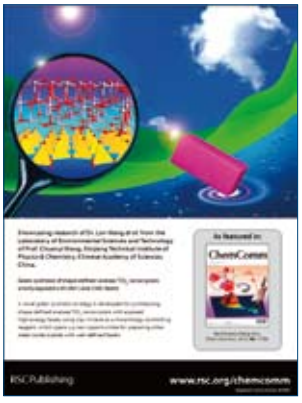
Quantitative Measurement of the Intrinsic Electric Fields in Ionic Liquids Using VSE Spectroscopy and MD Simulation

This work provides a systematic way to evaluate the ionic environment and the intrinsic electric fields in ILs and improves the understanding of the ionic nature of ILs. The findings have been published in *Chem. Eur. J.*, 2012, 18.

Owing to their unique properties, ionic liquids (ILs) nowadays are very fascinating in various fields, including organic synthesis, catalysis, inorganic chemistry, electrochemistry, and materials. The determination of the strength of the intrinsic electric fields in ILs is of fundamental importance to the understanding of the properties of ILs and their applications. Unfortunately, until now the intrinsic electric fields in ILs have remained poorly understood, and their identification and quantification are very challenging.

Researchers at R&D Center for Green Chemistry and Catalysis, CAS Lanzhou Institute of Chemical Physics, have, for the first time, successfully applied the vibrational Stark effect (VSE) spectroscopy to measure the intrinsic electric fields in ILs, and have carried out an evaluation of the results by performing molecular dynamics (MD) simulations. The results show that the electric fields of ionic liquids are only slightly higher than those of common molecular solvents, and are strongly structure-dependent. They noticeably decrease with the increasing of the size of anion and cation.

A New Green Anatase TiO_2 Nanocrystals Synthesized



This work is published in *Chem. Commun.*, 2012, 48, and highlighted on its back cover.

Titanium dioxide (TiO_2), as one of the most promising semiconductor materials, has become a topic of intensive study due to its important applications in a broad range of fields. However, the physicochemical properties of TiO_2 largely depend on the exposed crystal facets. In this scenario, many efforts have been directed to engineering the morphology of TiO_2 with specifically exposed crystal facets.

Dr. WANG Lan and colleagues, from the Laboratory of Environmental Sciences and Technology, the CAS Xinjiang Technical Institute of Physics & Chemistry, found a novel, environmentally benign synthetic strategy for shape-defined anatase TiO_2 nanocrystals wholly exposed with {001} and {100} facets.

They used titanium isopropoxide (TTIP) as the TiO_2 precursor, tetramethylammonium hydroxide (Me_4NOH) as a dual-functional reagent, and low cost acid-delaminated vermiculite (DVMT) as the hard template controlling the morphology and growth of the crystal facets. Combined optimization of such a reaction system leads to the formation of well-faceted anatase TiO_2 nanocrystals, for which the morphology and size of TiO_2 crystals can be controlled simply by adjusting the ratio of DVMT to TTIP in the hydrothermal reaction system. With increasing DVMT content, the 'hard template' effects are gradually enhanced, leading to the transformation from elongated nanorods to cube-like anatase TiO_2 particles.

These results reveal that the DVMT layers act as effective hard template selectively stabilizing the {001} facets of TiO_2. The present synthesis represents a green approach as no fluorine-containing reagents are involved, avoiding the environmental problems from F- ions. This is the first report of using a natural clay mineral for controlled synthesis of well shape-defined TiO_2 crystals with exposed high-energy facets, and the synthetic strategy is adoptable to other metal oxides.