Functional Materials by Design for Solar Energy Conversion

Bill Tumas
Associate Lab Director
Materials and Chemical Science and Technology
National Renewable Energy Laboratory
February 19, 2014
bill.tumas@nrel.gov
Acknowledgement: Center for Inverse Design EFRC

Director
W. Tumas (NREL)

Theory
A. Zunger, Chief Scientist-Theory (CU)
S. Lany, P. Graf (NREL); V. Stevanovic (CSM)
L. Yu, X. Zhang (CU), A.J. Freeman, G.Trimarchi (Northwestern)

Inorganic Synthesis
D.G. Ginley, Chief Scientist-Experiment (NREL)
J.D. Perkins, A Zakutayev, P. Ndione (NREL)

& Characterization
D.A. Keszler and J.F. Wager (Oregon State University);
K.R. Poeppelmeier and T.O. Mason (Northwestern University);
M.Toney (SLAC)

Program Integrator
L. Kazmerski, John Perkins
Global Energy Challenge: Sustainable Materials, Processes and Systems

- Greenhouse Gases
- Land Use
- Water Use
- Resources
- Hazards
- Waste

Sustainable development is development that meets the needs of the present without compromising the ability of future generations to meet their own needs

– UN Bruntland Commission
From Horse Power to Horsepower: The Great Horse-Manure Crisis of the 1890s

In 1898, delegates from across the globe gathered in New York City for the world’s first international urban planning conference. One topic dominated the discussion. It was not housing, land use, economic development, or infrastructure. The delegates were driven to desperation by horse manure. The situation seemed dire. In 1894, the Times of London estimated that by 1950 every street in the city would be buried nine feet deep in horse manure. One New York prognosticator of the 1890s concluded that by 1930 the horse droppings would rise to Manhattan’s third-story windows. A public health and sanitation crisis of almost unimaginable dimensions loomed.

And no possible solution could be devised. After all, the horse had

Shift Happens

- Eric Morris, UC Davis
Solar Energy Generation
AND
Storage/Use of Solar Energy

- Solar (light)
- Thermal (heat)
- Electrical (storage)
- Fuels (chemical)

Materials ➔ Processes/Components ➔ Devices ➔ Systems
Key Solar R&D Needs Addressed at NREL

- **Applied R&D**
  - Costs and efficiency, performance
  - Understanding and control defects and interfaces
  - Processing
- **Reliability**
  - Testing
  - Prediction, Mechanisms of degradation
- **Manufacturing**
- **Next Generation**
  - New absorbers/contacts
  - Advanced processing
  - New architectures, substrates, balance of system
- **Fundamental Research**
  - **New materials by design**
  - Efficiency beyond the Shockley-Queisser limit
  - Advanced manufacturing
Gap between Cell and Module Efficiencies

http://www.solarnavigator.net/solar_cells.htm
Target Functionalities – Solar Energy Conversion

Solar Absorber Materials
- **Strong solar absorption**
  Eg, absorptivity, SLME
- **Carrier Lifetimes**
- **Carrier Diffusion**
  recombination centers/defect
- **Doping**
- **Low cost, non-toxic**

**Transparent Conductors \( (n, p) \)**
- **Transparency (band-structure)**
  optical band gap > 3 eV
- **Conductivity (defects)**
  - Minimize hole-killer defects
dopability, avoid formation of O-vacancies
  - Maximize hole-producing defects
    intrinsic: vacancies, anti-sites, ...
    extrinsic: impurity doping
  - Enhance hole mobility
• Semiconductor “high-tech” is based on just a handful of basic species: Si, Ge, GaAs, ...

• These provide but a limited and sparse scale of band gaps:

\[
\begin{array}{ccccccc}
\text{InSb} & \text{Ge} & \text{Si} & \text{InP} & \text{GaAs} & \text{AlAs} \\
\end{array}
\]

\[
\begin{array}{cccccccc}
0 & 1 & 2 & 3 & \text{eV} \\
\end{array}
\]

Very, Very few ....
DOE Basic Research Needs Workshop report noted Missing Materials:

“... the range of materials currently available for use in photovoltaics is highly limited compared to the enormous number of semiconductor materials that can in principle be synthesized “. 

