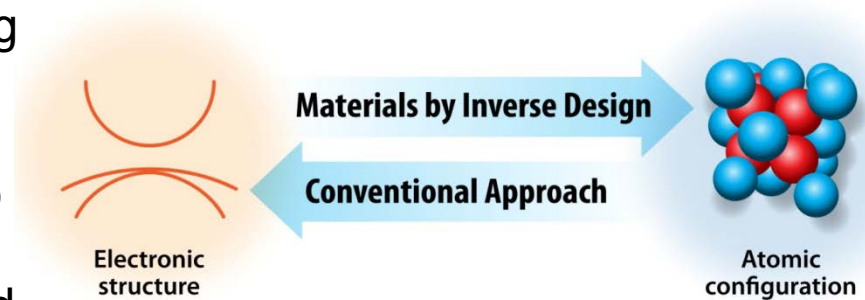


VISION: Revolutionary materials discovery—leading to developing better and even entirely new materials more rapidly—by (i) articulating needed material target properties, then (ii) using “Inverse Band Structure” quantum-mechanical methods and design principles to identify the structure having such properties, and (iii) employing combinatorial and targeted materials synthesis to realize such new materials experimentally.



The “materials by inverse design” approach (left to right), as compared to the conventional approach (right to left)

RESEARCH PLAN AND DIRECTIONS

We address the **Materials by Inverse Design grand challenge** (“Given the desired property, find the structure and composition”), rather than using the conventional approach (“Given the structure, find the electronic properties”). **Target properties** are optimized in the design of new semiconductor absorbers, transparent conductors, and nanostructures for energy sustainability. We study predictions iteratively using various synthetic approaches (e.g., high-throughput parallel materials science).