

After literature review, numerous areas were identified in Quantum Dot sensitized Solar Cells for improvement. These problems are related to the efficient sensitization of quantum dots in mesoporous electrode, transition metal doping of quantum dots to tune their optoelectronic properties for better photovoltaic response, identification of alternate photoelectrode material for quantum dot sensitized solar cells and possible theoretical window of improvement with detailed balance consideration of actual devices. Figure 3.1 represent schematically these issues/problems. Methodologies to tackle these problems will be discussed in the following sections.

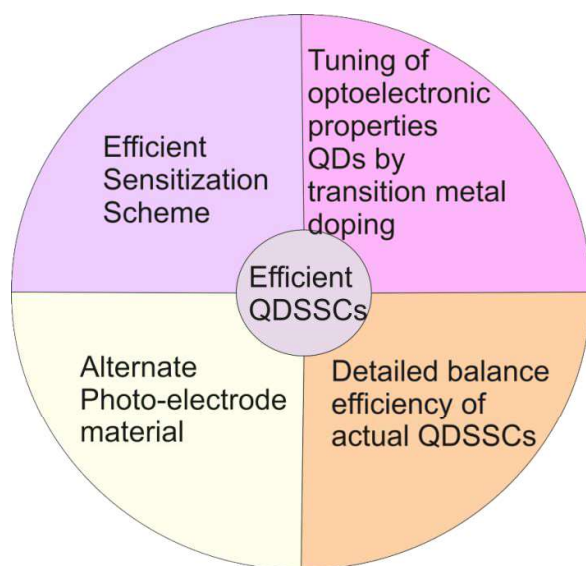


Figure 3.1: Schematic diagram for problems identified for improvement in quantum dot sensitized solar cells after literature review.

### 3.1 Sensitization of Mesoporous Electrode

Effective sensitization of mesoporous electrode has been the focus of research in quantum dot sensitized solar cells as discussed in section 2.1.3. Ideal sensitization scheme should be able to provide monolayer covering of quantum dots on mesoporous electrode with sufficient surface area to absorb all the incident solar radiation above bandgap of excitonic absorber along with suitable optoelectronic properties of quantum dot absorber. Water based CdTe quantum dots were synthesized and direct adsorption was tried initially. However, it was not leading to the successful sensitization. Further, electrophoretic deposition was also not a suitable choice for sensitization due to limited potential range for these water solvent based CdTe QDs. Considering these constraints, in-situ hydrothermal sensitization scheme was utilized for mesoporous electrode sensitization using CdTe quantum dots. In-situ hydrothermal

sensitized electrodes showed efficient penetration of quantum dots inside the mesoporous electrode matrix. In-situ sensitized photoelectrodes were characterized in details for structural properties using X-ray diffraction. Optical characterization was done using diffuse reflectance accessory along with UV-Vis spectrometer. Surface morphology of sensitized mesoporous electrode was studied using scanning electron microscopy and atomic force microscopy. Internal structure was also studied using transmission electron microscopy. Sensitized electrodes were utilized to prepare quantum dot sensitized solar cells and photovoltaic characterization was carried out using Autolab potentiostat under 1 Sun illumination. QDSSCs were also characterized using impedance spectroscopy under dark and measured spectra were fitted with equivalent circuit model for correlation with photovoltaic efficiency with extracted impedance parameters. A schematic diagram is shown in Figure 3.2 explaining in-situ hydrothermal sensitization of mesoporous electrode and their photovoltaic performance characterization.

