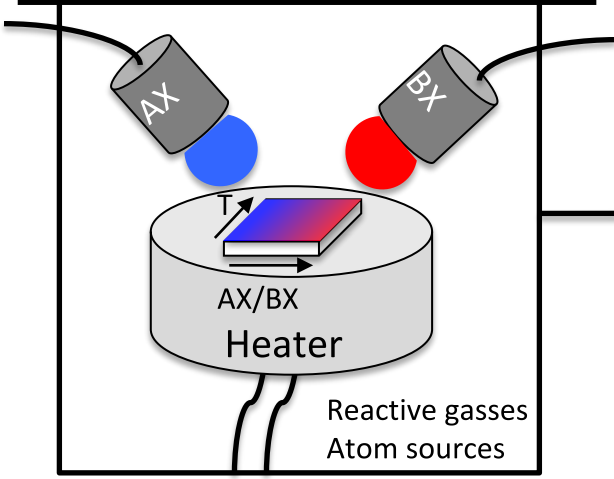
S. Lany, A. Zakutayev et al: Advanced Materials for Solar Energy Conversion, Journal of Optics, 18, 073004 (2016)

We work on all kinds of Novel Thin Films Inorganic PV Materials and PV Devices

High-Throughput Experimental Combinatorial Research Methods

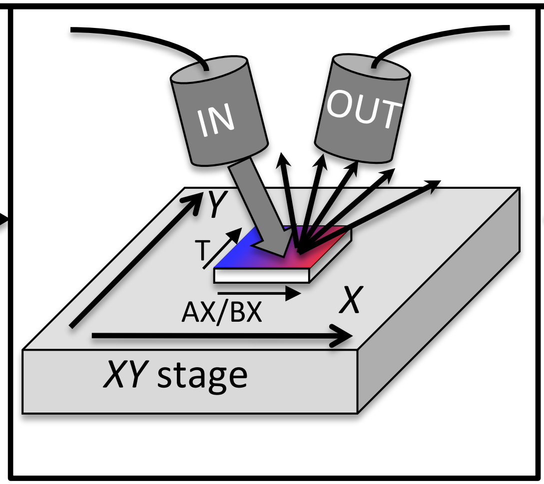
Combinatorial methods for novel PV material development

Thin Film Deposition



- RF co-sputtering, PLD
- Binary/metal targets
- Ar, N_2, H_2S, O_2
- S-, N-, O- atom sources
- Screening conditions:
  - Composition gradient
  - Temperature gradient
  - Thickness gradient

Physical property mapping



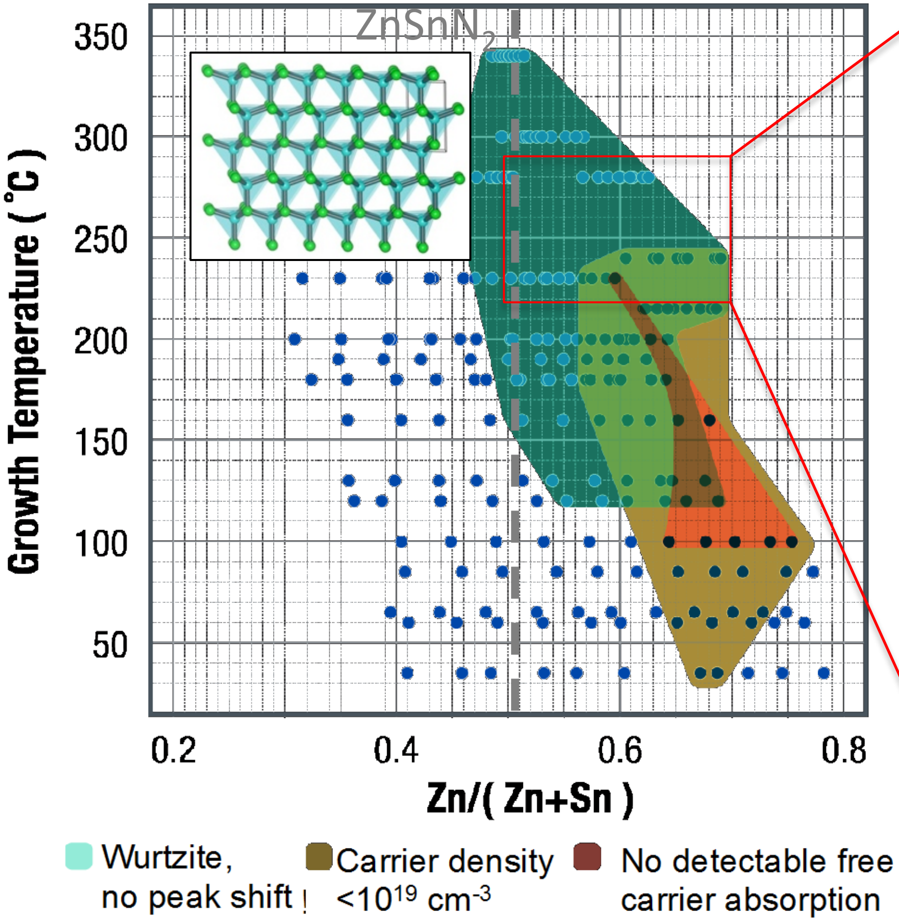
- Composition (XRF,RBS)
- Structure (XRD, Raman)
- Optical (uv-ir, FTIR, PL)
- Transport(4pp, Seebeck, PC)
- Surface (KP, PYS, XPS/UPS)
- Microscopy (SEM, AFM)
- PV devices (JV, CV)
- Thickness, Impedance

