Abstract

The energy crisis in the world today has led to in-depth research in the field of renewable energy, and the most promising technology within it is that of solar energy based photovoltaics (PV). Solar energy provides a powerful and limitless source of energy that is freely available to all, irrespective of their geographic location allowing for endless innovation in terms of emerging technologies to harness its capability. However, the device that is the solar cell, which converts the energy of the incoming photons into electrical power is the limiting factor in the successful and optimal utilization of solar power. The current devices available commercially are expensive as well as not very efficient therefore leading to a large loss of incident photons. Therefore, research groups world-wide are working on new materials and technologies that will allow the fabrication of high efficiency, low-cost and easy to manufacture solar cells. Nanostructured materials with their size and surface dependent optical and electronic properties are a novel methodology for improving the solar cell performance. It is important to understand the junction properties of single nanorod devices prior to applying these for practical solar cell devices. With these objectives, the current work examines single nanorod based heterojunctions and nanostructured thin films of different materials to study in detail their methods of synthesis, material properties and optical and electronic characterization. The first part of this study is based on single cadmium sulphide (CdS) nanorod based heterojunctions. Initially, the synthesis of pure CdS nanorods has been optimized with a control over their diameter and then current-voltage measurements carried out on them after vacuum and oxygen annealing. Photoconducting response measurements in CdS nanorods were found to show that the photoresponse depends on several parameters which are: (i) structural defects inherent in the semiconductor crystal, (ii) passivation of these defects by oxygen treatment, (iii) adsorption of oxygen to the nanorod’s surface leading to the removal of free electrons from the nanorod’s core and (iv) the magnitude of the Debye length of CdS in comparison to the nanorod’s diameter. Using these CdS nanorods as the base, a novel architecture for a length-wise single nanorod based junction has been demonstrated in two material pairs of CdS-CuxS and CdS-CZTS. Conducting AFM measurements of an individual CdS-CuxS nanorod shows a photovoltaic...
response with an open circuit voltage of ~320 mV and a short-circuit current density of ~5.5 mA/cm² under illumination. Kelvin probe force microscopy (KPFM) shows the emergence of interfacial regions in the light and it has been proven that the surface potential of these new interfacial regions also lies between those of the two materials which are topologically on either side of the interface. KPFM has also been used to measure a fall in surface potential on the surface of the samples under illumination due to the photo-generation of carriers and incomplete separation of charge at the junction leading to an overall accumulation of holes. At the same time the relative difference in surface potential values that develops under illumination is assigned to the development of photovoltage between them and a shifting of their Fermi levels.

In the second part of the study, CZTS thin films were fabricated with different wet-chemical techniques and the synthesis of stoichiometric CZTS was optimized. Elemental variation was carried out to demonstrate the ability to tune the entire band structure (band gap, work function, distance of Fermi level from valence band) of the material by simply changing precursor ratios. CZTS nanocrystalline inks were synthesized (stoichiometric and doped) and formed into films which were given various surface treatments and finally devices were fabricated and tested, allowing the emergence of an optimal ink and surface treatment combination which showed the overall best performance.