

Ligands on Nanocrystals: From Molecular Picture to Macroscopic Solubility

Zhenfeng Pang, Jun Zhang, Weicheng Cao, Haibing Zhang, Linjun Wang, Xiaogang Peng, Xueqian Kong,

Department of Chemistry, Zhejiang University, Hangzhou, China.

Correspondence: kxq@zju.edu.cn

For nanocrystals of semiconductor (often called quantum dots), the surface ligands play an important role in controlling their morphology, stability and many physicochemical properties. (Figure 1a)

In order to probe the coordination structure and geometric arrangement of surface ligands, we performed a full set of solid-state NMR (SSNMR) investigations. First, we combined ^{13}C NMR with Ab Initio calculation to quantitatively identify different coordination structures. Secondly, we uncovered the partitioning of mixed ligands using CODEX experiments taking advantage of ^{13}C homonuclear coupling (Figure 1b). Based on the static picture, we used ^2H NMR and ^1H - ^{13}C DIPSHIFT experiments (Figure 1c) to depict the dynamic picture of individual chain segments (Figure 1d). From the SSNMR investigation, the fundamental connection between microscopic molecular interaction and macroscopic thermodynamic parameters has been revealed.

Our work demonstrated the enormous potential of SSNMR on the understanding of surface chemistry of colloidal nanocrystals.

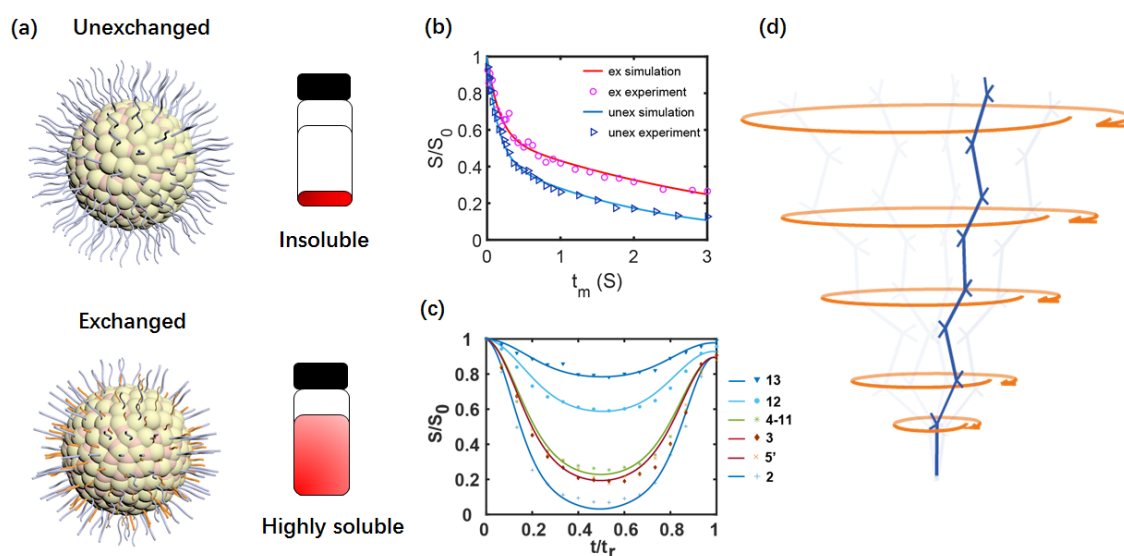


Figure 1. (a) The schematics of quantum dots with unexchanged and exchanged ligands, and their respective solubility. (b) the ^{13}C CODEX results. (c) the ^1H - ^{13}C DIPSHIFT results. (d) The illustration of ligand motion.