The Autonomous Formulation Laboratory: Automated SAXS and SANS for Formulation Discovery and Optimization

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Industrial liquid formulations from nanoparticle coatings to drug delivery vehicles are often strikingly complex, with large numbers of components (10-100), complex multistep processing, and a wide variety of design requirements for a functional product. This complexity often precludes physics-informed mapping between component fractions, processing, structure, leaving most formulation design to empirical trial-and-error or design of experiments strategies. I will discuss recent efforts by the Autonomous Formulation Laboratory (AFL) team at NIST to use machine learning driven, highly automated characterization to rapidly and intelligently map formulation phase space using structural characterization tools such as small-angle x-ray and neutron scattering (SAXS/SANS) together with secondary measurements, e.g. optical imaging, UV-vis-NIR and capillary viscometry. Our initial studies using the AFL at the Materials Support Network at CHESS (MSN-C) beamline and the NIST Center for Neutron Research 10m SANS have resulted in an order of magnitude reduction in the time needed to map a model phase diagram, and extensive mapping studies in an industrial coating formulation, a block copolymer-additive system, and other systems of interest from our personal care, biopharmaceutical, and alternative energy industrial collaborators. Future directions in algorithms and instrumentation to study the far-from-equilibrium self-assembly and processing steps that underlie many real products will also be discussed.