

Title: Titanium Dioxide Nanocrystals for green Hydrogen Production: Elucidation of the Crystallization path by Synchrotron Techniques.

Keywords: photocatalysis, nanoparticles, X-ray scattering, nucleation and growth

Scientific description:

The LIONS laboratory hosted at CEA Saclay is expert in Nanoscience, Physico-Chemistry and synchrotron characterizations. We are looking for a Master 2 student wants to advance the knowledge on the synthesis of nanocrystals used in green hydrogen production, via treatment of synchrotron data.

Among possible options, hydrogen production by photocatalysis is very promising given the possibility of using to sunlight, a cost-free and abundant source of energy. Today, materials with the best photocatalytic activity are nanostructured titanium dioxide (TiO₂), but their performances are still too low to allow realistic implementation. Further progress is hampered by a lack of knowledge on the synthesis of TiO₂ nanocrystals, and how to master relevant properties (crystal phase, defects, doping with metal ions, and nanostructure).

In view of these limitations, our main objective is to provide guidelines to optimize the synthesis of TiO₂-based nanoparticles, based on real-time, *in situ* measurements by X-ray scattering synchrotron data. We will assist the candidate to develop fitting routines (Python 3), model datasets, and prove / disprove different crystallization scenarios are at play in the different syntheses: S1) the amorphous precursors directly template the size and shape of the final nanocrystals, S2) alternatively, the nanocrystals form via a dissolution-precipitation of the amorphous phase, and S3) the metastable anatase phase transiently forms prior to the rutile phase and converts via a solid-solid transformation.

Application process:

A cursus in physico-chemistry or experimental physics with computational skills is required. Please send a resume to Dr David Carrière david.carriere@cea.fr at least 3 months before the expected start of the internship.

About the group:

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