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Stabilizing and Functionalizing Inorganic Nanocrystals via Metal-Ligand Coordination Interactions

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Colloidal nanocrystals made of transition metal cores, prepared via bottom-up solution growth routes, offer great promises for use in wide range of applications and as functional platforms for integration in biomedicine. Implementation of these concepts require optimal surface coating. We have developed a set of high affinity metal-coordinating polymers that are optimally-adapted for surface functionalizing a variety of inorganic nanocrystals. The ligand design exploits the effectiveness of the one-step nucleophilic addition reaction to simultaneously introduce several "custom-adapted" anchoring groups, along with solubilizing blocks and reactive functionalities into a single macromolecule. We have more recently used this strategy to test the ability of N-heterocyclic carbene (NHC)-modified ligands to coordinate and stabilize luminescent CdSe-ZnS core-shell quantum dots (QDs) and AuNPs alike. In particular, we probed the effects of ligand structure and coordination on the coating affinity to the nanocrystals. We find that such NHC-based ligands rapidly coordinate onto the nanocrystals (requiring ~ 10 min of reaction time), which reflects the soft Lewis base nature of the NHC groups, with its two electrons sharing capacity. Removal of the hydrophobic cap and promotion of carbene-driven coordination on the nanocrystals have been verified by ¹H NMR spectroscopy, while ¹³C NMR was used to identify the formation of carbene-metal complexes. We will discuss the ligand design, characterization and use of these colloids in a few specific applications.