Thiol Ligand Conformation and Dynamics on Gold Nanoparticles Investigated with NMR Spectra and Relaxation Analysis

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Several methods can identify the chemical species on nanomaterials' surfaces, yet less is known about the heterogeneity and dynamics of these surface ligands. In 2019, Murphy et. al. functionalized a series of gold nanospheres (AuNS) with one ligand (MTAB) featuring a thiol group, a 16-carbon alkyl chain, and a bulky trimethyl ammonium headgroup in a D2O environment; using NMR tools such as T2 (spin-spin relaxation) measurements, they determined that ligand motion sharply decreased as NP diameter increased due to the reduction in radius in curvature. This talk will feature a continuation of that work in which ligands analogous to MTAB but featuring shorter or longer alkyl chains are appended onto AuNSs and investigated with NMR spectroscopy to connect the effects of ligand length/van der Waals interactions on ligand conformation and dynamicity on AuNS. This work will create a fuller picture of ligand behavior on AuNS, which will inform many of their potential applications.