

## Center for Inverse Design

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**Lead Institution:** National Renewable Energy Laboratory

**Partner Institutions:**  
 • Oregon State University  
 • Northwestern University  
 • Stanford Synchrotron Radiation Lightsource / Stanford Linear Accelerator Center / Stanford University

**Mission Statement:** To revolutionize the discovery of materials by developing an inverse design approach powered by theory guiding experiment with an initial focus on materials for solar energy conversion.

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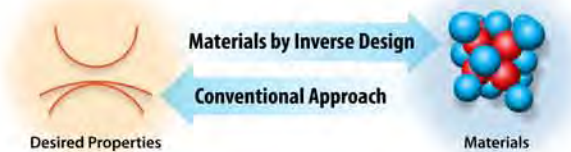
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### Achieving the Grand Challenge of Materials and Nanostructures by Design

**Mission:** To revolutionize the discovery of materials by developing an inverse design approach powered by theory guiding experiment with an initial focus on materials for solar energy conversion.

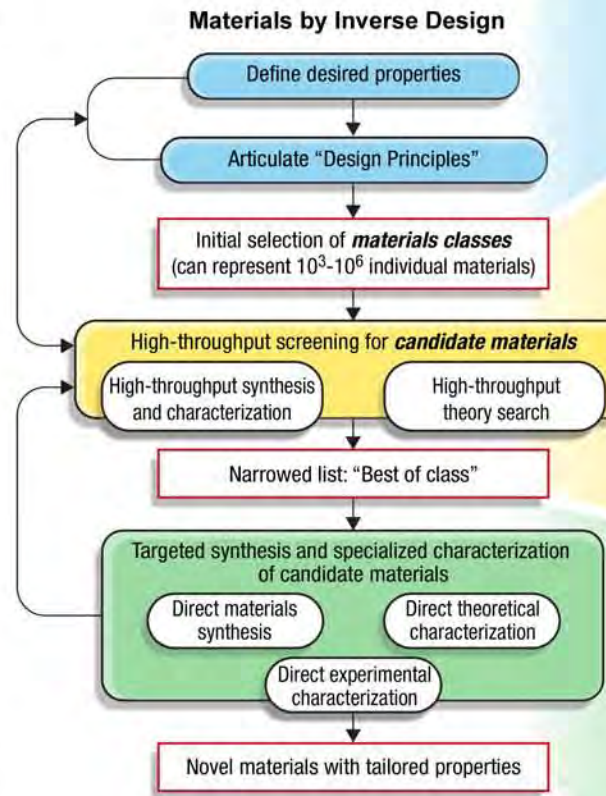


**Conventional Approach:** One chooses a material of a known composition and structure, which often was discovered by accident to have useful properties (e.g., electrical and optical properties). Then, one applies theory and targeted experiments to try to understand and explain the properties retrospectively. The discovery of new technologically relevant materials is unpredictable and slow.

**Inverse Design Approach:** We invert this process by first defining the desired application-specific properties. Based on general scientific "Design Principles," we select a broad materials class within which the desired properties are likely to be found. We then employ high-throughput theoretical and experimental screening to identify the most-promising candidate materials within this class. Finally, we do in-depth studies by means of targeted theory, synthesis, and characterization to go the last mile, making materials by inverse design a reality.

### Proposed Goals

- Goal A.** Develop Inverse Design methodology.
- Goal B.** Apply and refine Inverse Design to address the basic research needs for solar conversion materials.
- Goal C.** Promote Inverse Design methodology and tools to the scientific community as a user-friendly, transferable approach and tool set for solving materials science problems.

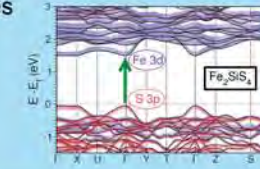


### Inverse Design Methodology

#### Step 1: Design Principles (DPs)

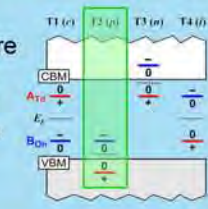
##### Solar Absorbers

- Need:** High optical absorption
- DP:** Use materials with high density of states due to empty d-states



##### p-type Transparent Conductors

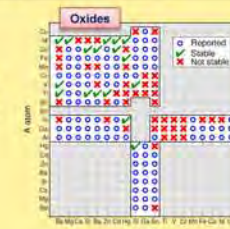
- Need:** Many acceptors (neg. charge), Few donors (pos. charge)
- DP:** Find materials where donor state is inactive (level inside valence band)