EERE invested in incremental refinement of the “usual-suspect materials” (Si, CdTe, CIS ...) Most involved accidental discoveries.

Need broad base of materials with optimized tailored properties not just few materials
Traditional approach:  “Given a material, what are the properties”
Inverse design:  “Given a desired property, what is the material”

“Inverse Design”: Declare first the functionality you need, then use theory-guided experiment to iteratively find the material that has this target functionality
Center for Inverse Design

* tight coupling of theory and experiment
* iterative attempts at a problem, teaching each other;
* synergism between theory, synthesis and characterization
Center for Inverse Design

1. Define target properties
2. Articulate "Design Principles"
3. Initial selection of *materials classes* (each representing $10^3$-$10^6$ individual compounds)
4. Screening of promising *individual candidate materials*
   - High-Throughput synthesis and characterization
   - Inverse-Band-Structure search
5. Narrowed list: "Best of class"
6. Targeted synthesis and specialized characterization of candidate compounds
   - Direct materials synthesis
   - Direct theoretical characterization
   - Direct experimental characterization
7. Novel inorganic materials with tailored properties
Properties of interest

- Thermodynamic stability - $\Delta H_f$
- Band structure and optical properties
- Defects and doping
- Carrier transport mechanism (band vs. small-polaron)
- ...

Electronic structure methods

- Density functional theory
  self-consistent charge density, total-energy
- Many body interactions in GW approximation
  Quasi-particle energies, optical properties
- Credit to VASP group
High-throughput combinatorial experimental approach

RF sputtering, PLD
Binary/metal targets
Ar/H₂S, Ar, N, O gasses
S, N atom sources
2x2” sample libraries

Composition (XRF, RBS)
Structure (XRD, Raman)
Transport(4pp, Seebeck)
Optical (uv-ir, PL)
Surface (KP, XPS/UPS)
Microscopy (SEM, AFM)

Igor PRO software framework
Custom-written package of functions
User-assisted analysis
Data mining/analysis


Thin film combi approach can do fast screening before bulk synthesis
Two Main Approaches for Inverse Design

**Design by Design Principles**
- Many material systems with known structure and composition (e.g. ICSD)
- Functionality unknown
- Complex target properties, e.g. PV absorptivity, efficiency, transparent conductivity
- Search via design principles for targeted functionalities

**Missing Materials**
- Many material systems, but structure unknown
- Many (~ 50–100) possible configurations, requiring energy minimization and stability analysis
- Target properties: first existence, then other properties
Implementing Inverse Design: Solar Absorbers

Inverse Design of Solar Absorbers

Design Principle for high absorption

- Desired: Very high absorption for cell design with very thin absorber
- Needed: High joint density of states

Materials Screening

- Theory screening of many candidate materials for band gap and absorption

Validate properties for “best of class”

- Theory, synthesis, and characterization

Define target properties

Articulate “Design Principles”

Initial selection of materials classes (each representing 10^3-10^6 individual compounds)

Screening of promising individual candidate materials

- High-Throughput synthesis and characterization
- Inverse-Band-Structure search

Narrowed list: "Best of class"

Targeted synthesis and specialized characterization of candidate compounds

- Direct materials synthesis
- Direct theoretical characterization
- Direct experimental characterization

Novel inorganic materials with tailored properties
Inorganic Crystal Structure Database: ICSD

> 166,000 crystal structures; updated semi-annually

http://www.fiz-karlsruhe.com/icsd.html
Selection Criteria: Spectroscopically Limited
Maximum Efficiency—SLME

