

Number of project: UK/3038/2025,

Name of the project: Electronic tuning and surface passivation of CdSe nanocrystals by ZnO shelling

Abstract:

Colloidal heterostructures composed of a metal chalcogenide core and a metal oxide shell combine the size-tunable absorption and emission of materials such as CdSe with the low toxicity and catalytic activity of oxides such as ZnO, and are attractive for optoelectronics, bio-imaging, and photocatalysis. Among the least explored members of this family are the CdSe/ZnO quantum dots, for which only one preparation has been reported, leaving open the way in which the core-shell interface and the size of the core govern the electronic behavior of the resulting particles. This is important because CdSe and ZnO have similar conduction band offsets, so the same pair of materials is expected to switch between two fundamentally different regimes, one where both charge carriers are confined in the core, and the other where the electron and the hole are separated between the core and shell, by changing the core size, shell thickness and the nature of the interface between them.

The project's goal is to systematically develop structure-property relationships. The design combined synthesis of CdSe cores over a wide size range by hot injection with controlled thermal decomposition of a zinc precursor to grow ZnO shells of increasing thickness, deliberately varying injection temperature, injection rate, annealing conditions, and core surface stoichiometry to tune the interface itself, rather than treating it as a fixed property. Characterization was designed around the question, not around any single technique: high-resolution electron microscopy with elemental mapping to verify shell formation and crystal structure, Raman spectroscopy to probe interfacial strain and sharpness, and absorption, emission and excited-state lifetime measurements to follow the optical consequences. These data were to be interpreted in terms of an effective mass model of the electronic structure, developed in collaboration with Los Alamos National Laboratory, allowing the two confinement regimes to be identified across the series.