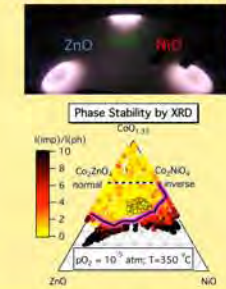
#### Step 2: High-Throughput Screening

##### Theory Search

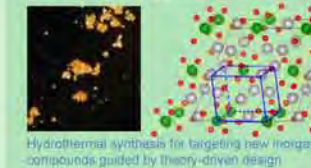
- Search for new  $A_2BX_4$  compounds (X = O, S, Se, Te): We predict structure and heat of formation of 107 stable new (previously not reported) materials.



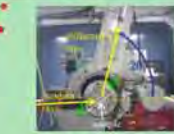
##### Experimental Screening



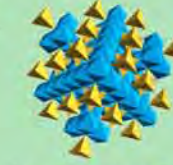
#### Step 3: Targeted Synthesis and Characterization



Hydrothermal synthesis for targeting new inorganic compounds guided by theory-driven design



SSRL Beamline 2-1



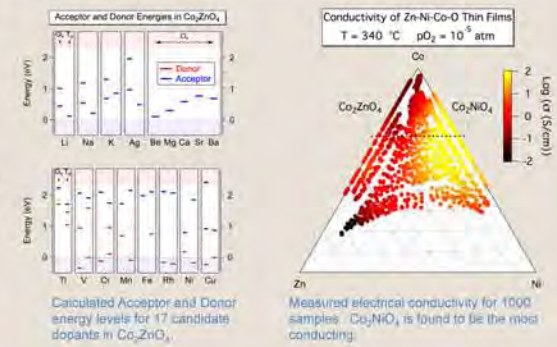
Zn = yellow (tetrahedral, T<sub>2</sub>), Co = blue (octahedral, O<sub>h</sub>)

- Based on design principles, computational methods guide the synthesis of new solar PV electrode and absorber materials with desired properties.
- Targeted synthesis and specialized characterization of candidate electrode and absorber PV materials are essential steps in demonstrating the Inverse Design process.

### Inverse Design Highlights

#### Transparent Conducting Oxides (TCOs)

n-type TCOs are well known. However, good p-type TCOs, which would enable improved photovoltaics (PV), are not. We are using combined theory and experiments in an Inverse Design approach to look for new p-TCOs.  $Co_2ZnO_4$ , a doping-type T2 spinel, and related materials is our starting point material in the Spinel class.



Calculated Acceptor and Donor energy levels for 17 candidate dopants in  $Co_2ZnO_4$ .

Measured electrical conductivity for 1000 samples.  $Co_2NiO_4$  is found to be the most conducting.

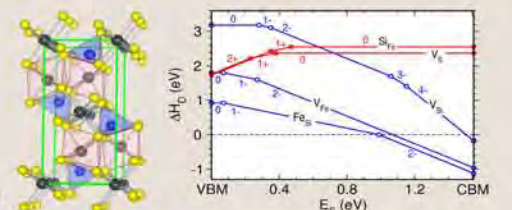
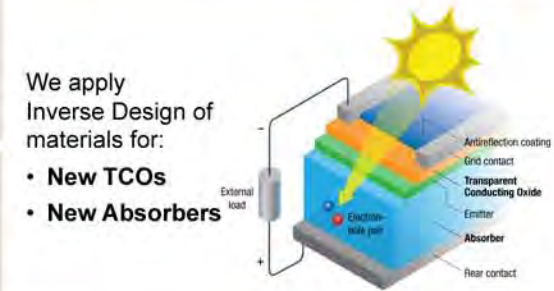
#### Earth Abundant Solar Absorbers

**Purpose:** Design ultra-thin film absorbers for high-efficiency solar cells.

- Intrinsic flaws of thin-film  $FeS_2$  identified by theory-guided experiments

#### New Design Principles:

- Avoid phase coexistence
- Octahedral coordination for  $Fe^{2+}$
- Incorporate electronegative elements



The formation energies of point defects in  $Fe_2Si_4$  as a function of Fermi energy at  $T \sim 550$  K. The red lines represent donor defects, and the blue lines represent acceptor defects.

**Outcome:** New family of absorbers represented by  $Fe_2Si_4$  with potential for efficient, high-voltage performance in thin-film solar cells