- Detailed balance between cell inside and outside
- Photon energy dependent absorption
- Optical band gap type factor $f(r)$ – non-radiative recombination

\[
\eta = \frac{P_m}{P_{in}}
\]

\[
J = J_{sc} - J_0 (1 - e^{eV/kT})
\]

\[
J_{sc} = e \int_0^\infty a(E) I_{sun}(E) \, dE
\]

\[
a(E) = 1 - e^{-2\alpha(E)L}
\]

\[
J_0 = J_{0nr} + J_{0r} = J_{0r} / f_r
\]

\[
J_{0r} = e\pi \int_0^\infty a(E) I_{bb}(E,T) \, dE
\]

\[
f_r = e^{-\Delta/kT} \quad \Delta = E_g^{da} - E_g
\]

Captures physics of absorption, emission and recombination
optical type, gaps and material-dependent non-radiative recombination loss

Absorption Screening

- **High Throughput screening:**
  - First-principles quasi-particle GW method (G0W0+HSE06)
  - Provides good band gap estimation

- **Input:**
  - ICSD structure
  - No element or stoichiometry restrictions

- **Output:**
  - Band gap type
  - Absorption spectra
  - Electronic structure
Developing new Metrics – Spectroscopic Limited Maximum Efficiency (SLME):

Generalized I-III-VI chalcopyrite group \( (I^p_{III}^q_{VII}^r) \)

Any possible \((p,q,r)\); oxidation states of III can be 1 or 3

\( (>300 \text{ compounds}) \)

\( CuInSe_2, \ CuGaSe_2, \ Cu(\text{In, Ga})Se_2 \)
High SLME materials include known absorbers
Other experimentally confirmed PV absorbers (less studied)

Previously unrecognized high SLME materials

In Cu-III-VI system:
\( \text{Cu}_3\text{Tl}^{1+}\text{Se}_2 \) has stronger absorption than \( \text{CuTl}^{3+}\text{Se}_2 \)

In \( \text{Cu}_3\text{Tl}^{1+}\text{Se}_2 \):
more Tl p in CB, more Tl s in VB

What controls the strength of optical absorption?

The direct transition rate (Fermi’s Golden rule):

\[ W_{i \rightarrow f} = \frac{2\pi}{\hbar} |M|^2 g(h\nu); \quad g(h\nu = E_f - E_i) \]

GaAs, CdTe

CuInSe₂ (CIS)

Cu-M-VI

- Increase p DOS near CBM and s DOS near VBM
Cu-III-VI $\rightarrow$ Cu-V-VI

<table>
<thead>
<tr>
<th>Cu-III($s^2p^1$)-VI</th>
<th>Cu-V($s^2p^3$)-VI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al (3+)</td>
<td>P (5+, 3+)</td>
</tr>
<tr>
<td>Ga (3+)</td>
<td>As (5+, 3+)</td>
</tr>
<tr>
<td>In (3+)</td>
<td>Sb (5+, 3+)</td>
</tr>
<tr>
<td>Tl (3+, 1+)</td>
<td>Bi (5+, 3+)</td>
</tr>
</tbody>
</table>

**Low valence compound:** Cu-V(3+)-VI  
**High valence compound:** Cu-V(5+)-VI
Case of Cu-Sb-S:

Cu-Sb$^{3+}$-S vs. Cu-Sb$^{5+}$-S vs. CuInSe$_2$ (CIS)

Both Cu$_3$SbS$_3$ and CuSbS$_2$ have stronger absorption than Cu$_3$SbS$_4$ and CIS for $h\nu > E_g + \Delta$.

$\Delta$ depends on the energy difference between indirect gap and direct gap

CuSbS$_2$: 0.05 ($E_g^d - E_g^i$)
Cu$_3$SbS$_3$: 0.13 ($E_g^d - E_g^i$)

VASP: $G_0W_0$@HSE06

Experiment shows same absorption trend in Cu-Sb-S case

By R. S Kokenyesi and D. A Keszler, Oregon State University

More $V\rho$ in Cu-V$^{3+}$-VI compounds near CBM
More $V_s$ in Cu-$V^{3+}$-VI compounds near VBM
Step 3: Experimental Realization

Low temperature synthesis
Polycrystalline absorbers with rapid onset of absorption
($\alpha>10^5$ cm$^{-1}$ at $E_G+0.5$ eV)