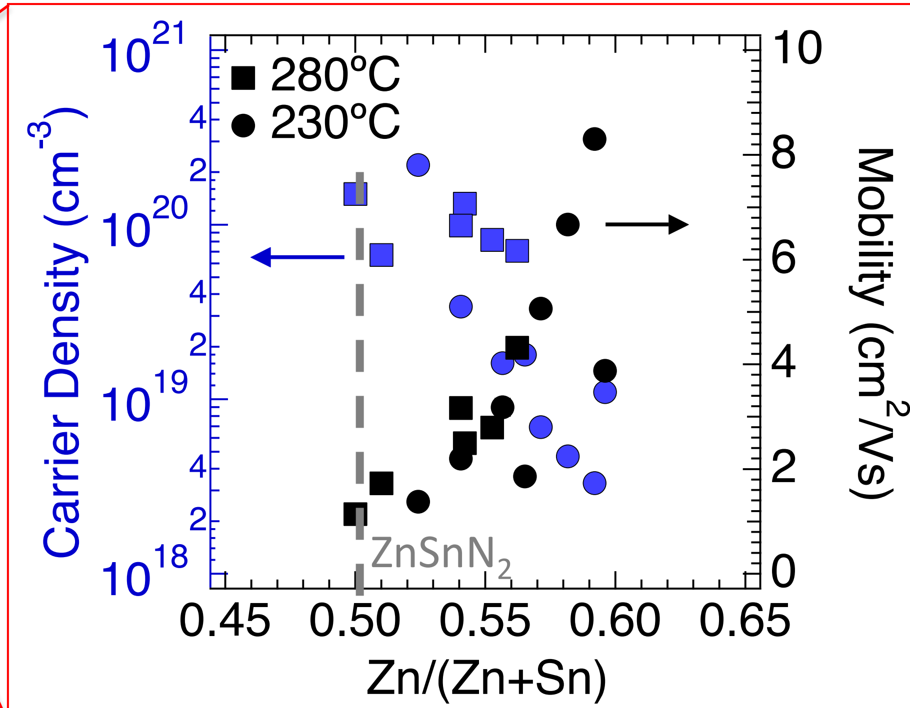
Data analysis and visualization

- Custom-written Igor PRO procedures/functions
- Data harvesting, management, databases
- Advanced analytics: data mining, machine learning
- Close comparison with theoretical calculations

