Center for Inverse Design

The Center for Inverse Design pursues a new approach to material science. Rather than using the conventional approach ("Given the structure, find the electronic properties"), we will pursue the "materials by inverse design" approach ("Given the desired property, find the structure"). The target properties include general semiconductor optical and electrical properties, and the desired materials functionalities include electron- and hole-conductive transparent conductors, solar absorbers, and nanostructures for energy sustainability. Predictions will be iteratively examined by various synthetic approaches, including high-throughput parallel materials science.

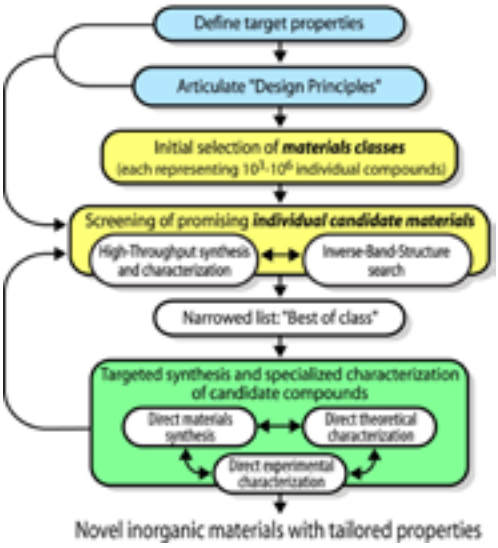
Comparison of "materials by inverse design" versus the conventional approach.

Additional information on the Center is provided in the following sections and in the links below:

- "DOE to establish Energy Frontier Research Center at NREL" (NREL news release, 5/27/09)
- "NREL gets $20M from DOE for solar" (Denver Business Journal, 8/6/09) (PDF 33 KB)
  Energy Frontier Research Center (summary slide) (PDF 78 KB)
- "NREL Center Turns Materials Design Upside Down" (NREL news feature, 8/14/09)
- Center for Inverse Design (fact sheet) (PDF 404 KB)
- Staffing for the Center for Inverse Design (PDF 28 KB)

Research Approach

The inverse materials design methodology integrates and combines the three components of (1) theory, or prediction, (2) synthesis, or realization, and (3) characterization, or validation. The result will be the acceleration—by orders of magnitude—in developing new materials. The following figure graphically illustrates the research approach described below.



Flow diagram of steps in the "materials by design" research approach within the Center for Inverse Design.

Articulate Target Properties and Design Principles (blue section in figure)

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

Optimize and Refine Screening of Materials Classes (yellow section in figure)

- Based on the design principles, we choose initial "classes of materials," which each represent 10^3 to 10^6 individual compounds.
- We use theoretical inverse-band structure (IBS) methods, in parallel with experimental high-throughput synthesis and characterization (HTSC) methods to narrow down 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.
- The target materials properties of interest are then measured using high-throughput mapping tools specifically developed for this purpose.
- Finally, advanced techniques and tools of data analysis and data mining are used to compare with the IBS results and to rationally identify the "best-of-class" materials.

Investigate Individual Candidates in Targeted, Direct Studies (green section in figure)

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

Participating Organizations and Researchers

Four participating institutions form the Center for Inverse Design, which is headed by Dr. Alex Zunger. Brief descriptions are given below of the principals at each institution, with links to full biographical sketches.

National Renewable Energy Laboratory (NREL)

- **Alex Zunger**—the EFRC Director, has led NREL's Solid State Theory group for 30 years, a group that has been a platform for state-of-the-art theory and modeling of semiconductors, insulators, metals, alloys, and nanostructures, including inverse-band structure methods. He is co-developer of the Plane-Wave Total Energy method, the first "first-principles" pseudopotentials, and LDA "Exchange Correlation" functionals. His scientific research covers all of the areas called for in this proposal, including photovoltaic materials, computational techniques, and nanostructures. Full bio (PDF 24 KB).
- **Lawrence L. Kazmerski**—the Program Integrator, has had over 30 years experience in line and program management at NREL. In his position as Director of NREL's National Center for Photovoltaics, he has had line management and technical leadership responsibility for a staff of 185 for the past 9 years (annual budget of ~$75 million).

Recently, he has been appointed as Executive Director for Science and Technology, with responsibilities for building partnerships with other laboratories in renewable energy worldwide. He has also had executive experience with several professional organizations, including that as elected President of the AVS in 1991. He is a member of the National Academy of Engineering, and a Fellow of the APS, the IEEE, and the AVS. Full bio (PDF 28 KB).