Keszler et al. Oregon State
Scientific approach of the “Rapid Development” project

State of the art research methods
From materials to devices (3 steps)
Predictive theoretical calculations
High-throughput combinatorial experiments

Broad scope of PV materials
Test-cases: Cu-Sn-S and Cu-Sb-S absorbers
Next-generation: oxide-based absorbers
Broadly applicable to wide range of materials
Exploration of Cu-Sn-S family of materials

- $\text{Cu}_4\text{SnS}_4$ - too many holes
- $\text{Cu}_4\text{Sn}_7\text{S}_{16}$ - Fermi level ($E_F$) pinning
- $\text{Cu}_2\text{SnS}_3$ - few holes, no $E_F$ pinning

$\text{Cu}_2\text{SnS}_3$ is a more promising PV absorbers than other Cu-Sn-S materials

Implementing Inverse Design

Designing p-Type Ternary Oxides

1. Define target properties
2. Articulate "Design Principles"
3. Initial selection of materials classes (each representing $10^3$-$10^6$ individual compounds)
4. Screening of promising individual candidate materials
   - High-Throughput synthesis and characterization
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   - Direct experimental characterization
7. Novel inorganic materials with tailored properties

DEVELOP p-type TCO design principles
SEARCH $A_2BO_4$ w.r.t. design principles
IMPROVE $Co_2ZnO_4$ based on design principles
**Modality 2 = Inverse Design By Design Principles**

<table>
<thead>
<tr>
<th>P-TCO PROPERTIES</th>
<th>DESIGN PRINCIPLES</th>
</tr>
</thead>
</table>
| *High hole concentration (defect calc.)* | • Absence of hole-killer defect  
  • Presence of hole-producing defects |
| *High hole mobility (polaron calc.)* | • Anti-bonding valence band maximum  
  • No bound polarons |
| *Transparency (band-structure calc.)* | • Optical band gap > 3 eV  
  • Wide ligand field splitting (some cases) |

Chose Search Space: \( \text{A}_2\text{BO}_4 \) Spinels – 40 in ICSD
Selection of Ternary $A_2BO_4$ Compounds
A broad class for materials discovery

Normal 3-2 Spinels:
$A^{+3}$ $O_h$ site (e.g., Al, Fe, Co)
$B^{+2}$ $T_d$ site (e.g., Mg, Zn, Fe)

Inverse 3-2 Spinels:
$A^{+3}$ $O_h$, $T_d$ sites (e.g., Fe, Co)
$B^{+2}$ $O_h$ site (e.g., Ni)

• Large family of compounds
• Wide range of physical and chemical properties; low oxygen vacancy
Role of Anti-Site Defects in Spinels

Ability to calculate defects and dopants is critical to electronic materials design (supercell approach)

Anti-site defects control properties:

\[ \text{A}^{3+} \text{ on Td is DONOR} \]
\[ \text{B}^{2+} \text{ on Oh is ACCEPTOR} \]

DT-2--No Intrinsic Hole Killer !!

\[ \text{Co}_2(\text{Zn,Ni})\text{O}_4 \text{ – best of class!} \]
12 of 40 $A_2BO_4$ Spinels Type 2 (Naturally P-Type)


Low Cost + Non-Toxic → Take $Co_2ZnO_4$ as Prototype
Sputtered $\text{Co}_2\text{ZnO}_4$ Can Be Zn-Rich

Non-Equilibrium Theory
- Excess Zn $\rightarrow$ $O_h$ Site
- AXRD Confirms

Sputtered Films ($T_s = 340^\circ\text{C}$)
- Zn-Rich Spinel Phase
- Conductivity Increases

Annealed Films
- Conductivity Decreases
- Reduced Antisite Defects?