Combinatorial methods increase throughput of novel PV materials research

Example: doping and transport in zinc tin nitride





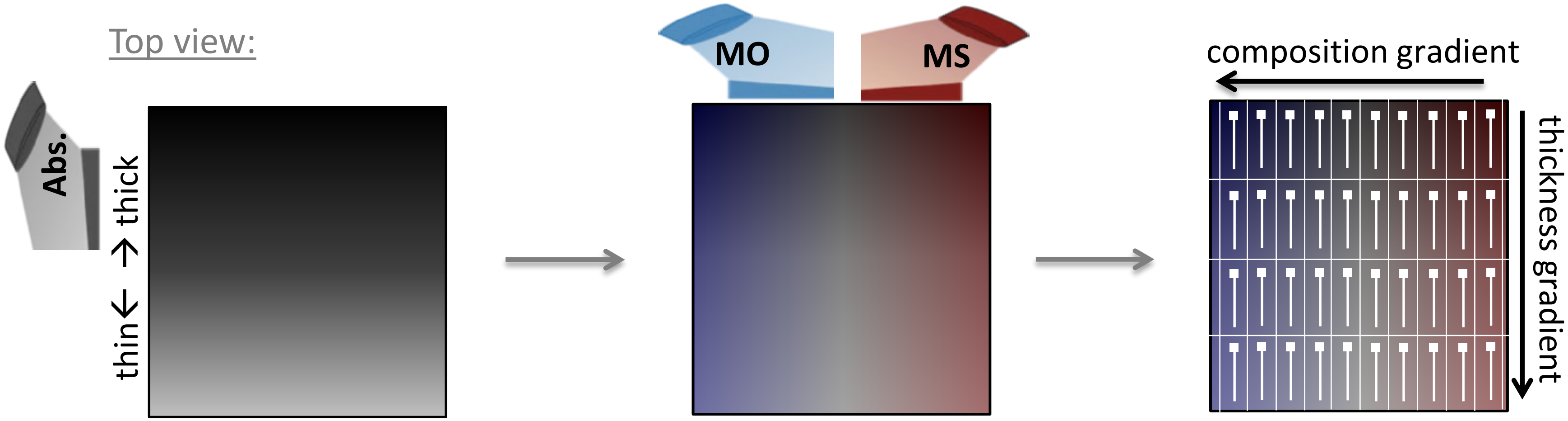
- Doping control by adjusting Zn/Sn ratio
- Disordered $ZnSnN_2$ mobility increases with increased off-stoichiometry

A. Fioretti et al J. Mater. Chem. C, 2015, 3, 11017

Combinatorial composition gradients enable $ZnSnN_2$ doping and transport control

Combinatorial methods for photovoltaic device prototyping

Top view:

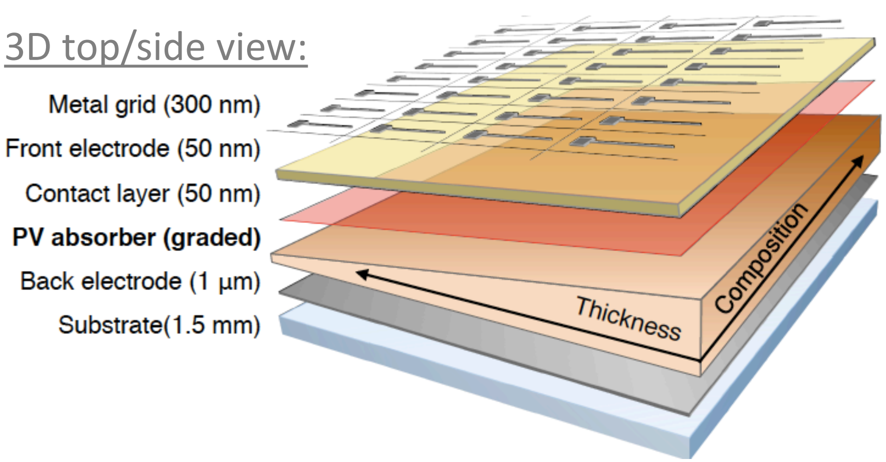


Vertical gradient in absorber thickness

Horizontal gradient in contact composition

Uniform front contact (TCO/metal/isolation)

3D top/side view:



Progress in Photovoltaics 24, 929, (2016)

Fabrication:

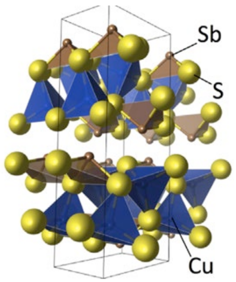
- 1 experiment=44 devices
- 50x50 mm device library
- Each device = 0.5 cm^2

Characterization:

- Automated JV and CV mapping
- Manual EQE measurements
- Automated data processing

