Resolving Correlated Reaction Pathways: A Multimodal Analytical Toolkit

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Understanding and controlling the function of materials systems, including catalysts, batteries, and materials synthesis reactions, requires that we unravel the interplay between structure and chemistry across multiple length scales. However, this can be challenging due to the limited scope and sensitivity of individual experimental tools. Multimodal experiments that combine insights from several complementary characterization tools have the potential to provide a solution, but they present new experimental and data analysis challenges.

This presentation describes our recent efforts to resolve the critical interplay between correlated phenomena during materials synthesis by combining simultaneous X-ray scattering (e.g., XRD, PDF, SAXS) and vibrational spectroscopies amongst other tools. To address the challenge of integrating insights from these multimodal experiments, we have employed an analytical toolkit that combines traditional, tool-specific analyses with tool- independent meta-analysis involving dimensional reduction algorithms (e.g., non-negative matrix factorization) and correlation analyses. This has allowed us to build a unified mechanistic picture that spans diverse chemistries and length scales, identifying key chemical drivers that control the reaction progress and outcome.

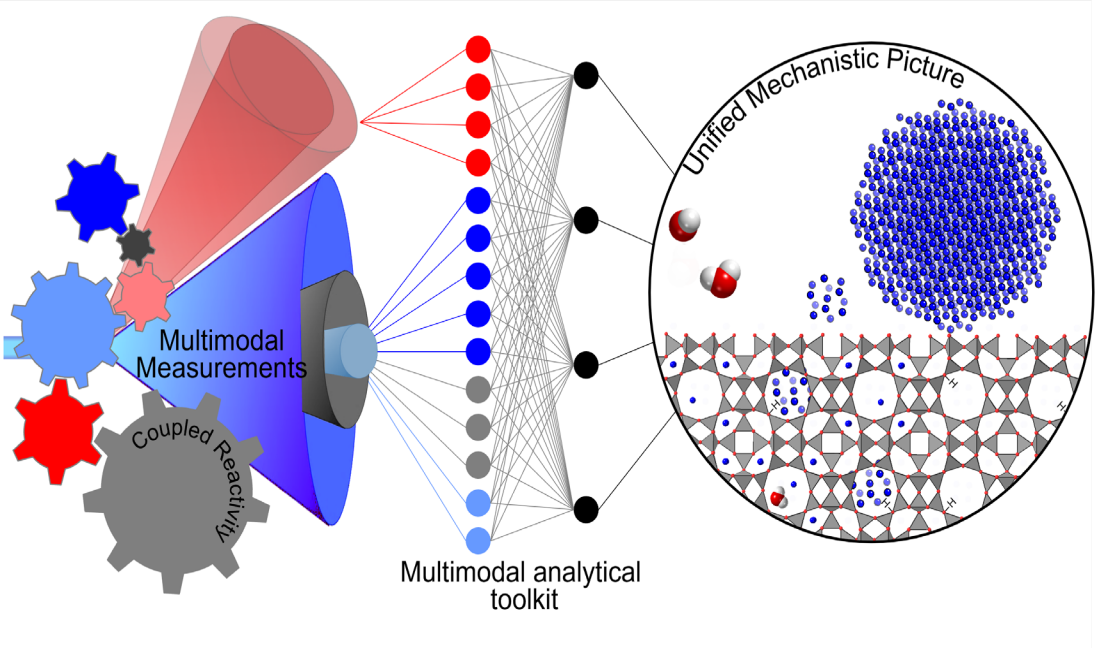

Figure 1