Center for Inverse Design (CID)
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***Mission Statement*:** *To revolutionize the discovery of new materials by design with tailored properties through the development and application of a novel inverse design approach powered by theory guiding experiment with an initial focus on solar energy conversion.*

Historically, developing new materials for technological applications has largely been based on trial-and-error searches or accidental discoveries. However, this practice may not be the best way to find game-changing technologies because: (i) in many cases, materials with fundamentally new properties are outside the chemical neighborhood of the "usual suspects" materials, and (ii) developing accidentally discovered materials may take a long time (since it takes a long time to determine what it is that has been discovered).

We prefer, in principle, *materials design* over materials discovery. Our center's revolutionary research uses quantum theory and high-performance computers to design new materials having desired properties. Then we use state-of-the-art high-throughput synthesis and targeted synthesis to converge on those materials in the laboratory.

Figure 1 shows that our approach resembles "Quantum Jeopardy": Given the answer (e.g., a certain unique and useful material property), find the question (e.g., what material is it?). Stated another way, traditional accidental discovery says: "Give us the structure; we'll study its properties," whereas our center's approach reverses this norm to: "If these are the properties we want, we'll find the structure."

Fig. 1. Inverse-design approach versus conventional (materials discovery) approach.

The vision of Inverse Materials Design could change the basic approach to materials research and potentially usher in a new era of materials science. The methodology combines and integrates theory (prediction), synthesis (realization), and characterization (validation). Its successful implementation will accelerate by orders of magnitude the development of new materials. The four steps that we are following are described below.

First, we articulate a set of desired, physical target properties. For *optoelectronic materials*, including solar semiconductors and insulators, the target properties might include achieving the following: a direct-bandgap system out of indirect-gap constituents (such as Si and Ge); a given positioning of band-edge energies with respect to certain redox potentials; a target anisotropy of the effective masses conducive to conductivity or thermoelectricity; or the ability to dope a material *p*-type or *n*-type. For *ferromagnets*, the target might be a desired Curie temperature. For *impurities in solids*, a target might be a certain energetic position of the impurity (donor or acceptor) levels with respect to the band edges. For *topological insulators*, a target might be to invert the order of conduction and valence bands; and

for *quantum wires and dots*, a target might be a certain Auger recombination, spin-splitting, or exciton-multiplication rate.

Second, for given target properties, we select an initial set of *broad material class*—based on "design principles" distilled from past insights and calculations—likely to encompass the required target properties. For new solar absorbers and transparent conductors, we have selected ternary chalcogenides and ternary oxides, including hundreds of candidate materials that are simply missing from standard material compilations. We ask: Are they missing for a good reason (e.g., they are intrinsically unstable), or have they simply been overlooked and could potentially be game-changing materials?

Third, we identify—via theoretical searching of the above-noted material and structure spaces—the sub-class whose electronic properties are close to the target property. The search-space might include either (i) *configurational degrees of freedom* at fixed composition (such as lattice decoration by Si and Ge atoms leading to direct gap), or (ii) *shape degrees of freedom* of quantum dots/wires leading to a given spectroscopic property, or (iii) *compositional degrees of freedom* (different elements constituting a compound). We use high-throughput electronic structure, defect and nanostructure calculations, and genetic or other biologically inspired search algorithms in conjunction with quantum-mechanical calculations. For example, we have performed such calculations for hundreds of A_2BX_4 and A_3BX_4 chalcogenides and ABX "filled tetrahedral structures." This work has uncovered previously unsuspected but stable "missing compounds," as well as fundamental "doping rules" that control carrier introduction into wide-gap oxides, rendering them "transparent conducting oxides."

Fourth, we study the candidate structures and materials narrowed down from an initial astronomical number to a more manageable range. We use both combinatorial synthesis and targeted synthesis, followed by material characterization. The latter steps involve an *iterative process* between experiment and theory—where 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—eventually converging on the target.

We believe our approach applies to a broad range of material properties (e.g., topological insulators, magnetism, ferroelectricity, superconductivity, transparent conductors) and structures (e.g., crystalline solids, alloys, nanostructures, molecular structures). Our center is generating general methodologies to be tested on specific cases, but that have future potential to open the door for much broader applications.

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