Anatase TiO_2 colloidal nanocrystal-based architectures: models to assess the role of porosity and nanocrystal morphology in Li battery electrode

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In the context of energy storage, our present research focuses on investigating how nanocrystals (NCs) can be efficiently used as active material in electrodes for lithium ion battery. The high surface area of the nanoparticles suggests an extended contact with the electrolyte and their small dimension shortens the diffusion path of both lithium ions and electrons. Combined, these two features should lead to a significant improvement in the overall charge and discharge rates of the battery.[1] However, when introduced in conventional electrodes (i.e. randomly packed active particles with carbon and a binder) NCs tend to form aggregates. It causes a loss of the nanosize benefit and it also prevents any conclusion about the actual electrochemical behavior of the NCs themselves.

In a previous work, we proposed a unique way to create tridimensional (3D) organized porous architectures of various colloidal nanocrystals by exploiting specific interactions between the bare surface of ligand stripped-NCs and a specifically designed block-copolymer.[2] In the context of the present study, 3D ordered NCs based-architectures are key because they represent a unique tool to discriminate the NCs' contribution to the battery performances from the contribution of the NCs' packing. Using the well-controlled architecture, we can therefore compare the electrochemical behavior of a large panel of NCs of different size, shape and composition for the same open architecture.

This way, we were able to study the influence of the NCs morphology on the electrochemical behavior of the anatase TiO_2 nanoparticles (Example for TiO_2 nanorods, figure 1). Anatase TiO_2 is a well-studied lithium insertion material, so our results can be compared with rigorous theoretical analysis of the anisotropic strain induced by lithiation, the facet-dependence of lithium insertion reactions, and the crystallographic direction-dependent lithium diffusion constant.[3] On this rigorous basis, the lessons learned about the relationship between architecture and electrochemical characteristics can suggest design rules also for other insertion electrode materials.

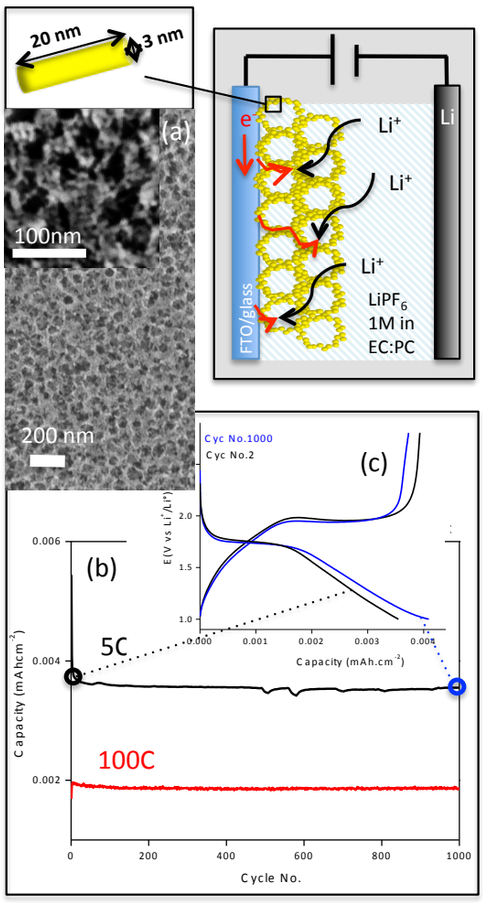

Figure 1. Nanocrystals based-architecture: unique tool to study electrochemical performances of nanocrystals. Example for anatase TiO_2 nanorods (a) SEM pictures, (b) cycling behavior at 5 and 10C and (c) charge discharge profiles at 5C for the 2d and 1000th cycles.

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