A Next Generation Synthesis Center (GENESIS)
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Lead Institution: Stony Brook University
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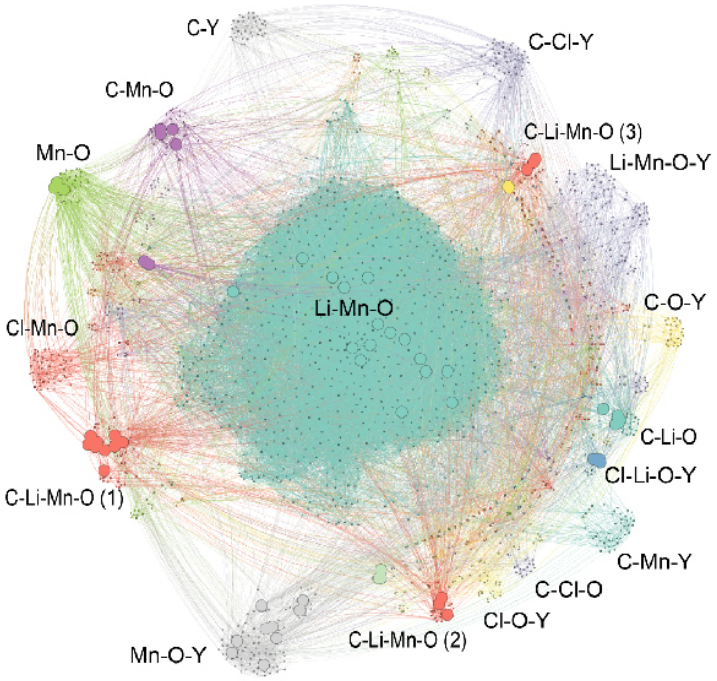
Mission Statement*: To develop a new paradigm for synthesis that accelerates the discovery of functional materials by integrating advanced in situ diagnostics and data science tools to interrogate, predict, and actively control the pathways that govern synthesis and lead to new materials.*

Our ability to solve application-driven energy problems—such as the production, conversion and storage of energy, or the design of tailored heterogeneous catalysts and catalyst substrates—depends on the development of next-generation functional materials with targeted properties. While computational materials discovery can now predict new hypothetical materials (and their functional properties), computation has struggled to predict the inherently non-equilibrium processes that govern their synthesis. Realizing these hypothetical functional materials through conventional intuition-guided synthesis is a slow, rate-limiting, iterative process.

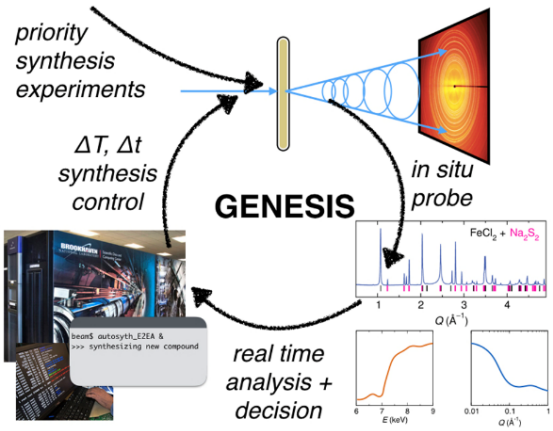


The reaction network for the C-Cl-Li-Mn-O-Y chemical system. The network contains 56 phases: 39 stable and 17 metastable. Chemical subsystems are labeled by color. The larger nodes indicate reactant nodes which are traversed on the 20 shortest pathways from precursors to targets in $YMnO_3$ synthesis.

To be *useful*, a material must be *made*, and its synthesis must then be optimized, regardless of how it was conceived or serendipitously discovered. Control over synthesis pathways and products is a critical requirement for materials design, without which concepts developed *in silico* cannot be brought into reality. Can we develop a data-driven approach to design synthesis pathways *ab initio?*

A radical rethinking of inorganic materials synthesis is needed; one that moves us forward from think-cook-look-repeat strategies to machine-predicted synthesis pathways, in a manner analogous to computational property-driven structure-prediction methods. Several emerging concepts in experimental and computational approaches, especially in combination, hint at ways forward.

Chemical reaction network models, constructed from thermochemistry databases, offer computationally tractable approaches for suggesting likely reaction pathways via application of pathfinding algorithms, presenting new opportunities for enabling reaction pathway prediction, rapid iteration between experimental/theoretical results, and ultimately, control of synthesis.



GENESIS workflow with in situ experimental probes analyzed in real time to enable controlled, next-generation synthesis.

Bright sources of X-rays and neutrons at National Facilities allow users to perform high-throughput studies to determine local and long-range atomic arrangements, site chemistries, stress-strain relationships, sample textures in inorganic materials as a function of p, T etc. Access to open searchable databases and powerful computational resources lead to lists of target structures, prioritized by the fundamental properties leading to the desired functionality, and synthesizability. Development and deployment of individual experimental and computational tools are not transformative in themselves. Their combination and a focus on the reaction pathway, rather than just the beginning and end points of a reaction, will produce a transformation in synthesis science.

The GENESIS effort complements other DOE efforts. Specifically, the *de novo* prediction and adaptive control of synthesis routes enabled by GENESIS can facilitate the realization of new materials identified within programs, including hypothetical materials identified through computational materials discovery or materials that implement new design rules. The tools for science-based synthesis, including at large DOE user facilities, serve a broader community to understand and control the synthesis different families of materials beyond those of specific interest to GENESIS. The GENESIS framework for understanding how to effectively access materials away from equilibrium and, build new infrastructure to rapidly collect and interpret *in situ* synthesis data that can be use by any researcher in this field.

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