

Ligand engineering of colloidal nanocrystals

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Quantum dots are small crystals, around a million times smaller than a human hair. At this scale, quantum effects occur which can drastically alter the properties of materials. They are synthesized in a liquid, surrounded by a shell of ligand molecules.

In the case of quantum dots, it is the luminescent behavior which is significantly changed. While normally, after absorption of UV light, a semiconductor can only emit light of a specific color (think red LEDs), in quantum dots this color becomes size-dependent.

This makes controlling the size an interesting goal which can be achieved using the ligand shell. Some ligand molecules will bind much stronger to the dots than others, affecting their growth. By quantifying these interactions with quantum mechanical simulations the synthesis can be fine-tuned, selecting specific sizes and obtaining the optimal emission of light.