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Distributed Strategies for Materials Development

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Through an advanced combination of "ab-initio", “data-mining high-throughput”, “cluster expansion”, "vibrational", and "electronic structure" techniques, we have parameterized the whole set of transition-metal binary intermetallics (435 alloys) and a list of ~6,000 inorganic crystals. The presentation will introduce methods, tools, standards, online-access, and the approach for automatic discovery of trends in material development. We will analyze rules for miscibility in metallic catalytic materials, electronic structure correlations in scintillators, high-throughput search of thermoelectric and topological insulators through the distributed network of data. If time allows, the presentation will also extend the hybrid method to study phenomena at the nanoscale, such as size-induced viscosity effects on the catalytic rate, self-consistent variational approaches to the shape of nano catalysts and size-dependent Wulff plots for tailoring catalysts compositions and size.