**Center for Inverse Design**
**EFRC Director: Alex Zunger**
**Lead Institution: National Renewable Energy Laboratory**

***Mission***: *Achieve the grand challenge of materials and nanostructures by design: Given the desired, target property, find the structure/configuration that has it, and then make the material.*

Historically, the development of new materials for technological applications has been based to a large extent on trial-and-error searches or accidental discoveries. This pattern is exemplified not only by the historic discovery of semiconductivity in Si and GaAs, but also, more recently, by the discovery of new materials with unsuspected physical and chemical properties, including: high-$T_C$ in cuprates or iron-based superconductors, high tensile strength in carbon nanotubes, and colossal magneto-resistance in manganites. Since (i) in many cases, materials with fundamentally new properties are found outside the chemical neighborhood of the "usual suspects" materials, and (ii) the development of accidentally-discovered materials may take a long time (because it takes a long time to figure out what it is that has been discovered), the current practice of materials-by-discovery may not be the best way to lead to game-changing technologies. We will prefer materials design over materials discovery. As far as theory is concerned, our strategy is to reverse the conventional approach of "given the structure of a solid or molecule, predict its electronic properties", into "given the target electronic properties (required for a given technological application), find the structure that has such properties" (Fig.1).

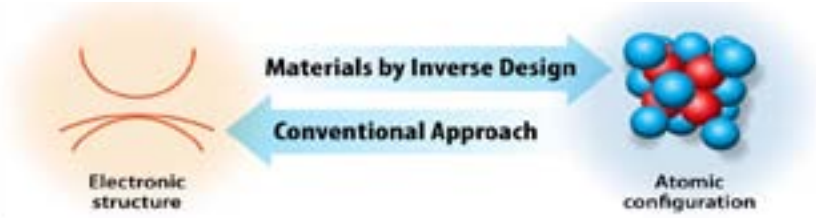


Fig. 1. Inverse-Design approach versus conventional approach to materials discovery.

The vision of "Inverse Design" could change the basic approach to materials research and potentially usher in a new era of materials science .To accomplish this vision we will conduct three steps.

**First,** we will articulate a set of desired, physical target properties. For optoelectronic semiconductors the target properties might be, for example, a given value of the band gap and effective masses, the ability to dope a material *p*-type or *n*-type, or a certain thermoelectric (ZT) response. For ferromagnets , the target might be a desired Curie temperature; for impurities in solids or surface states this might be a certain energetic position of the gap levels with respect to the band edges; for quantum dots a target might be a certain Auger recombination or exciton–multiplication rates. One might start by certain, broad classes of solids /alloys/nanostructures, initially selected on the basis of "Design Principles", which determine rather broad classes of materials (e.g, containing $10^6$-$10^8$ individual compounds) likely to encompass the required target properties. The initial selection might be done on the basis of physical mechanisms that have been identified in past theoretical or experimental research.

**Second**, we will identify, via theoretical search of the above noted astronomic spaces of structures, the sub-class of atomic configurations whose electronic properties are close to the

target property. This will be done e.g, using genetic or other biologically-inspired search algorithms in conjunction with quantum-mechanical calculations of the electronic structure. For example, for optoelectronic semiconductors we might find the atomic short-range or long-range order in a multi-component alloy that has given band gap or effective-masses; for magnetic ions in insulators we might find their spatial arrangement that has a given Curie temperature. Preliminary examples include (i) *Band gap design in superlattices:* A. Franceschetti and A. Zunger, Nature 402, 60 (1999); (ii) *Impurity design in insulators:* S.V. Dudiy and A. Zunger, Phys. Rev. Lett. 97, 046401 (2006); (iii) *Design of Curie temperatures in ferromagnets:* A. Franceschetti, S.V. Dudiy, S.V. Barabash, A. Zunger, J. Xu, and M. van Schilfgaarde, Phys. Rev. Lett. 97, 047202 (2007); and (iv) *Design of optical transitions and strain in nanostructures:* P. Piquini, P.A. Graf, and A. Zunger, Phys. Rev. Lett. 100, 186403 (2008).

**Third,** having narrowed down the range of candidate structures and materials from an initial astronomic number to a hopefully manageable range, we will employ both combinatorial synthesis and targeted synthesis, followed by material characterization, studying the material systems that fulfill the target properties. We envision the second and third steps to involve an iterative process between experiment and theory, whereby theoretically proposed structures are scrutinized by experiment and experimentally obtained feedback is used by theory to refine and further narrow the search of new materials.

*The Inverse Materials Design Methodology integrates and combines all three components of Theory (prediction), Synthesis (realization), and Characterization (validation). The result will be orders of magnitude acceleration in the development of new materials.* The general research concept for Inverse Design of materials is illustrated in Fig. 2:

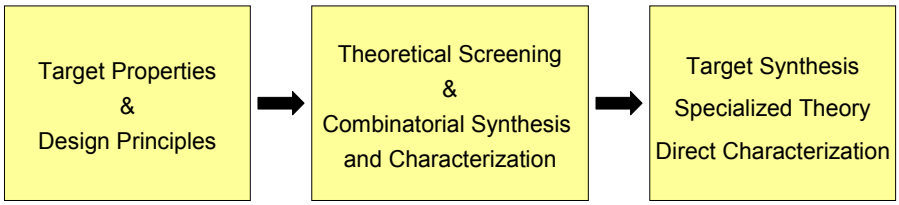


Fig. 2. The three components of the Inverse-Design approach.

We think that this philosophy is applicable to broad type of material properties (magnetism, ferroelectricity, superconductivity, transparent-conductors, to name a few) and to a broad range of structures (solids, alloys, polymers, molecular structures). The center will attempt to develop general methodologies that will be tested on specific cases, but will hopefully open the door for much broader applications in the future.

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