PREFACE

The potential features of core-shell QDs, that are not accessible with their mono-component counterparts, make them highly demandable in various fields such as photovoltaics, light emitting diodes, optical switches, spintronic devices, low-threshold lasers, bio-labeling agents, etc. Depending on the band alignment of the core and shell materials, three types of core-shell systems are identified, viz. type-I, type-$I^{1/2}$ and type-II, possessing different functional features.

In a type-II system, which is the focus of our study, the valence and conduction band edges of one of the components (core/shell) lie lower in energy than the corresponding band edges of the other component, i.e., there exists a staggered band alignment at the materials interface. A gifted advantage of these systems is that the band gap offset in them spatially separates photo-generated carriers within the structure such that the electron-wave function resides largely in one material and the hole-wave function in the other, which is of particular interest in photovoltaics. The energy offset can then be tuned by a judicious control of the composition, size and shape of each component which offers the possibility of directly controlling the electron-hole wave function overlap, tailoring the optoelectronic properties of the devices based on them. The staggered band alignment helps in improving the power conversion efficiency of photovoltaic cells by preventing the back electron transfer. This also causes a reduction in the oscillator strength of wave functions leading to longer lifetimes of the excited state. The exciplex state of type-II QDs can raise the light absorption rate too.

Two novel type-II core-shell QDs: CdSe-Cu_2Se and $CuInS_2$-In_2Se_3 QDs were synthesized in our work. Another type-II system, ZnTe-ZnSe, prepared using some modifications of a reported procedure, was also included in our study. To be in line with "green energy" initiatives, we adopted a "green" phosphine free organometallic colloidal hot injection method for the new materials synthesis. The colloidal procedures have the potential to control the size and shape of QDs effectively along with their cost effectiveness. Oleylamine/oleic acid was used as the capping agent to stabilize the QDs, which are also cost effective and phosphine free. We have explored photoinduced charge transfer between CdSe-Cu_2Se and ZnTe-ZnSe QDs and a molecular adsorbate methyl viologen (MV^{2+}) from a photovoltaic point of view. The possibility of electron/hole transfer under photo-excitation is an essential requirement of core-shell systems for employing them in photovoltaic applications. A detailed understanding of the charge transfer processes is also important in designing devices based on them. We have also fabricated Quantum Dot Sensitized Solar Cells (QDSSCs) based on CdSe-Cu_2Se QDs.

The structural and optical properties of the core-shell QDs were investigated using UV-Vis-NIR absorption spectroscopy, photoluminescence spectroscopy (PL), X-ray diffraction (XRD), high resolution transmission electron microscopy (HRTEM), selected area electron diffraction (SAED), energy dispersive X-ray spectroscopy (EDS), inductive coupled plasma atomic emission spectroscopy (ICP-AES), cyclic voltammometry (CV) and X-ray photoelectron spectroscopy (XPS). The charge transfer studies were performed by monitoring the luminescence of the QDs in presence of the molecular adsorbate and investigated by steady state and time-correlated single photon counting (TCSPC) studies. The solar cells were characherized using absorption spectroscopy, HRTEM, EDS, field emission scanning electron microscopy (FE- SEM) and solar simulator.