A365 CHIMIA 2021, 75, NO. 5 COLLOIDAL NANOCRYSTALS

Editorial



Prof. Jonathan De Roo

Colloidal nanocrystals are typically hybrid objects with an inorganic, crystalline core and a disordered organic ligand shell. Depending on the inorganic core, these materials have fascinating optical, magnetic, or catalytic properties and thus many different applications are possible. The field is inherently multidisciplinary. One can argue that chemistry is really at the core of this field since colloidal, bottom-up synthesis has been providing a wide variety of structures, shapes and compositions to the community. And the attainable complexity keeps increasing.

Switzerland has a rich history in the area of nanomaterial research and possesses several structures (e.g. the Swiss Nanoscience Institute) embedding this strategic direction in the scientific landscape. Also the new NCCR Catalysis makes use of colloidal nanocrystals to achieve their goals.

This issue highlights excellent research performed in the colloidal nanocrystal field. It reflects the broad range of chemists that are part of this community: from theoretical chemists, over organic synthetic chemists, to material scientists. In the first contribution by *Kirsten Jensen*, she lays out the challenge of characterizing nanocrystals. They are typically only a few nanometers in size and clearly do not satisfy the 'infinite periodicity' requirement for regular X-ray diffraction, as performed on single crystals or bulk powders. Her group focuses on Pair Distribution Function (PDF) analysis which is a total scattering technique, allowing the analyst to study the local nanostructure. In the second contribution by Pedro López-Dominguez and Isabel Van Driessche, the authors review the bottom-up synthetic routes to oxide perovskite nanocrystals of the type BaTiO₃. Designing chemical reactions with the correct kinetics to form double-metal oxide nanocrystals is a challenging task. In the third contribution by Florian Putz and coworkers, the authors discuss the concept of using colloidal nanocrystals as building blocks to create macroscopic materials with a specific nanostructure. Supercrystals are discussed where colloidal nanocrystals are used as superatoms. In addition, both ordered and disordered porous materials, built from nanocrystals, are reviewed. In the contribution of *Maksym* Yarema, Vanessa Wood and coworkers, the authors focus on lead sulfide Quantum Dots, and take us on a journey from nanocrystal synthesis, over thin film fabrication, to finally nanocrystal-based devices (e.g. solar cells or infrared LEDs). They show how the synthetic approach and the surface chemistry of the nanocrystals directly translates in device characteristics. E. Henrik Peters and Marcel Mayor further underscore the importance of the nanocrystal surface chemistry. Focusing on gold nanocrystals, they address the question on how to achieve monofunctionalization, i.e. attaching a single chemical functionality to the nanocrystal surface. They consider different approaches such as ligand exchange or single-ligand stabilization. Finally, the contribution of Ivan Infante and coworkers provides us with a historic overview of the computational studies on semiconducting nanocrystals. There have been exciting developments where the methods and computational power have been improved up to the point that realistic nanocrystal models can now be calculated, even with Density Functional Theory (DFT). The authors review computational efforts regarding the surface chemistry of the classical II-VI and IV-VI semiconductors, and also of the III-V materials, and the perovskite metal halides which received recently a lot of attention.

This issue thus brings together many different facets from colloidal nanocrystals: experimental synthesis and characterization, surface chemistry, theoretical calculations, and materials and device fabrication. We hope it will provide inspiration to the reader.

Prof. Jonathan De Roo University of Basel