Predicted Extrinsic Dopability

- 17 Dopants Evaluated by Theory
- Li, Ni, Mg best
- Equilibrium Solubility Limit ~ 5%

**Optical and Electrical: Region of Interest**

Optical and Electrical properties are optimized in a non-trivial composition region.
Three ways to improve conductivity in Co spinels

1. Non-equilibrium growth
   - 2+ on $O_h$ site produces holes
   - Maximize this to increase conductivity
   - 5x improvement

2. Extrinsic dopants
   - 20x improvement

3. Induce inverse spinel phase
   - 10000x improvement
Zn-Co-O as a hole transport layer (HTL) for OPV

- Performance comparable to PEDOT:PSS on the first try

"Zn-Ni-Co-O wide-bandgap p-type conductive oxides with high work functions"
Missing Materials

- New materials are likely to have new properties
- Properties have previously been extracted in literature from an incomplete set of materials (e.g. ICSD)
- Many have calculated properties for unknown compounds (e.g. ABX half-Heusler compounds) but haven’t determined their stability (i.e. existence)
- Candidate materials for alloying
Challenge 1: Structure of an unknown compound

General solution: Global Space Group Optimization (GSGO)

Alternative:
- 39 structures-types for 800 known $A_2BX_4$
- GGA+U to sort out the ground-state structure

<table>
<thead>
<tr>
<th>No.</th>
<th>Name (example)</th>
<th>Space Group</th>
<th>Occurrence</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>Spinel (Al$_2$MgO$_4$)</td>
<td>Fd3m</td>
<td>255</td>
</tr>
<tr>
<td>2.</td>
<td>NN (Th$_3$P$_4$)</td>
<td>I43d</td>
<td>87</td>
</tr>
<tr>
<td>3.</td>
<td>Olivine (Al$_2$BeO$_4$)</td>
<td>Pnma</td>
<td>48</td>
</tr>
<tr>
<td>4.</td>
<td>Hausmanite (Mn$_3$O$_4$)</td>
<td>I4/amd</td>
<td>27</td>
</tr>
<tr>
<td>5.</td>
<td>Phenakite (Li$_2$WO$_4$)</td>
<td>R3</td>
<td>14</td>
</tr>
</tbody>
</table>

...
High - Throughput calculations

**Scope:**
- 406 $A_2BX_4$
- 39 structure-types for each $A_2BX_4$
- Several magnetic configurations

$\Rightarrow$

$\sim80,000$ GGA+U calculations
$\sim10^6$ CPUh
using
Red Mesa HPC

**Software development:**
1) Setting up automatically the crystalline and magnetic structure for each potential ground state
2) Automatic detection of errors
3) Automatic extraction of properties
Challenge 2: Stability with respect to competing phases

\[ \Delta H_f(A_m B_n X_l) = E_{\text{tot}}(A_m B_n X_l) - (m\mu^0_A + n\mu^0_B + l\mu^0_X) \]

Total energy

Elemental reference energies

\[ 2 \, A + B + 4 \, X \]

\[ A_2BX_4 \]

\[ \cdots \]

\[ A_2X_3 + BX \]

\[ \cdots \]

\[ ABX_3 + \frac{1}{2} A_2X + \frac{1}{2} X \]
Correcting DFT for accurate $\Delta H_f$ – FERE

- Fitted Elemental-phase Reference Energies (FERE) + GGA+U
- 50 $\mu^0$-values fit to 252 binary compounds with measured $\Delta H_f$
50 $\mu^0$ values fitted using measured $\Delta H_f$ values of 252 binary pnictides, chalcogenides and halides

$$\mu^0 \text{(FERE)} = \mu^0 \text{(GGA+U)} + \delta \mu^0 \text{(FERE)}$$

FERE Validation - Ternaries

Example: Mn$_2$SiO$_4$

**Theory:**
Structure: Olivine
$\Delta H_f = -2.53$ eV/atom

**Experiment:**
Structure: Olivine
$\Delta H_f = -2.56$ eV/atom

Competing phases:
Mn, Si, O$_2$
How it Works: Mn$_2$SiO$_4$

**Theory:**
Structure: Olivine
$\Delta H_f = -2.53$ eV/atom

**Experiment:**
Structure: Olivine
$\Delta H_f = -2.56$ eV/atom

Competing phases:
Mn, Si, O$_2$
MnO
Example: Mn$_2$SiO$_4$

**Theory:**
- Structure: Olivine
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**Experiment:**
- Structure: Olivine
- $\Delta H_f = -2.56$ eV/atom

Competing phases:
- Mn, Si, O$_2$
- MnO, MnO$_2$, Mn$_2$O$_3$
- Mn$_3$O$_4$, SiO$_2$
Example: Mn$_2$SiO$_4$

**Theory:**
Structure: Olivine
$\Delta H_f = -2.53$ eV/atom

**Experiment:**
Structure: Olivine
$\Delta H_f = -2.56$ eV/atom

Finch et al.