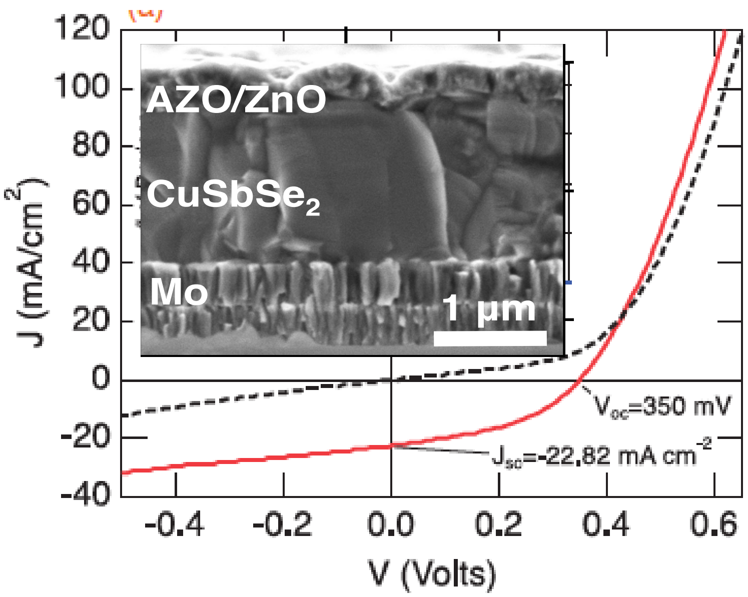
HTE combinatorial approach can be extended from single materials to their integration

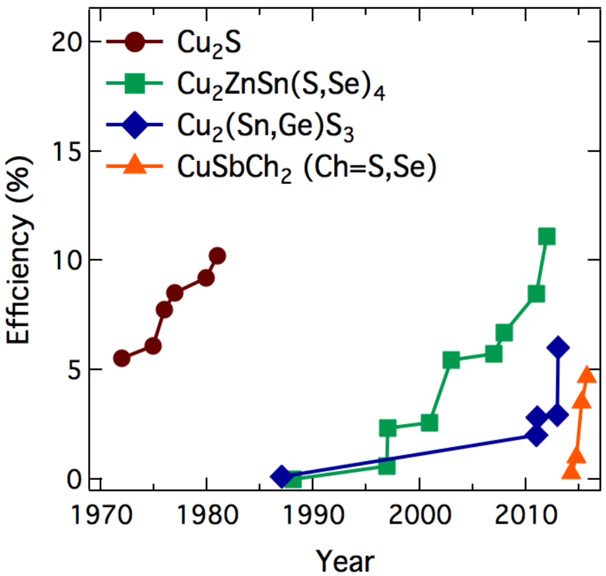
Example: rapid prototyping of $CuSbSe_2$/CdS PV devices



- $CuSbQ_2$ (Q=S,Se) has layered crystal structure, unlike Cu(In,Ga)Se_2
- Promising optical properties (E_g = 1.1 - 1.5 eV), intrinsic p-type doping
- Stronger optical absorber but weaker charge transport than CIGS

Sol. En. Mat.. 132, 499 (2015)





Appl. Phys. Exp. 8, 082301 (2015)

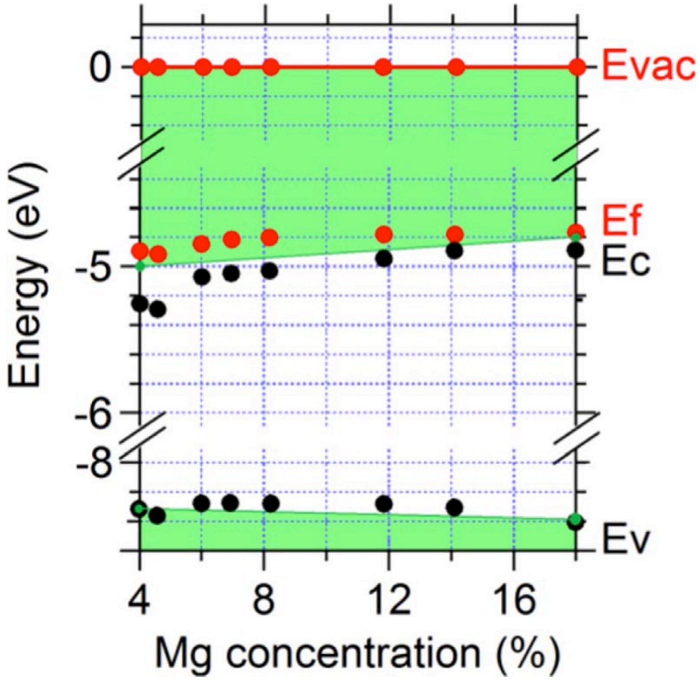
~**5% $CuSbQ_2$** efficiency was achieved in 1.5 years, material has much more potential

Combinatorial research methods helped accelerate $CuSbQ_2$ PV device development

Example of results from prior collaboration

Example 1a: combinatorial PV contact development

Combinatorial sputtering of Ga-doped (Zn,Mg)O for contact applications in solar cells



