

MAR14-2013-020623

Abstract for an Invited Paper
for the MAR14 Meeting of
the American Physical Society

The “Missing Compounds” affair in functionality-driven material discovery¹

ALEX ZUNGER, University of Colorado, Boulder, Colorado 80309

In the paradigm of “data-driven discovery,” underlying one of the leading streams of the Material Genome Initiative (MGI), one attempts to compute high-throughput style as many of the properties of as many of the N (about 10^{*5} - 10^{*6}) compounds listed in databases of previously known compounds. One then inspects the ensuing Big Data, searching for useful trends. The alternative and complimentary paradigm of “functionality-directed search and optimization” used here, searches instead for the n much smaller than N configurations and compositions that have the desired value of the target functionality. Examples include the use of genetic and other search methods that optimize the structure or identity of atoms on lattice sites, using atomistic electronic structure (such as first-principles) approaches in search of a given electronic property. This addresses a few of the bottlenecks that have faced the alternative, data-driven/high throughput/Big Data philosophy: (i) When the configuration space is theoretically of infinite size, building a complete data base as in data-driven discovery is impossible, yet searching for the optimum functionality, is still a well-posed problem. (ii) The configuration space that we explore might include artificially grown, kinetically stabilized systems (such as 2D layer stacks; superlattices; colloidal nanostructures; Fullerenes) that are not listed in compound databases (used by data-driven approaches), (iii) a large fraction of chemically plausible compounds have not been experimentally synthesized, so in the data-driven approach these are often skipped. In our approach we search explicitly for such “Missing Compounds”. It is likely that many interesting material properties will be found in cases (i)-(iii) that elude high throughput searches based on databases encapsulating existing knowledge. I will illustrate (a) Functionality-driven discovery of topological insulators and valley-split quantum-computer semiconductors, as well as (b) Use of “first principles thermodynamics” to discern which of the previously “missing compounds” should, in fact exist and in which structure. Synthesis efforts by Poeppelmeier group at NU realized 20 never-before-made half-Heusler compounds out of the 20 predicted ones, in our predicted space groups. This type of theory-led experimental search of designed materials with target functionalities may shorten the current process of discovery of interesting functional materials.

¹Supported by DOE ,Office of Science, Energy Frontier Research Center for Inverse Design