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Correlated Materials Characterization *via* Multimodal Chemical Imaging and Data Analytics

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Multimodal chemical imaging simultaneously offers high resolution chemical and physical information with nanoscale, and in select cases atomic resolution. By coupling modalities that collect physical and chemical information, we can address scientific problems faced system spanning both biological and material. The combined systems enable local correlation of material properties with chemical makeup, making fundamental questions in how chemistry and structure drive functionality approachable.

Understanding the complex functionality of inorganics and ceramics, soft and polymeric materials, and especially biological systems necessitates multiple sources of information, placed in the context of sample history (preparation conditions, medical history, etc.) that are related to properties; and likely future behaviors. Furthermore, while much of the dynamic chemistry can be studied on macro-scale systems, there is a lack of means to localize chemical measurements and correlate them to nanoscale structure of the material. Therefore, we have focused our research on the unique merger of advanced scanning probe and microscopy with mass spectrometry that allow nanoscale chemical and functional material characterization. However, the complicated nature of the multidimensional data generated with these techniques requires innovative machine learning and control algorithms, to understand the interplay between chemical and physical functionality.

Here, I will discuss how we are combing imaging modalities with advanced data analytics approaches to correlate changes in chemical composition with structural and functional information on combined atomic force microscope (AFM) and mass spectrometry (MS) systems. Challenges associated with the use of data originated by the combinatorial hardware, analysis, and machine learning as well as processing tools necessary for interpretation of multidimensional data acquired from multimodal studies will also be presented. Overall, using multimodal data analytics we are able to understand and predict material behavior from the corelated imaging modalities to better grasp the physical properties of materials and the mechanistic physics-chemistry interplay behind their properties.