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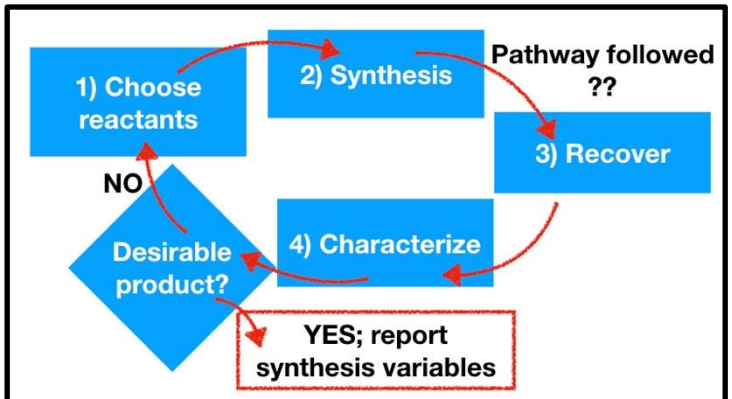
Mission Statement*: To develop a new paradigm for synthesis that accelerates the discovery of functional materials by integrating advanced in situ diagnostics and data science tools to interrogate, predict, and control the pathways that govern synthesis and lead to new materials.*

The "cook-and-look" technique remains the mainstay of materials research and development. Researchers seal chemical reactants in a vessel, "cook" to initiate a reaction and after some time "look" at the recovered products to determine if they are in a form required to be useful.

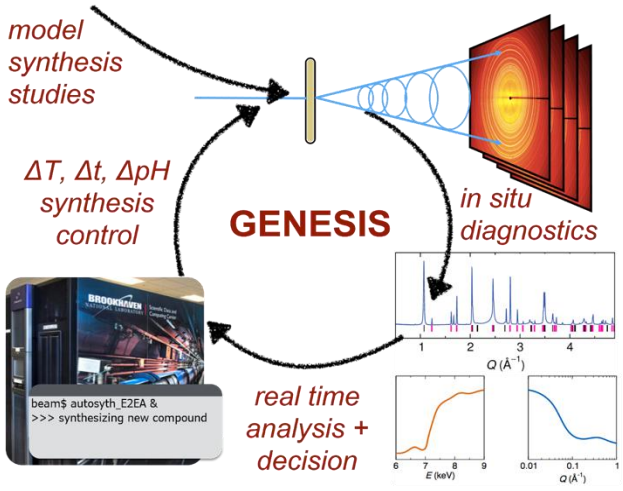


Schematic of historical practice for synthesis of materials.

The formidable task of repeated synthesis-recovery-characterization can be accelerated using modern in situ techniques that allow us to "look inside" the reaction vessel. The paths taken by a reaction from starting materials to final functional product are opaque to researchers without the use of in situ techniques. However, the data, such as those collected using beams capable of penetrating reaction vessels at DOE X-ray and neutron User Facilities, are mostly analyzed off-line. During reactions transient species form, grow and transform to other species. These processes are critical to the final product and all are invisible without the ability to follow them in situ *and* in real time. Observation of the reaction pathway and real time analysis of data reveals the fundamental mechanisms that result in the final product, at the molecular level and step by step. The science of synthesis lies in not only mapping the reaction pathway but also in understanding at the atomic level the underlying operational mechanisms that occur all the way along the pathway; determining, at the speed of the reaction, which atoms are doing what. That requires the development of computational approaches that identify what phases are forming when. In order to speed the development of transformational materials the challenge of tracking the evolution of phases along the reaction pathways must be met. Importantly, knowing the details of the reaction pathway allows us to steer the reaction in new directions, towards novel functional materials not yet realized.

Beyond implementation of computational approaches for the real time analysis of reaction pathways can we develop a data-driven approach to initiate desired synthesis pathways on-demand? Because theory struggles to describe the non-equilibrium diffusional processes governing real syntheses due to the incredibly complex, dynamically-evolving, defect-driven multi-dimensional parameter space associated with the synthesis mechanism of real materials, a data science approach is going to be more fruitful. Can we build a framework that moves us forward from think-cook-look-repeat strategies to machine-suggested synthesis pathways, in a manner analogous to now-mature computational structure- and properties-prediction methods?

The tremendous amounts of minable data on reaction pathways produced by in situ experiments, not only by GENESIS but by the community of scientist worldwide, can be mined using Natural Language (NL) searches. GENESIS will capture all synthesis parameters, including temperature history, process gas composition and flow rates, concentrations of all liquid species, and the composition, into structured-data databases. These data will become features for supervised learning algorithms in NL that will enable us to use an efficient, data-intensive approach and find elements for new pathways in publications and databases: the structure, defects, and morphological parameters (size, crystallinity) of solid phases thus discovered will also be captured.



GENESIS workflow illustrating that in situ probes are analyzed in real time to yield controlled, next-generation synthesis.

By this approach, GENESIS builds the tools and understanding to discover new materials more rapidly. In the end, to be useful, a material must be made, and control over synthesis pathways and products is a critical requirement for materials design, without which concepts developed in computers cannot be brought into reality. Computational approaches can now identify a library of potential materials; however, synthesis and physical realization of these new predicted materials remains a critical limit. The GENESIS approach eliminates this bottleneck by exploiting advanced real time diagnostics coupled with data science tools and, thereby, accelerate the synthesis of new materials. The acquisition of large databases of high value synthetic data will be accelerated if the input parameter space is searched in a "smart" way, rather than by brute force. Indeed, the high dimensionality of the input parameter space makes this essential. A longer-term goal of GENESIS is to develop adaptive experiment controls-- the ability of the control software to "steer" reactions in real time based on the results of just run experiments. These tools will be made available to the wider community so that different groups can carry out similar investigations using the hardware and computational infrastructure developed in GENESIS.

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