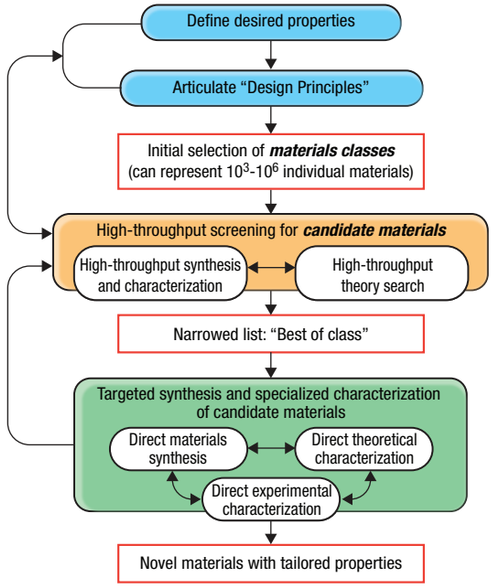
Materials by Design in Three Steps

During this Summer School, we will discuss the three key steps and further details of the inverse design approach described below:



Step 1: Design Principles

- Articulate target properties for a given desired functionality.
- Employ and further develop a set of overarching "design principles." These physical mechanisms have been identified in previous theoretical research efforts.

Step 2: High-Throughput Screening

- Based on the design principles, choose initial "classes of materials," each representing 10^3 to 10^6 individual compounds.
- Use theoretical inverse band structure (IBS) methods, in parallel with experimental high-throughput synthesis and characterization (HTSC) methods, to narrow these classes to a list of promising individual candidate ("best of class") compounds. For example:
  - IBS identifies the optimal compositions (x,y) and/or atomic arrangements that maximize the hole concentration while maintaining optical transparency.
  - HTSC provides validation and complementary information by synthesizing 10^3 to 10^4 samples per class using either composition-spread physical vapor deposition or combinatorial hydrothermal synthesis approaches.
- Measure the target materials properties of interest using high-throughput mapping tools specifically developed for this purpose.
- Finally, use advanced techniques and tools of data analysis and data mining to compare with the IBS results and to identify the "best-of-class" materials rationally.

Step 3: Targeted Synthesis and Characterization

- Use targeted synthesis, specialized theory, and direct characterization to investigate individual candidates in greater detail. For example, explore the materials synthesis routes, defect structures and models, and fine-tuning of the target properties.
- Feed back the results of these scrutinized investigations into a second optimization loop, if needed.

Inverse Design Summer School

September 13-14, 2011

Denver Marriott West • 1717 Denver West Blvd. • Golden, CO 80401
1-888-238-1803 (toll-free) • 303-279-9100 (local)

The Center for Inverse Design—an Energy Frontier Research Center of the U.S. Department of Energy—is offering a no-cost, two-day summer school on inverse design. We invite you to attend if you are a:

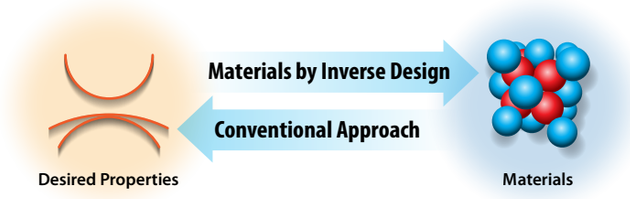
- Scientist or engineer interested in materials design and discovery
- Technical leader in materials, electronics, or chemical science
- Leader of a large, interdisciplinary center and organization
- Student or post-doctoral researcher in science and technology.

The overall purpose is to introduce the inverse design methodology *(see back page)* and tools to the scientific community as a user-friendly, transferable approach and tool set for solving materials science problems.

Specific purposes of this summer school are to:

- Answer the question, "What is inverse design?"
- Understand how inverse design differs from historical approaches to materials discovery
- Introduce the tools for screening materials from the vast universe of materials
- Introduce the tools for targeted synthesis and characterization
- Examine the applications of inverse design within the solar/photovoltaic discipline
- Discuss what inverse design can do for you.

For more information, contact L.L. Kazmerski, NREL (kaz@nrel.gov)



The vision of the Center for Inverse Design is to revolutionize the discovery of materials, replacing the conventional approach with the inverse design approach.

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.

AGENDA: Inverse Design Summer School

Tuesday, September 13

7:30 – 8:00	Breakfast *(provided)*	
8:00 – 8:30	Introduction/Welcome	B. Tumas
Morning:	***What is inverse design?***	**Chair: B. Tumas**
8:30 – 9:20	The vision of inverse design	A. Zunger
9:30 – 10:20	A history of theory for materials	S. Lany
10:30 – 11:20	Challenges and research needs for PV	D. Ginley
11:30 – 1:00	Lunch with students/postdocs	P. Thiyagarajan
11:30 – 1:00	PI working lunch meeting	PIs
Afternoon:	***Tools for screening materials from a large phase space***	**Chair: D. Keszler**
1:00 – 1:50	High-throughput theory	M. d'Avezac, V. Stevanovic
2:00 – 2:50	High-throughput experiment:	
	Synthesis *(25 min)*	A. Zakutayev
	Characterization *(25 min)*	J. Perkins
3:00 – 3:50	Verification by specialized theory	S. Lany
4:00 – 5:30	Time for informal project discussions	all
Evening:	***Activities in the Center for Inverse Design***	
6:30 – 8:30	Poster session and buffet	

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Wednesday, September 14

7:30 – 8:00	Breakfast *(provided)*	
Morning:	***Tools for targeted synthesis and characterization***	**Chair: S. Lany**
8:00 – 9:20	Transparent conducting oxides:	
	Bulk methods *(40 min)*	T. Mason, N. Perry
	Hydro-thermal methods *(40 min)*	K. Poeppelmeier, V. Cloet
9:30 – 10:20	Chalcogenide solar absorbers:	
	Bulk methods *(25 min)*	D. Keszler
	Thin-film methods *(25 min)*	R. Kykyneshi
10:30 – 11:20	Synchrotron-based methods	M. Toney
11:30 – 1:00	Lunch with PIs	P. Thiyagarajan
11:30 – 1:00	Students/postdocs working lunch meeting	student/postdocs
Afternoon:	***Application of Inverse Design***	**Chair: T. Mason**
1:00 – 1:50	CO-based p-type TCOs	A. Zakutayev, N. Perry, Y. Shi, S. Lany
2:00 – 2:50	Fe-based absorbers	L. Yu, R. Kykyneshi
3:00 – 3:50	Ag- and Cu-vanadates as p-type TCOs	G. Trimarchi, H. Peng, A. Raw
4:00 – 5:30	***Inverse Design: Which way forward?***	**Chairs: D. Ginley, S. Lany**

EFRCcouncil members give short talks to begin general discussion on following topics:

- Where are opportunities for inverse design?
- What are the challenges ahead?
- What does success look like?
- Comparison with activities of competitors

Evening:		
6:00 – 8:30	Student/postdoc dinner *(informal)*	
6:00 – 8:30	EFRC council dinner *(location TBD)*	
9:00 –	Informal after-work gathering *(Yard House, Colorado Mills Mall)*	