In situ diffraction informed by structure prediction for the discovery of novel functional materials.

J. B. Parise[1] (John.Parise@stonybrook.edu) Department of Geosciences, Stony Brook University, Stony Brook, NY, 11794-2100.

Discoveries of new inorganic and hybrid materials with enhanced properties drive advances in condensed matter science and engineering. The strategies employed in exploratory synthesis often relying on "cook-and-look" techniques and empirically derived structure-property relationships. In those cases where the synthesis is onerous – recovery of samples from high pressure conditions for example – and/or where post synthesis testing is arduous – determination of sorption isotherms, for example –*in situ* techniques, coupled to theory, greatly narrows searches for new materials and enhanced properties. The talk will review two generic areas of research positively impacted by *in situ* techniques*:* 1) The application of modern structure prediction tools and in situ synchrotron x-ray diffraction to enhance the throughput for pressure exploratory synthesis[1]. 2) The application of database search, simultaneous calorimetry-XRD and *in situ* gas loading with synchrotron-based x-ray powder scattering to identify optimal materials for gas separation[2].

The systematic search for novel semiconductors for photocatalytic overall water splitting is a representative case where quench high-pressure synthesis informed by theoretical calculations is useful, and sometimes necessary, in order to efficiently identify and synthesize target compounds. The increasing availability of community-based databases and *ab initio* theory provides new opportunities for structure search based on desired properties, such as band gap and band edge position. By employing *in situ* laboratory and synchrotron-based x-ray scattering techniques, synthesis target lists can be rapidly surveyed to speed up the discovery and optimization of novel compounds.

Many of the strategies developed can be adapted to a varied of problems in materials chemistry.

References:

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