- **Mayeul d'Avezac—**is a post-doctoral researcher in Alex Zunger's the Solid State Theory group. During his post-doc appointment, he developed and applied novel search methods for material design, and implemented novel fitting-models used in conjunction with accurate, but computer-intensive, first-principles methods. Full bio (PDF 18 KB).

- **Alberto Franceschetti—**is a Senior Scientist at NREL who has more than 15 years experience in computational and theoretical condensed matter physics. He is co-author of the *Nature* article "The Inverse Band-Structure Problem of Finding an Atomic Configuration with Given Electronic Properties," which lies at the heart of this proposal. He also has a long history in electronic structure calculations for nanostructures. Full bio (PDF 22 KB).

- **David S. Ginley—**is a Research Fellow and group manager of the Process Technology and Advanced Concepts group at NREL in the National Center for Photovoltaics. He has over 30 years experience in developing new solar energy materials specifically with respect to oxides, photo-electrochemistry, and novel solar absorber materials and processing. His group currently consists of about 30 staff, post docs, and graduate students in the areas of organic photovoltaics, transparent conducting oxides, combinatorial high-throughput materials science, solution-based precursors to electronic materials, and novel process technologies for photovoltaic and related devices including batteries and fuel cells. Full bio (PDF 24 KB).

- **Peter A. Graf—**is a staff Scientist at NREL and has more than 15 years experience as a professional programmer and in developing and applying mathematical algorithms. His work at NREL focuses on simulation optimization and data analysis. He has been among the original designers of a data management, analysis, and mining system for high-throughput materials science which is currently under growing use and increasing development at NREL. Full bio (PDF 22 KB).

- **Stephan Lany—**is a Senior Scientist at NREL with 10 years experience in computational materials science. He has developed and applied methods to predict materials properties based on first-principles calculations, including improved accuracies of formation energies, bandgap correction methods, and the prediction of the materials stoichiometry, defect concentrations, and Fermi level. Full bio (PDF 20 KB).

- **John D. Perkins—**has more than 15 years experience in developing mixed metal oxide thin-film materials including more than 10 years on transparent conducting oxide materials. He also has 8 years experience in developing and applying high-throughput synthesis and characterization approaches to optical-quality thin-film materials. Full bio (PDF 25 KB).

Oregon State University (OSU)

- **John F. Wager**—is a Professor of the Department of Electrical and Computer Engineering EECS at OSU. He has almost 30 years experience in the areas of compound semiconductor materials and devices, solar cells, transparent electronics, thin-film electroluminescence, thin-film transistors, surface and interface analysis, and semiconductor defects. His current research thrusts include transparent electronics, printed electronics, and photovoltaics. Full bio (PDF 23 KB).

- **Douglas A. Keszler—**is Distinguished Professor of Chemistry at OSU. He joined the Department of Chemistry at OSU in 1985, where he has maintained research and education programs directed to the synthesis and study of new nonlinear optical materials, phosphors, wide-gap semiconductors, dielectrics, transparent electronics, and printed electronics. Full bio (PDF 23 KB).

Northwestern University (NU)

- **Kenneth R. Poeppelmeier**—has been Professor at the Department of Chemistry at NU since 1988. His research emphasizes the connections between the synthesis and structure of new materials, the physical properties of new materials, and the technological advances that can result from these discoveries. Full bio (PDF 32 KB)

- **Arthur J. Freeman—**is world-renowned pioneering proponent and developer of computational quantum materials science and engineering. The most apt designation for this emergent field is that it enables the "virtual fabrication" of new materials. His Electronic Structure/Condensed Matter Theory Group has been a leading research group in electronic structure theory for more than 40 years at NU and at MIT. Full bio (PDF 26 KB).

- **Thomas O. Mason—**has been Professor at the Department of Materials Science and Engineering at NU since 1989, where his group investigates fundamental structure property relationships in technologically important electro-ceramics, including transparent conducting oxides, transparent oxide semiconductors, ionic ceramics, and mixed ionic/electronic ceramics. Full bio (PDF 21 KB).

Stanford University / Stanford Synchrotron Radiation Lightsource (SSRL) / Stanford Linear Accelerator Center (SLAC).

- **Michael F. Toney**—has more than 20 years experience in synchrotron X-ray methods of materials characterization. He is an expert in thin-film, surface, and interface studies with X-ray and neutron scattering techniques. He was one of the pioneers, while at IBM, in the use of surface diffraction for investigations of atomic structure at solid/liquid interfaces and organic thin films. Full bio (PDF 25 KB).