Functionalization of Silicon Quantum Dots with Ferrocene Derivatives

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Silicon nanocrystals (SiNCs) are non-toxic quantum dots with size- and ligand-dependent optical and electronic properties.[1] The preparation of hydride-terminated SiNCs developed by the Veinot Group is based on the thermal processing of hydrogen silsesquioxane under a reducing environment.[1] Functionalization of the SiNCs with a variety of ligands imparts both stability and optical tunability. For example, UV excitation (*ca*. 340 nm) of alkyl-terminated 3 nm SiNCs results in photoluminescence centered near 700 nm. Ferrocene, an organometallic compound, is well-known for both its stability and redox activity. The purpose of this study was to investigate the potential combination of the optical properties of SiNCs with the redox properties of ferrocene. This was done via the co-functionalization of SiNCs with a 10:1 ratio of 1-dodecene and an alkene-terminated ferrocene (Figure 1):

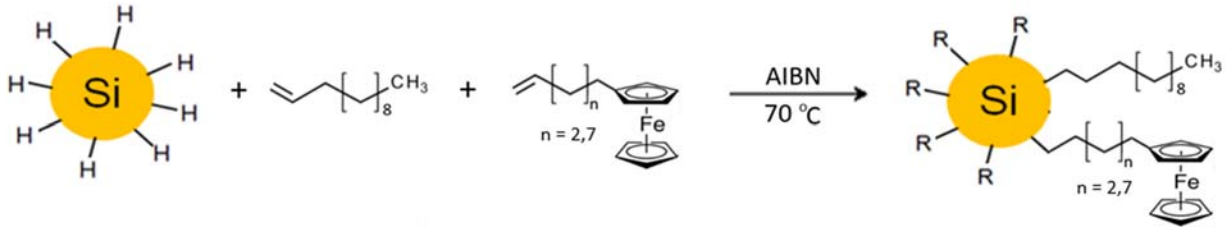

Figure 1. Co-functionalization of 3 nm SiNCs with 1-dodecene/alkene-terminated ferrocene.

Initial work focused on the syntheses of alkene-terminated ferrocene derivatives and their subsequent characterization using a variety of spectroscopic techniques (e.g. IR, NMR, UV-Visible). Hydride-terminated 3 nm diameter SiNCs were then co-functionalized with a mixture of 1-dodecene and the corresponding alkene-terminated ferrocene derivative. Characterization included TEM and IR studies but subsequent investigations were more heavily focused on the PL properties of the SiNCs which were significantly affected by the presence of the ferrocene molecule.[2] The presence of ferrocene at the surface effectively quenches the UV excitation PL pathway, however, excitation into the visible absorption band of the surface ferrocene (*ca*. 510 nm) results in the return of photoluminescence at *ca*. 740 nm. This effect of surface ferrocene on the PL properties of the SiNCs is under current investigation.

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2. Dorokhin, D.; Tomczak, N.; Velders A. H.; Reinhoudt, N. G.; Vancso, J. G. Photoluminescence Quenching of CdSe/ZnS Quantum Dots by Molecular Ferrocene and Ferrocenyl Thiol Ligands. *J. Phys. Chem. C* 2009, *113,* 18676–18680.