Nanoparticles for advanced materials: synthesis, characterization and applications

Date: November 22, 2012
Time: 14:00-15:30
Place: Room 0223(Y), Building no.2, Nagoya Institute of Technology
Program: “Nanoparticles for advanced materials:synthesis, characterization and applications”

Wolfgang Peukert
Institute of Particle Technology and cluster of excellence “Engineering of Advanced Materials” University of Erlangen, Germany

Abstract:
Advanced materials with properties tailored on the molecular and mesoscales are expected to stimulate evolutionary advances and revolutionary breakthroughs in emerging key-technology areas such as information and communication as well as catalysis, energy, and transportation. The creation of tailor-made products made from nanoscale building blocks is one of the grand challenges in nanotechnology. Nanoparticles as building blocks are controlled by surface and interparticle forces. Therefore, the microscopic control of the interfaces is a key requirement for product design and formulation of nanoparticles. This approach may create large effects, for instance in colloidal stability and aggregation, by even minor system changes. We present a multi-scale view from the molecular level towards macroscopic effects and applications. A highly relevant question is how product quality evolves along the process and how process structure-functions influence the product quality, i.e. the related structure-property functions. These are studied within the excellence cluster “Engineering of Advanced Materials – Hierarchical Structure Formation for Functional Devices” which is funded within the German excellence initiative. The vision of the cluster is to bridge the gap between fundamental research and real-world applications of modern high-performance materials in key scientific and engineering areas.

We develop process technologies for synthesis, handling and application of quantum dot (QD) systems for printable electronics including field effect transistors\(^1\) and solar cells.\(^2\) The contribution introduces a novel method for full size characterization of direct semiconducting quantum dots by UV-Vis spectroscopy.\(^3\) In case of ZnO, we follow the particle formation in detail and describe the formation kinetics by population balance equations (PBE).\(^4\) From the kinetics it becomes clear that the formation mechanism of ZnO is not dominated by the presence of a thermodynamic energy barrier but by reaction kinetics and subsequent oriented attachment of discrete clusters. Based on dimensional analysis we derive also maps for the colloidal stability.\(^5\) This enables an \textit{a priori} prediction if a suspension will be stable or not within a given time interval which is a prerequisite for any successful process design. In the next step, the UV-Vis method is transferred to other QD systems including PbS (NIR), CdTe (Vis) and ZnS (UV) and applied \textit{e.g.} for the quantitative evaluation of size selective precipitation, an efficient and scalable classification process which depends on fine-tuning of particle interactions via addition of anti-solvents to the suspension. We show that very sharp separations are achieved that narrow the size distribution to below 1 nm.
Moreover, only by the quantitative analysis of typical parameters like separation sharpness and yield a further optimization and subsequent scale-up of such post-synthetic process steps is possible. Thus, the rapid in-situ measurement of the particle size distribution can promote design and optimization of the QD formation and formulation processes, key steps in the development of advanced processes for this promising class of new materials.

In order to gain a detailed understanding of colloidal solutions it is not only necessary to obtain information on size and shape of the particles, but also on surface properties such as surface adsorbed molecules, charge density and interfacial molecular structure. Addressing these interfacial properties in-situ and in real time is of great importance for many processes relevant to particle technology. This task is, however, highly challenging since the interface cannot unambiguously separated from the bulk in most experimental techniques that do not require other experimental constraints. Nonlinear optical techniques in particular second-harmonic generation (SHG) and vibrational sum-frequency generation (SFG) spectroscopy are inherently surface sensitive and are powerful tools in interface science. As a result of recent developments in our laboratory, angle-resolved second harmonic (SH) experiments on bare particles in aqueous suspension could be performed for the first time without the use of highly nonlinear active markers and the results were corroborated by a novel nonlinear Mie model that allows for the quantitative analysis of SH scattering profiles. For charged particles the SH signal is generated predominately by water molecules that are polar ordered within the electric field of the particle’s electrical double layer. Furthermore, SHG can be applied to track particle formation and (shape) transformations in-situ.

In contrast to SHG, SFG vibrational spectroscopy accesses interfacial properties at the molecular level via vibrational fingerprints that allow for the in-situ determination of composition and conformation of surface-adsorbed molecules. We have applied these intrinsic properties of SFG to study the link between microscopic molecular structure and macroscopic properties. The formation of thin functional films, e.g. for transparent conductive coatings or for printed field effect transistors on flexible substrates will be discussed.