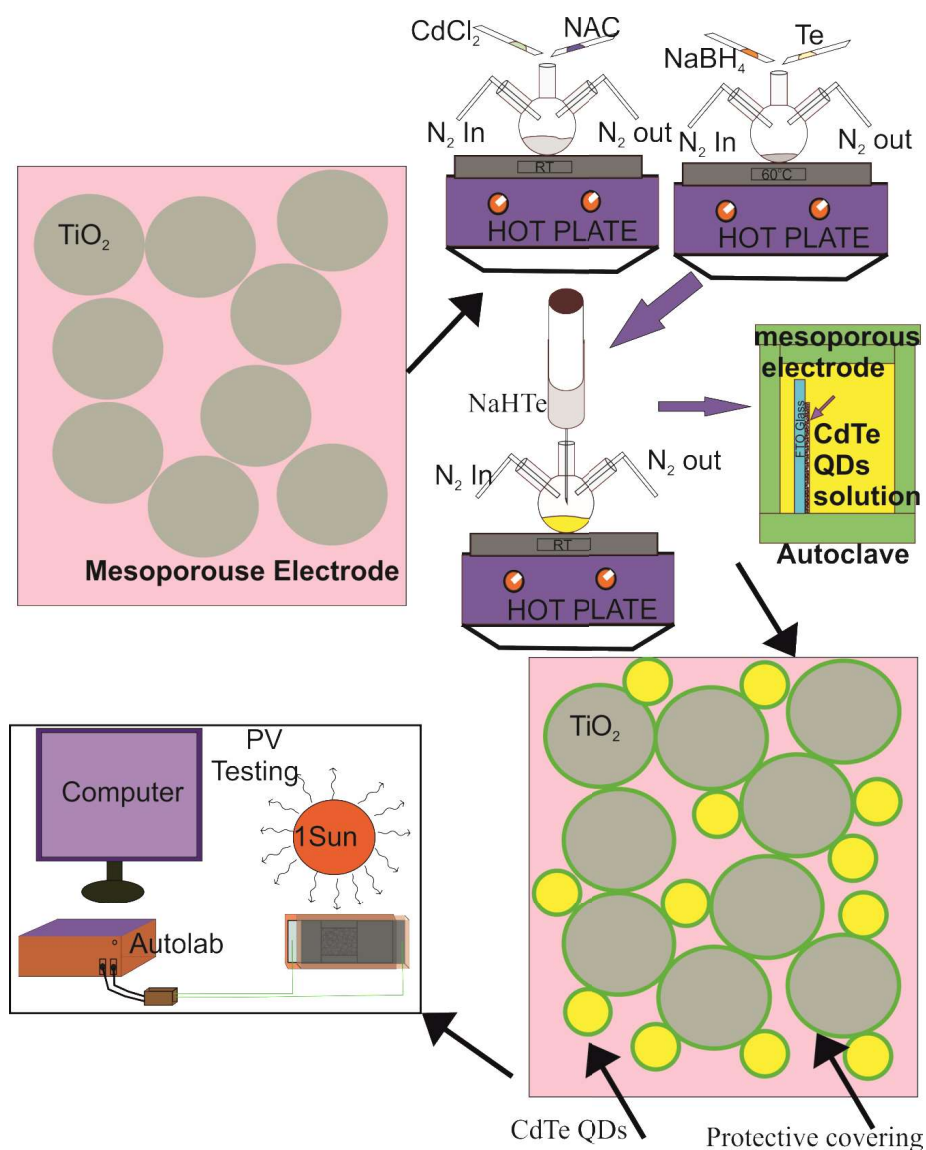


Figure 3.2: Schematic diagram for in-situ hydrothermal sensitization of mesoporous electrode along with their photovoltaic characterization.

### 3.2 Transition Metal Doping in Cadmium Sulfide Quantum Dots in QDSSCs

Transition metal doping has been an effective strategy to improve photovoltaic performance of QDs absorber considering enhanced absorption by quantum dots after doping and efficient carrier transport at interfaces. Cadmium sulfide quantum dots were investigated to address rationale behind selection of suitable transition metal for doping in quantum dots. Successive Ionic Layer Adsorption and Reaction (SILAR) process was utilized for CdS sensitization of mesoporous electrodes and transition metal doping was carried out by dissolving the desired transition metal precursor in cadmium precursor. The transition metals were chosen in such a way that their Fermi energy should fall either close to conduction band minima of electron transport material or close to electrochemical potential of redox electrolyte or in between electron transport material conduction band minima and redox level of hole transport material. Figure 3.3 shows schematic representation of transition metal doping using SILAR and photovoltaic characterization after solar cell preparation.

