Theoretical study of cyanidin dye using DFT and TDDFT methods showed that the ground and excited state oxidation potential energies as well as electron injection of the dye show that this dye has potential to be a good photosensitizer in DSSC. The nanocrysalline ZnO was prepared by the hydrothermal method with a different capping agent. X-ray diffraction results show that the all of the synthesized ZnO nanomaterials are of hexagonal structure with the size of 32.1 nm. We found that the solar cell device exhibited a short circuit current (I SC\_ 3.5 μA cm−2), open circuit potential(V OC\_ 0.045 V), fill factor (FF \_ 0.35), and overall light to electricity conversion efficiency (η \_ 0.006%) under white light (100 mWcm−2) illumination. The results showed that the conversion efficiency was increased with the increase dye adsorption time, and the highest efficiency (η \_ 1.5%) had been obtained at a time of 8 h.