NANOSCIENCE COLLOQUIUM

Materials on the nanoscale: Total scattering analysis for nanoparticle chemistry

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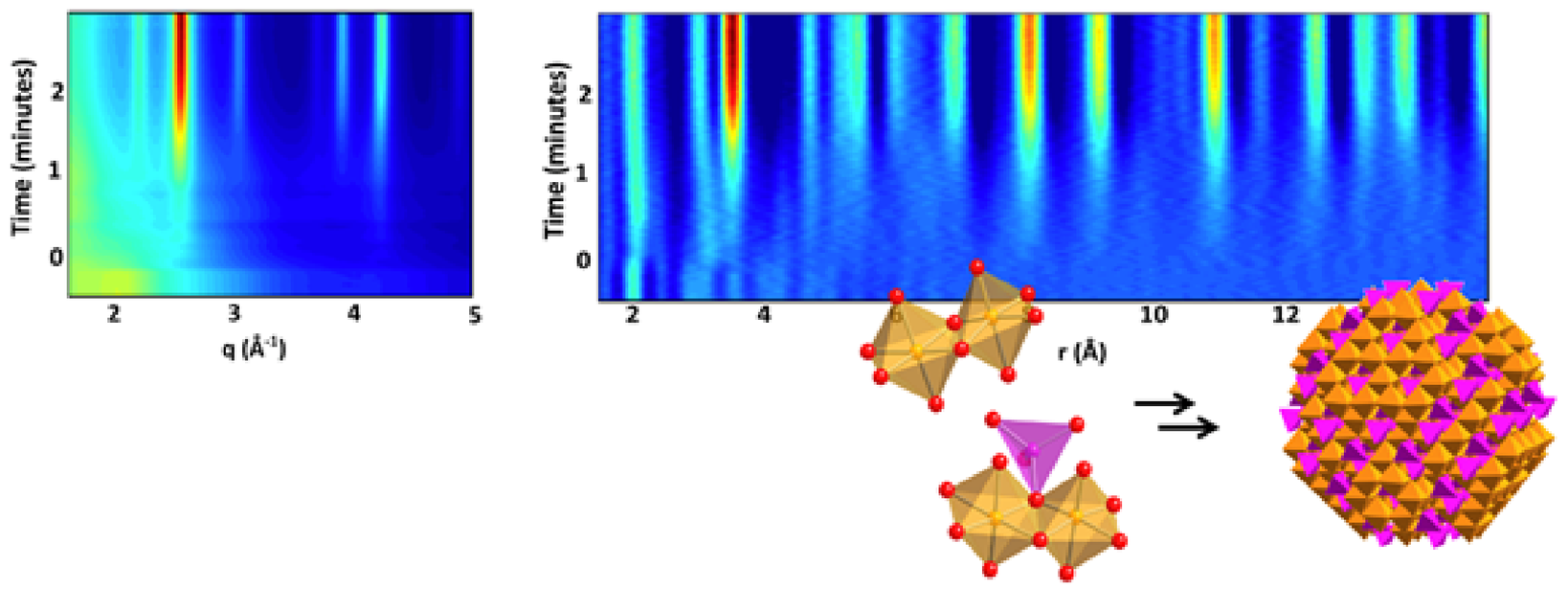
Abstract: When looking back on the developments in materials chemistry over the past decades, it is clear that the discovery and advancement of new functional materials for advanced applications in e.g. energy technologies and many other fields has paralleled the ability of scientists to characterize atomic structure in materials. The developments in materials chemistry relies on understanding the relation between atomic structure and properties, and structural characterization is thus key in materials chemistry. For many nanomaterials, the lack of long-range order challenges the use of crystallographic methods. Nanochemists have therefore had to look towards other methods for structural characterization and here, total scattering with Pair Distribution Function (PDF) analysis has come to play a large role.1 Here, I will present recent work illustrating how we use x-ray total scattering to study atomic structure in advanced nanomaterials, with special focus on metal oxide nanoparticles such as molybdenum and tungsten oxides. We observe that new structural motifs, unstable in the bulk form, become dominant in nanoscale materials,2 wich can be used for new material design.

Apart from studying the synthesized nanoparticles, I will also show how in situ x-ray total scattering allows following the formation of materials. Despite decades of research into nucleation processes, very little is known on how nanoparticle formation during solvothermal synthesis takes places on the atomic scale. We have developed methods which allows using in situ synchrotron X-ray Total Scattering and Pair Distribution Function analysis to follow nanoparticle nucleation and growth in situ.3-6 Using x-ray total scattering, we deduce the atomic structure of prenucleation clusters, present in the processes just before the crystalline nanoparticles have formed. We show that the solvent and synthesis conditions have large influence on the nucleation pathway and the structure of the nano-scale clusters in the synthetic pathway.



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