Noncovalent Control of the Electrostatic Potential of Quantum Dots through the Formation of Interfacial Ion Pairs

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For nanoparticle solutions, electrostatics plays a vital role in determining (1) the particles’ solubility, (2) their tendency to self-assemble into superlattices and functional materials, (3) their permeability and binding affinity to charged small molecules or macromolecules, and (4) the particles’ interaction with biomembranes. We report an approach for controlling the electrostatic interaction between the quantum dots (QD) by exploiting the van der Waals and excluded volume interactions between the screening counterions and the ligand shell of the QD. This is important because non-covalent chemistry imparts great tunability to the properties of QDs in aqueous dispersions without the need for additional covalent functionalization of their surfaces.

Figure: (left) PbS QDs coated by negatively charged ligands are neutralized by positively charged counterions NR₄. (right) Computer simulations show that the electrostatic potential at the slipping plane decreases as the chain length of the R groups increases, which is in excellent agreement with experimental measurements and theoretical predictions.