THE NANOSTRUCTURE AND NUCLEATION PROBLEMS: USING TOTAL SCATTERING TO UNDERSTAND NANOMATERIALS AND HOW THEY FORM.

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The properties of a material are intimately linked to its atomic structure. Therefore, to understand and improve material properties it is crucial to establish how the atoms of a material are arranged. Traditionally this has been done through crystallographic methods, but for a range of modern materials, notably nanomaterials, the crystallographic approach breaks down.[1] Instead the approach of total scattering with Pair Distribution Function (PDF) analysis has proven to be a powerful method to study the structures hidden from conventional crystallography[1, 2] However knowing the atomic structure is not enough to improve the properties of a material. Instead, material scientists need to know how to change the atomic structure to form a material with the desired properties. Unfortunately, even in modern science material synthesis is often a black box where precursors go in and a material comes out. This means that the development of new materials relies on large parameter studies, trial and error, as well as a good deal of luck. To move toward a more rational design of materials it is necessary to understand the chemistry of materials formation and PDF has proven to be a powerful method to determine the formation pathway of materials.[3, 4]

In this talk I will give several examples of how total scattering and PDF can give unique insights into the formation and structure of several types of nanomaterials.[2-4] Because PDF can give structural information from both crystalline and non-crystalline systems it enables us to map the chemistry of hydrothermal formation of tungsten oxide and establish the formation mechanism of sol-gel derived MAX phases. Using this strength of PDF, I will also show how PDF can determine a size dependent amorphous structure in tungsten oxide nanoparticles and local disorder in crystalline materials for example small molecules trapped inside the crystal.

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Picture of Author	Short Biography of Author
	Mikkel Juelsholt did his Ph.D. with Kirsten Jensen at the University of Copenhagen studying the formation of nanoparticles in solvothermal synthesis using *in situ* Pair Distribution Function. He also spend time with Katrine Page at Oak Ridge National Laboratory using X-ray and neutron total scattering to study the atomic structure of nanoparticles and MAX phases in collaboration with Christina Birkel. Mikkel Juelsholt is currently a PostDoc with Peter Bruce at the University of Oxford and is interested in the local structural rearrangements required for anionic redox in Li-ion batteries.