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OA-25

STRUCTURAL CHARACTERIZATION OF $LaFeO_3$ PEROVSKITE NANOPARTICLES

Jeremias Geiss, Markus Winterer

Nanoparticle Process Technology (NPPT), University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

e-mail: jeremias.geiss@uni-due.de

Under the irradiation of sunlight, colloidal nanocrystals can split water efficiently by photocatalysis. Suitable nanoparticles for this application absorb the sunlight and allow the transport of excited charge carriers to active sites on the surface where the reactions take place. Besides an acceptable performance, colloidal reactors must compose of abundant elements to compete economically.

$LaFeO_3$ nanoparticles are among the class of promising photocatalysts for water-splitting. However, the lack of understanding of the structure-activity relationship remains the most significant obstacle in increasing the catalytic performance. Extended X-Ray Absorption Fine Structure (EXAFS) measurements can probe the local structure of the bulk and the surface of small nanoparticles.

The presentation is focused on EXAFS measurements and data analysis by Reverse Monte Carlo (RMC) analysis of $LaFeO_3$ nanoparticles which provide partial pair distribution functions that contain the structural evolution of the local structure.

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OC-26

EFFECTS OF CITRIC ION ON HEXAGONAL $NaYF_4$: Yb/Er PHASE FORMATION DURING SOLVOTHERMAL SYNTHESIS

Ivana Dinic[1], Marina Vukovic[1], Predrag Vulic[2], Marko Nikolic[3], Lidija Mancic[4], Olivera Milosevic[4]

[1]*Innovation Center of the Faculty of Chemistry, University of Belgrade, Serbia*

[2]*Faculty of Mining and Geology, University of Belgrade, Serbia*

[3]*Photonic Center, Institute of Physics Belgrade, University of Belgrade, Serbia*

e-mail: ica.dinic@gmail.com; ivanad@chem.bg.ac.rs

Up-converting nanoparticles (UCNPs) which have ability to emit a visible light upon excitation with NIR photons are with wide applications in optoelectronic devices, forensic, biomedicine and security. The synthesis of the most efficient hexagonal β-$NaYF_4$:Yb/Er phase in shape of uniformly sized spherical nanoparticles is usually

performed through thermal decomposition of complex organic precursor in high-boiling organic solvents, which rise deep concerns regarding their potential citotoxicity**.** In this work, citric acid and Na-citrate are used for the stabilization of hexagonal polymorph during solvothermal processing of $NaYF_4$:Yb/Er phase from common inorganic precursor (rare earth nitrate salts). Additionally, effect of precipitation agent, i.e. fluorine source (NaF, NH_4F and NH_4HF_2) on the final particle morphology is deduced based on comprehensive scanning and transmission electron microscopy analyses. Detailed refinement of the X-ray powder diffraction data (XRPD) revealed simultaneous nucleation of a cubic and hexagonal phase during solvothermal reaction. The use of citric acid resulted in formation of micro- and nano- spherical particles of a hexagonal and cubic $NaYF_4$:Yb/Er phase, respectively, while Na-citrate provoked nucleation of well crystallized hexagonal crystals of β-$NaYF_4$:Yb/Er phase. Size of the crystallites is determined by the choice of the precipitant, and is smallest in the case when NH_4F is used. All synthesized powders emit bright and intense green light due to the intensification of the $^2H_{11/2}$,$^4S_{3/2}$ $\rightarrow$$^4I_{15/2}$ electronic transitions upon the excitation by the infrared light (λ=978 nm).

OA-27

LIGHT SCATTERING IN TRANSPARENT CERAMICS: USE AND VALIDITY OF MIE THEORY APPROXIMATIONS

Soňa Hříbalová, Willi Pabst

Department of Glass and Ceramics, University of Chemistry and Technology, Technická 5, Prague, 166 28, Czech Republic
e-mail: sona.hribalova@vscht.cz

Introduction: The main obstacle in the preparation of transparent ceramics is the elimination of residual porosity and other phases, which cause light scattering and therefore a reduction of transmittance. Mie theory is a useful tool for modeling light scattering in heterogeneous systems (such as transparent ceramics with a small content of pores or inclusions) and for the prediction of their level of transparency. However, Mie theory requires numerical calculations, and for some purposes it is more convenient to dispose of analytical tools for modeling and prediction purposes. There are popular approximations of Mie theory that can be used in specific contexts (Rayleigh, Fraunhofer), but their validity is strongly limited with respect to the range of wavelengths, scatterer sizes and refractive indices. On the other hand, a less well known approximation published by van de Hulst [1] has a much wider range of validity and seems to be a suitable approximation for at least some of the cases where the other popular approximations fail.

Aims: The main goals of this contribution are: comparison of the results obtained by Mie theory and its approximations (Rayleigh, Fraunhofer, van de Hulst) in the ranges of wavelengths, scatterer sizes and refractive indices relevant to transparent ceramics, comparison of the results of Mie theory and its approximations for suspensions with