Observing Crystallization Pathways In situ

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Understanding of crystallization pathways, which often proceed through metastable phases, offers a rich opportunity for materials engineering, as metastable phases can often exhibit superior properties to their stable counterparts. X-ray scattering and spectroscopies offer tremendous opportunism for observing these processes in situ and in real time. While this has been recognized for decades, the need for new materials for energy technologies drives more widespread adoption of this “panoramic synthesis” approach. In this talk, I will give two examples where we have using X-ray scattering and spectroscopies to follow the reaction pathways through metastable states during materials synthesis. The first concerns the hyper-popular hybrid organic metal halide perovskites solar absorbers, where we show that the formation of a metastable crystalline MA_2PbI_3Cl regulates the reaction to form $MAPbI_3$, the desired end-product (MA is NH_3CH_3+). The second involves hydrothermal synthesis of MnO_2 polymorphs where we combine density functional theory and in situ X-ray scattering to demonstrate a novel, predictive framework for materials synthesis through multistage metastable intermediates.