$T = 1600$ K, $p_{O_2} = 10^{-10}$ atm
$\rightarrow \Delta \mu_O = -3.45$ eV

$-4.18$ eV $< \Delta \mu_O < -3.16$ eV
Example: $\text{Mn}_2\text{SiO}_4$, growth conditions

**Theory:**
- Structure: Olivine
- $\Delta H_f = -2.53 \text{ eV/atom}$

**Experiment:**
- Structure: Olivine
- $\Delta H_f = -2.56 \text{ eV/atom}$
- Growth:
  - $T = 1600 \text{ K}$
  - $p_{O_2} = 10^{-10} \text{ atm}$
High-throughput Discovery of New $\text{A}_2\text{BX}_4$ Compounds

Rules:
1. Only one transition metal at a time
2. Respect possible oxidation states

Total 656 possible combinations
- 250 are reported
- 406 are not reported ("missing compounds")
Predicted New $\text{A}_2\text{BO}_4$

Out of 63 missing oxides
- 46 not stable
- 17 stable

Newly predicted:
- $\text{Hg}_2\text{SiO}_4$
- $\text{In}_2\text{HgO}_4$
- $\text{Ti}_2\text{BeO}_4$
- $\text{Ti}_2\text{SrO}_4$
- $\text{Ti}_2\text{BaO}_4$
- $\text{Ti}_2\text{ZnO}_4$
- $\text{V}_2\text{BeO}_4$
- $\text{V}_2\text{SiO}_4$

$\text{A}_2\text{BX}_4$ search:
- ~80000 individual total-energy calculations
  (incl. structures and magnetic configurations)

7 already predicted by Hautier et al., Chem. Mater., 2010
Results – Sulfides

We predict:

- $\text{Hg}_2\text{GeS}_4$,
- $\text{Al}_2\text{TiS}_4$,
- $\text{Al}_2\text{VS}_4$,
- $\text{Al}_2\text{CoS}_4$,
- $\text{Al}_2\text{NiS}_4$,
- $\text{In}_2\text{VS}_4$,
- $\text{Sc}_2\text{BaS}_4$,
- $\text{Ti}_2\text{MgS}_4$, ...

Out of 92 not reported:

- 34 stable,
- 1 undermined,
- 57 not stable.
CID Predicted Ternary Materials

**A$_2$BX$_4$ materials main group and 3d elements:**
Out of 684 variations, 429 are unreported

100 predicted stable, 11 undetermined, and 318 predicted not stable


**ABX materials with 8 electrons:**
Out of 714 variations, 488 are unreported

235 predicted stable, 18 undetermined, and 235 predicted not stable

Identification of ABX ternary materials

X-ray diffraction is usually the preliminary tool to identify a new material.

A fast identification of the new ABX compounds in multiphasic samples is possible by simulating the pattern of the predicted structure.

58 Stable and NOT reported ABX 18 electron compounds

1 compound P4_2/mmc
1 compound P-3m1
2 compounds P6_3/mmc
1 compound Imm2
2 compounds R-3m
30 compounds F-43m
15 compounds Pnma
6 compounds P2_1/c

The symmetry of a predicted stable compound makes possible:

1) Simulation of diffraction pattern
2) Fast identification in the experimental pattern
Identification of ABX ternary materials

HfIrSb, ZrRhBi, ScRhTe, TaCoSn, TaIrGe, VIrSi, VRhSi and HfRhP have been shown to crystallize in their predicted crystal structure.

