Priority Programme

“Material Synthesis near Room Temperature”

Project Description – Project Proposal

Understanding solution based syntheses of inorganic materials in ionic liquids: Peering into the reaction mechanism from birth to age

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Summary of proposal

In recent years, a variety of ionic-liquid-based syntheses of crystalline inorganic materials has been developed, offering advantageous properties and protocols in comparison to conventional syntheses, which however still lack mechanistic understanding. We aim at elucidating the synthesis of unusual modifications of TiO2, namely the Bronze phase (TiO2(B)) and a recently synthesized hexagonal Ti oxyhydroxy fluoride, which are both obtained by surprisingly mild reaction conditions using mixtures of common ionic liquids with water, and TiCl4 as precursor. Our previous experiments proved the importance of ionic liquids containing fluorine in the anion and mixtures of different side-chain lengths attached to the cationic head groups.

The main task of the project is to mechanistically understand the connections between the molecular structure of the IL-containing precursor solution and the generation of titanium fluoro hydroxo complexes and further the cluster formation on the molecular level, as well as their transformation into metal oxide nuclei and growth into nanoparticles. We will approach this task by variation of experimental parameters, i.e. the constituents in the ionic liquid (using [F]- instead of [BF4]-) and employing other Ti precursors such as [NH4][TiF6]. In-situ

methods (Raman, X-ray diffraction, small-angle scattering) are applied to probe the relevant species on the molecular and nanometer scale. At the same time this birth as well as the aging process will be calculated by special techniques providing a molecular level insight and confirming or correcting assumptions from experiments. For this purpose also new interaction potentials will be parametrized next to the application of techniques which evaluate the electronic structure on the fly and thus work without a priori parametrization. Additional computer experiments will be set up addressing key data, which are hardly accessible to experiments, for instance local polarity, specific interactions, and stability of intermediate complexes/clusters.