Science for our Nation's Energy Future

Energy Frontier Research Centers
Summit & Forum

Center for Inverse Design

Director
Bill Tumas (interim)

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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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.

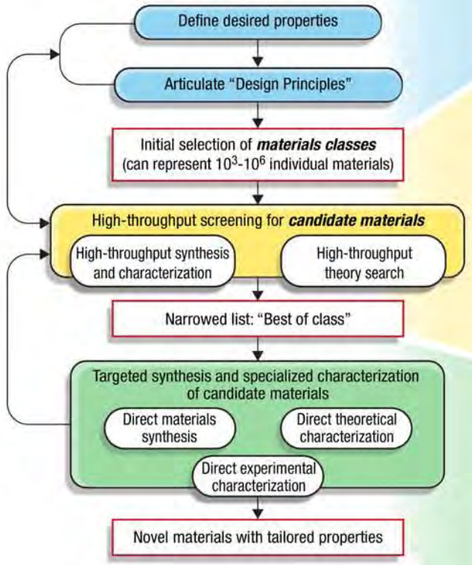
Proposed Goals

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.

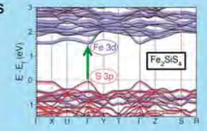
Materials by Inverse Design



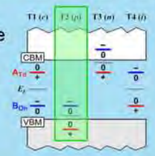
Inverse Design Methodology

Step 1: Design Principles (DPs)

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

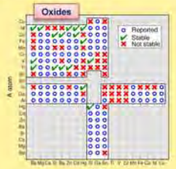


p-type Transparent Conductors
- **Need:** *Many* acceptors (neg. charge), *Few* donors (pos. charge)
- **DP:** Find materials where donor state is inactive (level inside valence band)



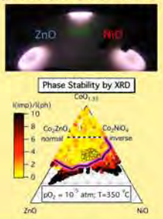
Step 2: High-Throughput Screening

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.

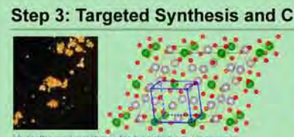


Among the 856 A_2BX_4 combinations considered for X = O, S, Se, Te, 406 are "missing" (not reported). We predict 107 new stable materials, whereas the remaining 299 are found to be unstable.

Experimental Screening



Step 3: Targeted Synthesis and Characterization



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

SSRL Beamline 2-1

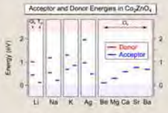
Zn = yellow (tetrahedral, T_d)
Co = blue (octahedral, O_h)

- 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.

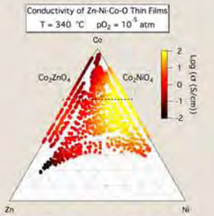
Inverse Design Highlights

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.



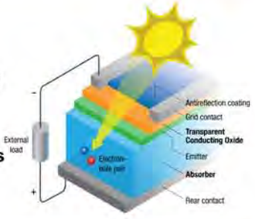
Measured electrical conductivity for 1000 samples. Co_2NiO_4 is found to be the most conducting.

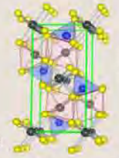
Earth Abundant Solar Absorbers

Purpose: Design ultra-thin film absorbers for high-efficiency solar cells.
- Intrinsic flaws of thin-film FeS_2 identified by theory-guided experiments

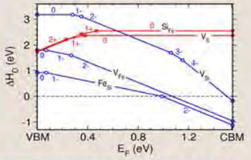
New Design Principles:
- Avoid phase coexistence
- Octahedral coordination for Fe^{2+}
- Incorporate electronegative elements

We apply Inverse Design of materials for:
- **New TCOs**
- **New Absorbers**





Fe_2SiS_4



The formation energies of point defects in Fe_2SiS_4 as a function of Fermi energy at T ~550 K. The red lines represent donor defects, and the blue lines represent acceptors defects.

Outcome: New family of absorbers represented by Fe_2SiS_4 with potential for efficient, high-voltage performance in thin-film solar cells

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