**Example:**

HfIrSb

F-43m

The symmetry of a predicted stable compound makes possible:

1) Simulation of diffraction pattern
2) Fast identification in the experimental pattern

**With Confirmation By Electron diffraction**

Fast identification in multiphasic sample

X. Zhang et al. submitted to Nature Materials
Functionality of ABX ternary materials

Theoretical calculations on predicted (and then synthesized) ABX materials provide information about their properties.

**Example:** TaCoSn – A Semiconductor from 3 metals

- Indirect band gap of 1.3 eV
- Absorption onset at 1.6 eV
- High absorption above 1.8 eV

**Experiment:**
- Thin film growth
- Potential absorber applications

Missing TaCoSn Compound

Not known in ICSD or ICDD

Large stability range

Predicted to have semi-conducting gap $\sim 1.3$ eV (GGA + U)
Validation: Growth of New TaCoSn

Predicted Structure

TaCoSn Grown

XRD: Predicted & Measured

Inverse Design provides a scientific framework to accelerate the discovery of new materials.
Summary

- Inverse Design
  Theory ↔ Experiment Coupling is Critical
  Theory and Experimental Tools
- Design via Design Principles
  Selection criteria for PV absorbers
  $\text{Co}_2\text{ZnO}_4$ from $\text{A}_2\text{BX}_4 \rightarrow \text{p-type TCO}$
  Search for missing materials and their functionality
- Materials Design Approach Broadly Applicable
  Other Functionalities
- Metastability, Synthesizability
cooperation and innovation “without borders” to develop and ready emerging and revolutionary solar electricity technologies toward the extended-time success of India’s Jawaharlal Nehru National Solar Mission and the U.S. DOE SunShot Program

SERIIUS

serius.org
SERIIUS R&D Thrusts

Research Thrusts

- **Sustainable Photovoltaics (PV)**
  - Earth Abundant PV
  - Advanced Process/Technology
  - Multiscale Modeling and Reliability

- **Multiscale Concentrated Solar Power (CSP)**
  - High-T, Closed-Cycle, Bravton Cycle
  - Low-T Organic Rankine Cycle
  - Thermal Storage & Hybridization

- **Solar Energy Integration (SEI)**
  - Roadmapping, Analysis and Assessment
  - Grid Integration and Energy Storage

- **Core Projects**
- **Consortium Projects**

- **CONSORTIUM PROJECTS:** disruptive, transformative R&D
- **CORE PROJECTS:** core industry partner-led and focused
Developing Low Cost Atmospheric Processing

Inks and synthesis
- Understanding metalorganic decomposition
- Molecular precursor design
- Synthesis to desired materials
- Inks:
  - Absorbers
  - Transparent conductors
  - Contacts/Packaging

Deposition
- Desired precursor with no residual organics
- Designed to densify with and allow grain growth
  - Compatible with other layers

Processing
- Device quality:
  - Rapid thermal processing
  - Optical Processing

Integration
- Materials/devices integrated onto flexible substrates
# Acknowledgements: CID EFRC

<table>
<thead>
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<th>Partner</th>
<th>Senior Investigators, *Staff and Students, Graduates/Alumni</th>
</tr>
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<tr>
<td>NREL</td>
<td>Dave Ginley, John Perkins, Stephan Lany, Andriy Zakutayev, Peter Graf, Jun Wei Luo, Paul Ndione, Haowei Peng, Vince Bollinger, Josh Martin, Mayeul d’Avezac, Alberto Franceschetti, Arkadiy Mikhaylushkin</td>
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Summary

- Inverse Design
  Theory \leftrightarrow Experiment Coupling is Critical
  Theory and Experimental Tools
- Design via Design Principles
  Selection criteria for PV absorbers
  \( \text{Co}_2\text{ZnO}_4 \) from \( A_2BX_4 \) \( \rightarrow \) p-type TCO
  Search for missing materials and their functionality
- Materials Design Approach Broadly Applicable
  Other Functionalities
- Metastability, Synthesizability
# Acknowledgements: CID EFRC

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