diffusion-fundamentals
The Open-Access Journal for the Basic Principles of Diffusion Theory, Experiment and Application

Characterizing Colloidal Nanocrystals with NMR looking at the Capping Ligand

Bernd Fritzinger[1], *Iwan Moreels*[2], *Petra Lommens*[2], *Zeger Hens*[2] *and José C. Martins*[1]

[1] NMR and Structure Analysis Unit, Department of Organic Chemistry and
[2] Physical Chemistry of Nanomaterials, Department of Inorganic and Physical Chemistry,
Universiteit Gent, Krijgslaan 281 S4, B-9000 Gent, Belgium,
E-Mail: Bernd.Fritzinger@UGent.be

1. Introduction

In this project the potential of solution NMR techniques to characterize colloidal nanocrystal systems from the capping ligands point of view (i.e. InP, PbSe and ZnO quantum dots) was investigated [1]. The techniques used were mainly diffusion pulsed field gradient spectroscopy and NOESY/ROESY spectroscopy. Depending on the system, the signal of the capping ligand was determined in free and bound state or in exchange between both states. The exchange regime could be determined relative to the frequency and diffusion timescale.

2. Different exchange regimes

For slowly exchanging systems (InP quantum dots with trioctylphosphine oxide (TOPO) ligands), the density of the ligands on the nanocrystal surface could be quantified. The existence of an equilibrium between bound and free ligands can be established by using ^{1}H NMR. The corresponding adsorption isotherm leads to an estimation of the free energy of adsorption and the free energy of ligand-ligand interaction at the nanocrystals surface. Thus solution NMR allows an independent avenue to important physical-chemical properties of such colloidal dispersions [2, 3].
In case of a fast exchange (ZnO with Octylamine ligands) some assumptions are necessary for the interpretation.
For non-exchanging systems (PbSe quantum dots with Oleic acid ligand) an estimate of the structure of the ligand shell can be postulated using a NOESY study in combination with diffusion NMR.

References

[1] G. Schmid, Nanoparticles – From Theory to Application, Wiley VCH, 2004.
[2] Z. Hens, I. Moreels, J.C. Martins, ChemPhysChem 6 (2005), 2578-2584.
[3] I. Moreels, J.C. Martins, Z. Hens, ChemPhysChem 7 (2006), 1028-1031.