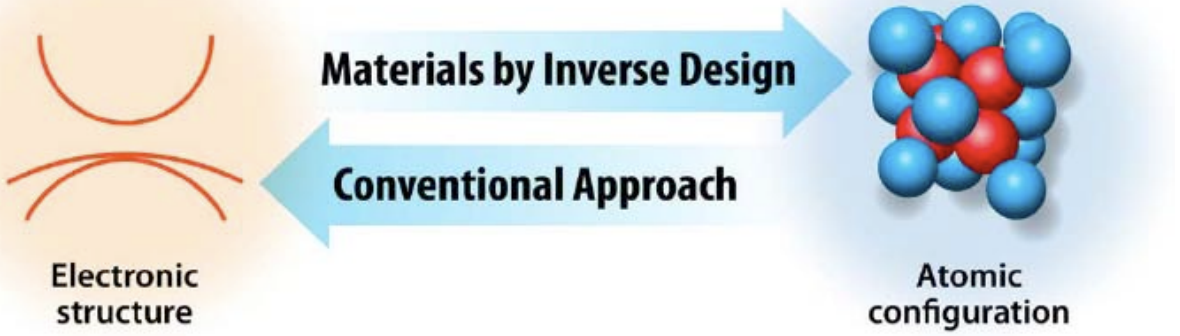
U.S. DEPARTMENT OF ENERGY

Energy Frontier Research Center
Alex Zunger (NREL)

Summary statement:

We will focus on material discovery via an "Inverse Band Structure" (IBS) methodology to theoretically identify promising structures and compositions and then apply a combination of high-throughput and targeted materials synthesis to experimentally converge on the optimum properties.



RESEARCH PLAN AND DIRECTIONS

Rather than use the conventional approach "given the structure, find the electronic properties," this center will employ the Materials by Inverse Design approach "given the desired property, find the structure." The target properties include general semi-conductor 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.