P. P. Rajbhandar … T. P. Dhakal, A. Zakutayev
Solar Energy Materials & Solar Cells 159 (2017) 219

Combinatorial Chemical Bath Deposition of CdS Contacts for Chalcogenide Photovoltaics

K. Mokurala, …, P. Bhargava, and A. Zakutayev
ACS Combinatorial Science 18, 583, (2016)

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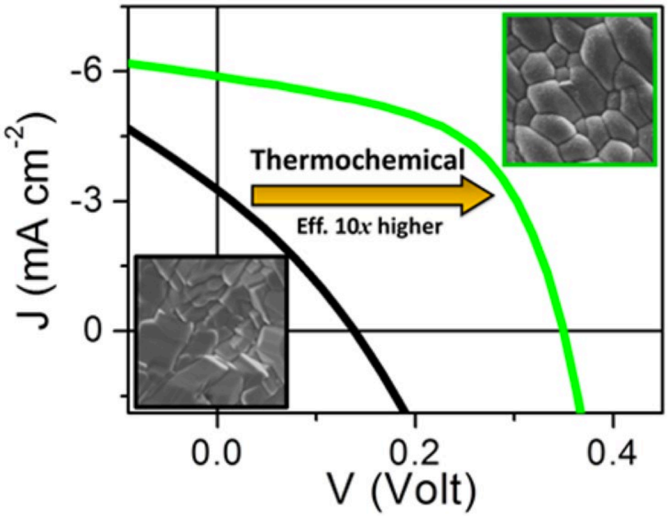
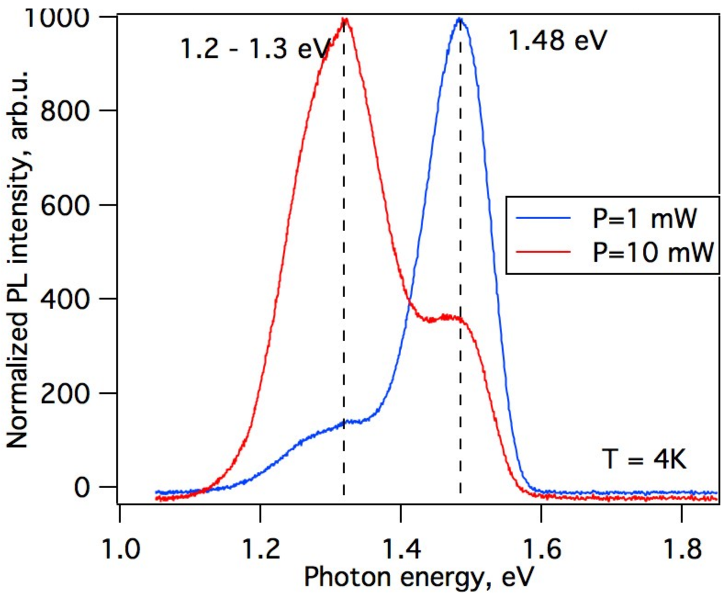
Example 1b: $CuSbS_2$ absorber post-deposition annealing

Effects of Thermochemical Treatment on $CuSbS_2$ Photovoltaic Absorber



W. Lucas, ... L. Mascaro, A. Zakutayev
J. Phys. Chem. C, 120, 18377 (2016)

Study of the performance of $CuSbS_2$ thin film solar cells by defect characterization



W. Lucas, ... L. Mascaro, A. Zakutayev
In preparation

FAPESP SÃO PAULO RESEARCH FOUNDATION

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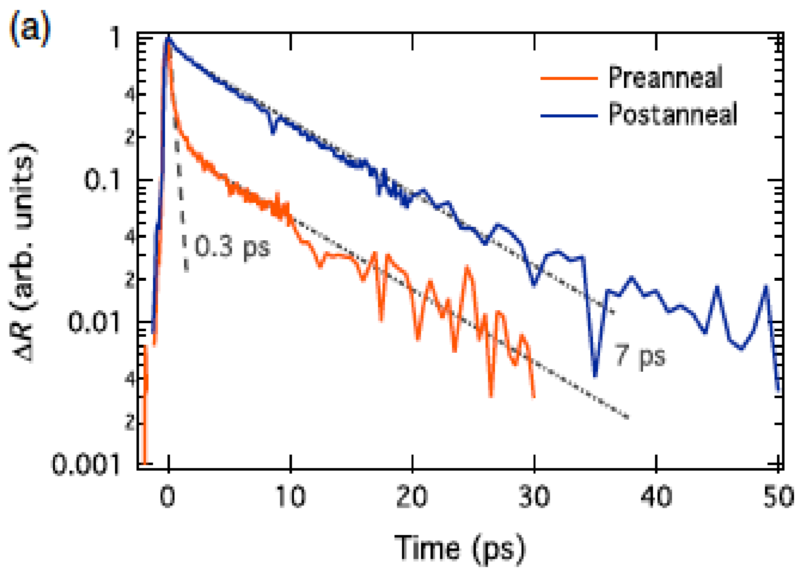
Typical productivity rate for an exchange student at NREL is 2 papers/year

