Mechanistic Understanding Coupled with the Discovery of Multifunctional Energy Materials

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Abstract: From the Stone Age to today’s Silicon Age, materials have had a historical impact on society and their manipulation has been the engine of societal advancement. With the ultimate goal to transition society to sustainable energy technologies and to improve our collective quality of life, there is a need for novel functional materials. This includes the discovery of new materials, understanding, controlling and manipulating their assembly and resulting functional properties on different time and lengths scales. In this talk I will introduce state-of-the-art in situ multimodal synthesis capabilities to characterize the chemical transformation of solution processed halide perovskite thin films for photovoltaic, LED, and detector applications amongst others. Establishing the relationships between synthesis condition and film properties will enable active control of synthesis parameters and increase reproducibility. The formation of halide perovskites from colloidal precursors including the initial stages of formation and the physicochemical evolution of properties via polydisperse nanocrystal nucleation and solvent-complexation will be discussed. We identified for example how the precursor and antisolvent influence the crystallization pathway, how morphology can be templated, and how additives can aid room temperature processing. By correlating diffraction and photoluminescence (PL) measurements, it will be demonstrated how in situ PL can reveal subtle changes throughout all synthesis steps. Lastly, I will describe our joint effort in setting up a robotic platform, SpinBot One, to synthesize and characterize halide perovskite thin films coupled to neural networks which learn time-dependent processes to optimize the optical properties of the material under study. SpinBot One fabricates halide perovskite thin films via spin coating and thermal annealing followed by build-in optical characterization (UV Vis, photoluminescence) and external X-ray diffraction measurements. Ultimately, coupling automated synthesis platforms with in situ characterization will enable autonomous experimentation and materials discovery with unprecedented pace.

Bio: Dr. Carolin M. Sutter-Fella is a Staff Scientist in the Molecular Foundry at the Lawrence Berkeley National Laboratory (LBNL). Before joining the Foundry she built her research program enabled by LBNL’s Glenn Seaborg Early Career Fellowship (2017). Her research focuses on synthesis of functional materials and understanding synthesis-property relationships using multimodal in situ techniques as well as development of an automated thin film synthesis and characterization platform. She received her Ph.D. in Electrical Engineering from ETH Zürich, Switzerland, in 2014 where she worked on the synthesis of chalcogenide thin film solar cells. Before joining LBNL, she was a Swiss NSF postdoctoral fellow at UC Berkeley.