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Abstract for an Invited Paper
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Distributed Strategies for Materials Development

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Through appropriate combinations 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 ∼10,000 inorganic crystals. The presentation will introduce the method, the tools, the standards, 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, and high-throughput search of thermoelectric materials and topological insulator through the distributed network of data, accessible to the scientific community. The presentation will also extend the hybrid method to study phenomena at the nanoscale, like 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 (Sponsors: ONR, NSF, DHS, Teragrid).