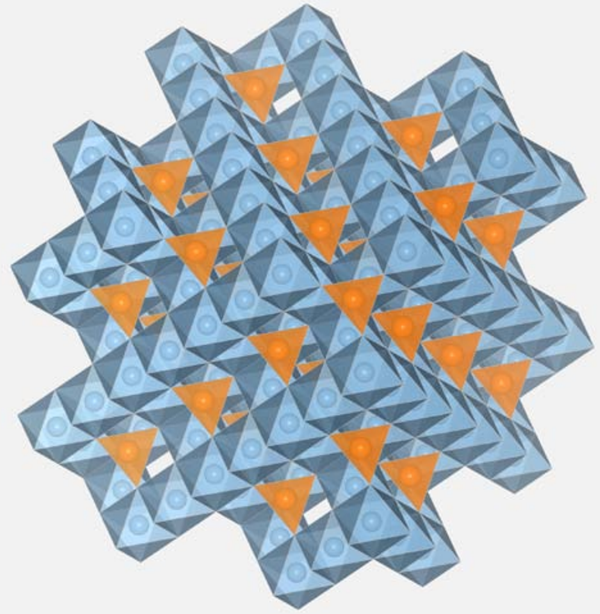
Scientific Innovation Without Borders

Theory probes the truth, while experiment tests the truth. Taking this concept to heart, scientists in the NREL-led Center for Inverse Design are addressing the crucial grand challenge of *materials by design* with an approach that integrates theoretical and experimental pursuits – essentially, innovation without borders.

The center's approach to materials science reverses the direction of the conventional paradigm to get the following: "Given the desired property of a material, find the structure of that material." Operationally, the center seeks to make significant progress with this approach by uniting theorists and experimentalists into a single band of allies.

Earlier this year, researchers within the center gathered at Northwestern University to review first-year accomplishments in four "entry-point" projects. Alex Zunger, director of the center, asked the researchers to provide "integrated experiment/theory presentations on each project, rather than two monologues." The resulting presentations reflected an impressive collaboration of theory and experiment – providing one story line, not two, on scientific advances in materials by design.

The first project focuses on so-called A_2BO_4 (or spinel) materials, which are p-type transparent conducting oxides (TCOs). The motivation for studying these materials is especially for greater design flexibility and higher efficiency of inorganic/organic solar cells, but also for their use in functional windows and transparent electronics. To many scientists, highly transparent conductive p-type TCOs are considered the "holy grail of TCOs."



Visualizing one form of an A_2BO_4 spinel structure.

Exemplifying this "borderless" approach, the review for this project wove together the results of seven presenters. Typically alternating a theorist and experimentalist, the presentation represented the work being conducted at three different institutions – Northwestern University, Stanford Synchrotron Research Laboratory, and NREL.

In the first section of the presentation, NREL scientists detailed work to identify regions of thermodynamic stability for desired material phases and which materials could be eliminated from further consideration for failing to have desired properties. A conclusion of this initial theoretical study was that self doping in cobalt zinc oxide spinel is not effective.

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The next section focused on thin-film combinatorial exploration, with studies by experimentalists from NREL and Northwestern corroborating the theoretical conclusion that self-doping indeed does not work well. Instead, one must consider extrinsic dopants to produce suitable spinels.

The final section covered work by scientists involved in materials characterization, who described the fundamental properties of bulk materials. They concluded that a solid solution exists between Co_3O_4 and Co_2ZnO_4; furthermore, only zinc-poor compositions are stable at high temperature.

A similar approach, for study and presentation, is being followed within the other three "entry-point" projects. And the theoretical and experimental scientists in the Center for Inverse Design – at the partner institutions of NREL, Northwestern, Oregon State University, and Stanford – are confident that this "borderless" approach to operations will help lead to success in developing materials by design.

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