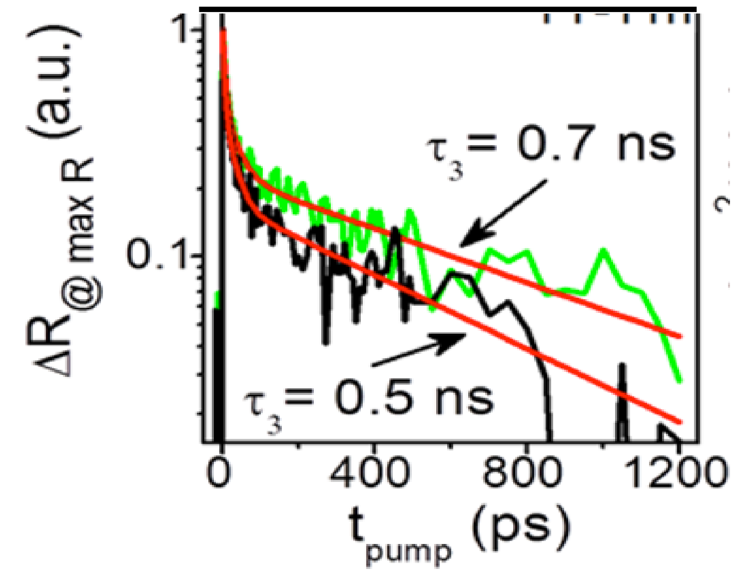
Example 2: optical pump THz probe spectroscopy at HZB

Effects of Disorder on Carrier Transport in Cu_2SnS_3



Phys. Rev. Appl. 4, 044017 (2015)

Effects of Thermochemical Treatment on $CuSbS_2$ Photovoltaic Absorber



J. Phys. Chem. C, 120, 18377 (2016)

HZB Helmholtz Zentrum Berlin

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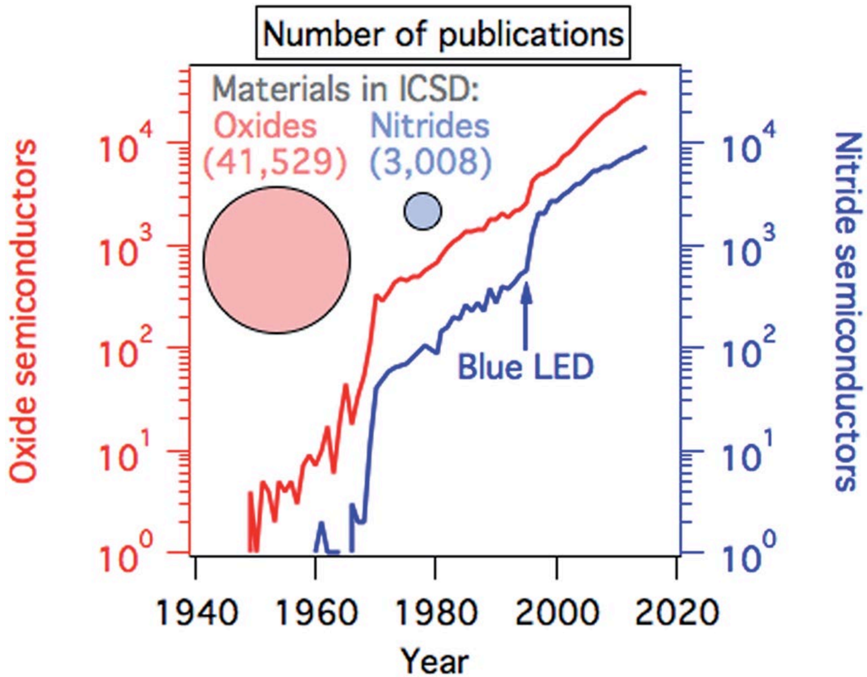
A single collaboration led to 2 publications, 1 more under review, 1 patent in preparation

