Opportunities in Novel Thin Films
Inorganic PV Materials

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Why We Need Novel Thin Films Inorganic PV Materials?

- 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

<table>
<thead>
<tr>
<th>Technology</th>
<th>Cost, c/m²</th>
<th>Effi. W/m²</th>
<th>Lifetime, y.</th>
<th>Capital exp.</th>
<th>Abundance</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
<td>🔴</td>
<td>✔</td>
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<tr>
<td>CdTe, CIGS</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
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<tr>
<td>CZTS</td>
<td>✔</td>
<td>🔴</td>
<td>✔</td>
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<tr>
<td>Perovsk.</td>
<td>✔</td>
<td>✔</td>
<td>🔴</td>
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<tr>
<td>III-V</td>
<td>🔴</td>
<td>✔</td>
<td>✔</td>
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<tr>
<td>“Disruptive”</td>
<td>✔</td>
<td>✔</td>
<td>✔</td>
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<td>✔</td>
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What materials does it take to make a photovoltaic solar cell?

**Solar cells are made of materials:**

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

**Requirements for each material:**

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


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**
- AX
- BX
- AX/BX
- Heater
- Reactive gases
- Atom sources

**Physical property mapping**
- IN
- OUT
- Y
- T
- X
- XY stage
- AX/BX

**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

- RF co-sputtering, PLD
- Binary/metal targets
- Ar, N₂, H₂S, O₂
- S-, N-, O- atom sources
- Screening conditions:
  - Composition gradient
  - Temperature gradient
  - Thickness gradient

- 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

Combinatorial methods increase throughput of novel PV materials research
Example: doping and transport in zinc tin nitride

Combinatorial composition gradients enable ZnSnN$_2$ doping and transport control

- Doping control by adjusting Zn/Sn ratio
- Disordered ZnSnN$_2$ mobility increases with increased off-stoichiometry

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:
- Metal grid (300 nm)
- Front electrode (50 nm)
- Contact layer (50 nm)
- PV absorber (graded)
- Back electrode (1 μm)
- Substrate (1.5 mm)

Fabrication:
- 1 experiment = 44 devices
- 50x50 mm device library
- Each device = 0.5 cm²

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

Progress in Photovoltaics 24, 929, (2016)

HTE combinatorial approach can be extended from single materials to their integration
Example: rapid prototyping of CuSbSe₂/CdS PV devices

- CuSbQ₂ (Q=S,Se) has layered crystal structure, unlike Cu(In,Ga)Se₂
- Promising optical properties (E_g = 1.1 - 1.5 eV), intrinsic p-type doping
- Stronger optical absorber but weaker charge transport than CIGS


~5% CuSbQ₂ efficiency was achieved in 1.5 years, material has much more potential

Combinatorial research methods helped accelerate CuSbQ₂ 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

Combinatorial Chemical Bath Deposition of CdS Contacts for Chalcogenide Photovoltaics

P. P. Rajbhandar ... T. P. Dhakal, A. Zakutayev

K. Mokurala, ..., P. Bhargava, and A. Zakutayev
ACS Combinatorial Science 18, 583, (2016)
Example 1b: CuSbS$_2$ absorber post-deposition annealing

Effects of Thermochemical Treatment on CuSbS$_2$ Photovoltaic Absorber

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

Study of the performance of CuSbS$_2$ thin film solar cells by defect characterization

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

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$_2$SnS$_3$


Effects of Thermochemical Treatment on CuSbS$_2$ Photovoltaic Absorber

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

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

**Design of Chalcogenide Alloys**
and characterization method development

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

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

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