

**Title:** Colloidal semiconductor nanocrystals for solar cell devices

**Proposer:** Stefano Ossicini

**Tutors:** Stefano Ossicini

**Type:** Theoretical

**Abstract:**

Colloidal semiconductor nanocrystals (CS-NC) are highly appropriate for device fabrication, owing to their narrow-bandwidth, their remarkably broad absorption spectrum (extending in some case till the mid-infrared) and their high stability under ambient conditions. In narrow band-gap semiconductors like PbS, PbSe, CdS, CdSe etc. the band-gap can be enlarged of 1-1.5 eV continuously from the bulk value exploiting the effect of quantum confinement in small nanocrystals. The surface of CS-NC is usually passivated with a shell of organic molecules coordinate to the surface allowing an easy dissolution of the material in common solvents. Besides the elevated interest for these systems several fundamental physical properties are unknown. We intend, with the use of ab-initio methods (DFT and MBPT like TDDFT and/or GW+BSE) to calculate the electronic and optical properties of different CS-NC as a function of size and of different surface ligands. Actually, a precise knowledge of these properties is highly relevant for the exploitation of these systems in devices application.

**Collaborations:** Collaboration with R. Del Sole (Univ. Tor Vergata, Rome) and ETSF (European Theoretical Spectroscopy Facility).

**Coworkers:** (at UniMORE) Dr. Elena Degoli, Dr. Nicola Spallanzani

**Extra-bourse ( about 15keuro/year) available:** no