Related activities in Materials by Design

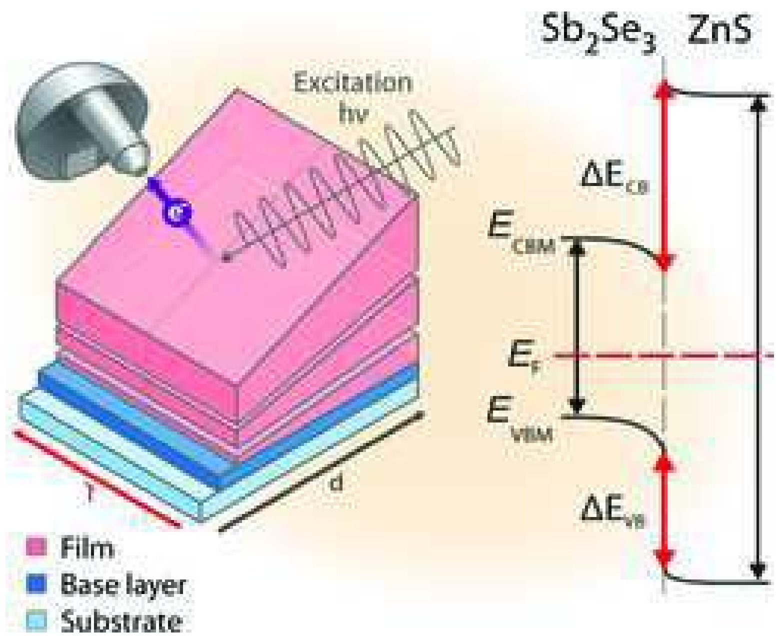
Materials by Design – Energy Frontier Research Center

Discovery of Nitride Compound
and deposition method development



J. Mater. Chem. A 4, 6742 (2016)

Design of Chalcogenide Alloys
and characterization method development



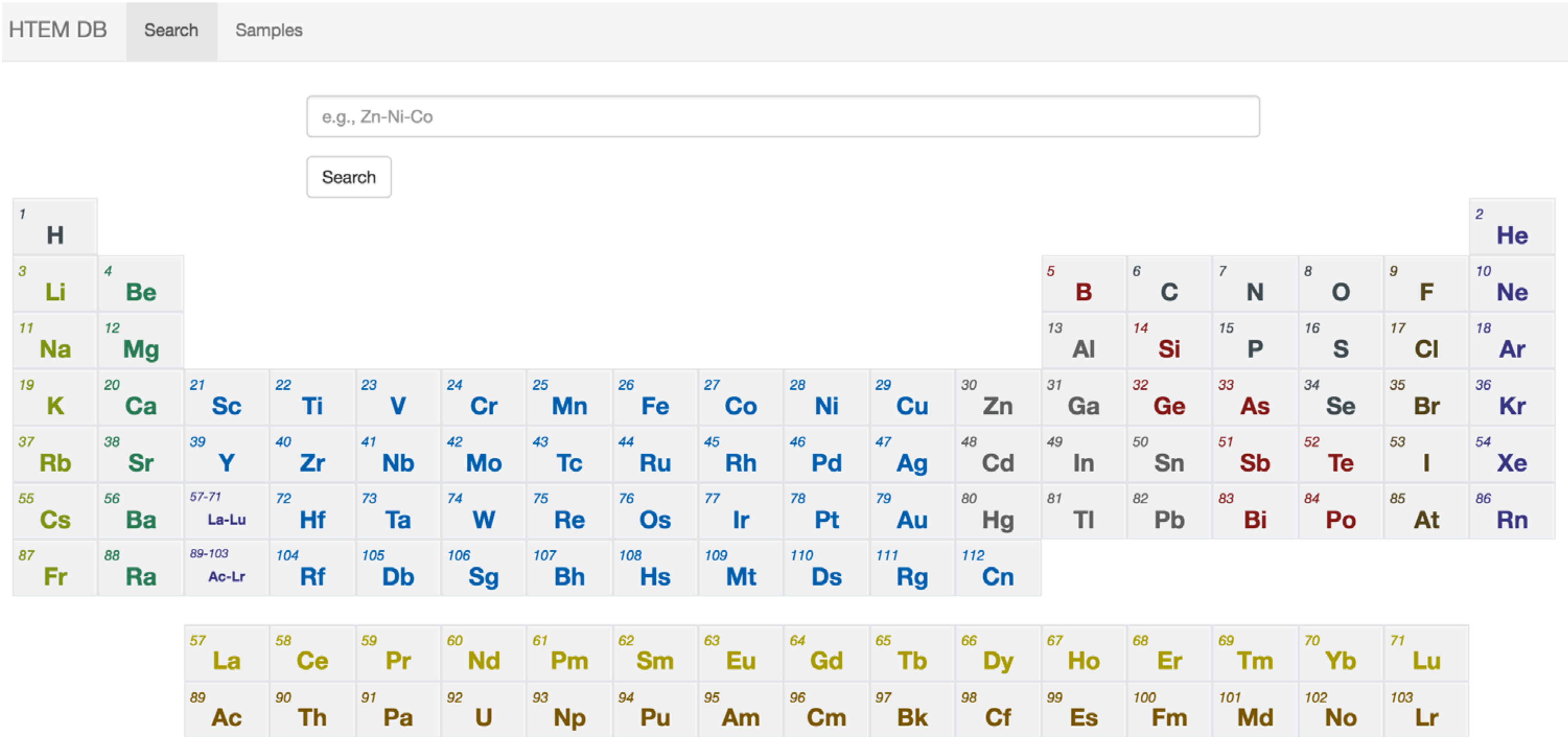
Adv. Mater. Int. 2016, 10.1002/admi.201600755

