From single atoms to nanoscale clusters: in-situ probes to link the electronic properties and structure of nanomaterials

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Understanding the connection between the electronic properties and the structure of nanomaterials is crucial to move from an empirical approach to materials discovery to the design-driven synthesis of nanomaterials with tailored properties. Over the last four years, we have focused on developing a set of in-situ capabilities that allow us to probe at the structure and properties of nanomaterials, and in particular the way that they evolve from isolated single cation clusters towards the formation of nanoparticles, and beyond. Our approach is based on leveraging the reproducibility of atomic layer deposition (ALD) to examine the evolution of nanomaterials in-situ using a combination of in-situ synchrotron techniques such as XAFS, PDF, GISAXS, with other techniques such as photoemission, photoluminescence, FTIR, and STM. A key feature of ALD is that it relies on the self-limited, sequential adsorption of monomers to form inorganic and hybrid organic/inorganic materials in a way that it is independent of reactor geometry. Here we use these properties to prepare in-situ decorated surfaces and nanomaterials starting from isolated single atom clusters. A primary focus of our research is the study of the electronic properties of semiconductor oxide and novel metal nanomaterials, and their connection with catalysis, solar, and energy storage applications.