U.S. DEPARTMENT OF ENERGY

http://www.cngmd-efrc.org/

CNGMD Incorporating Metastability

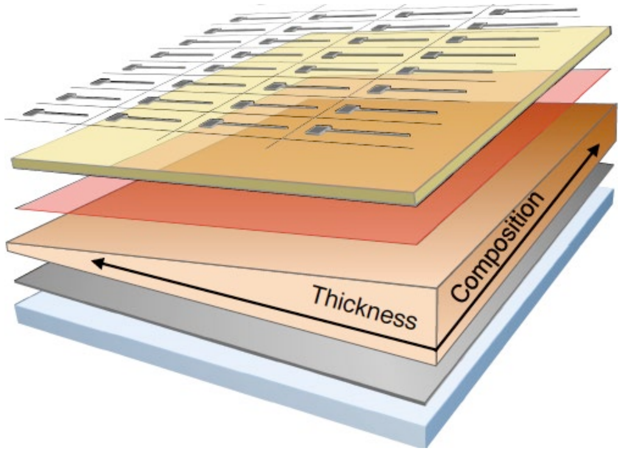
High Throughput Experimental materials database



The database currently contains 3159 libraries with 76753 unique samples.

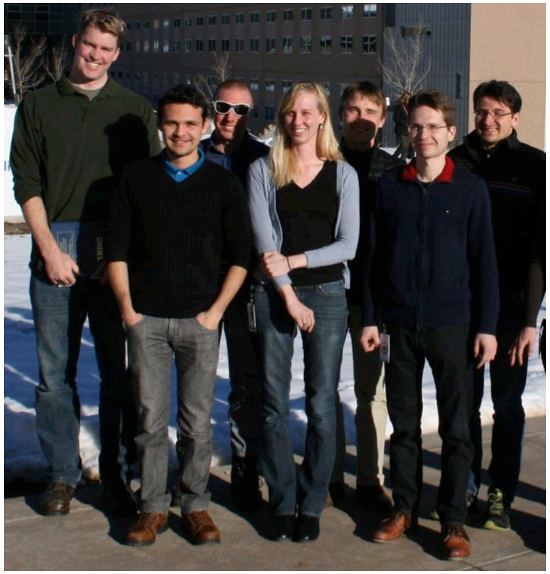
Summary and Conclusions

Summary and Conclusions



Summary: what research we do

- Novel Thin Films Inorganic PV Materials
- Absorbers, Contacts, Interfaces, Devices
- Oxides, Nitrides, Sulfides, Selenides
- High-Throughput Combinatorial Research Methods
- Materials by Design Energy Frontier Research Center
- High Throughput Experimental materials database



Conclusions: modes of collaboration

- Common materials research interest
- Your materials made/studied at NREL
- NREL materials studied at University
- Student research at (6-12 months)
- Postdoc research (3-6 month)

More information:

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http://www.nrel.gov/materials-science/materials-discovery.html

www.nrel.gov

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