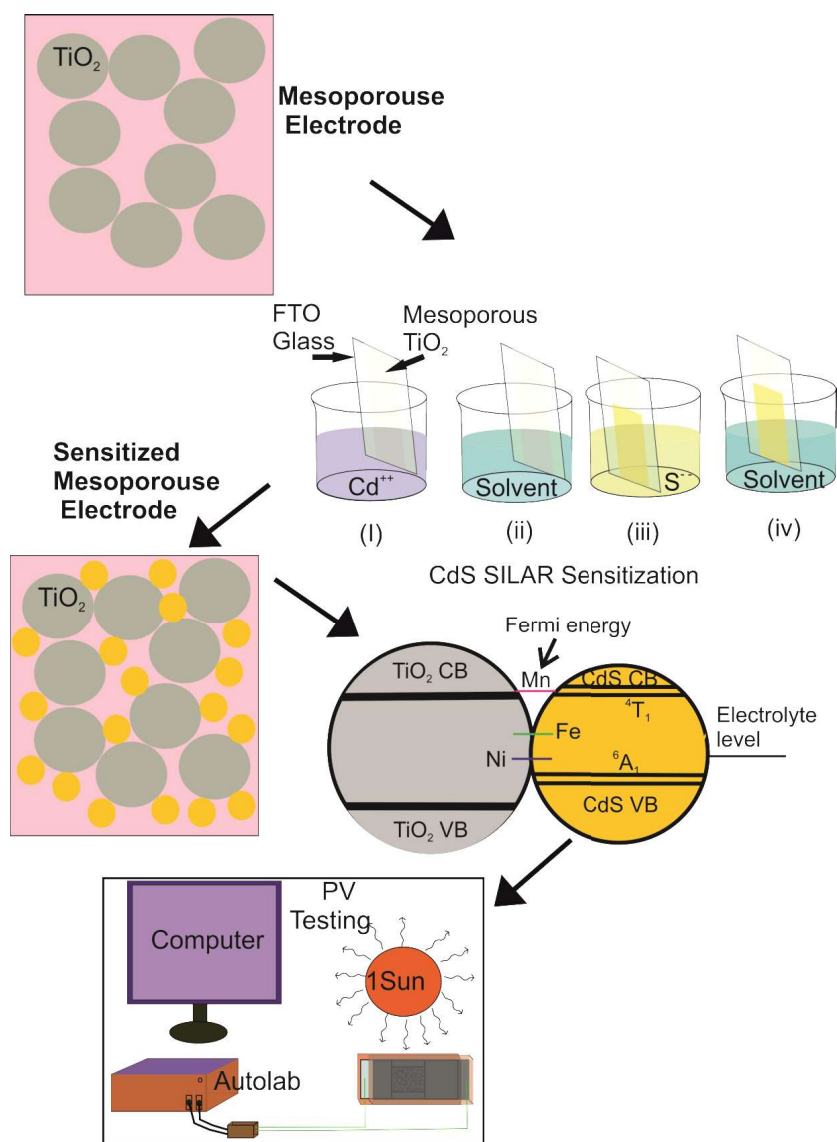


Figure 3.3 Schematic diagram showing transition metal doping in CdS sensitized quantum dot solar cells and their photovoltaic performance evaluation.

Sensitized mesoporous electrode was characterized for structural properties using X-ray diffraction. Optical properties of sensitized mesoporous electrode were investigated using diffuse reflectance accessory for absorption of sensitized electrode using UV-Vis spectrometer. Surface morphology of sensitized mesoporous electrode was studied using scanning electron microscopy and atomic force microscopy. The optimized sensitized mesoporous electrodes were utilized to prepare quantum dot sensitized solar cells and detailed photovoltaic characterization was carried out using Autolab potentiostat under 1 Sun illumination. Prepared QDSSCs were also characterized using impedance spectroscopy by making use of FRA 32 module of Autolab PGSTAT302N.

### 3.3 Photoelectrode Material for Efficient QDSSCs

Numerous photoelectrode materials have been explored in past for quantum dot sensitized solar cells as discussed in section 2.1.2. Figure 3.4 shows process flow chart for material's synthesis and device preparation along with intensive device characterization. Zinc titanate nano particles were synthesized using sol-gel for photoelectrode material application in QDSSCs. Prepared zinc titanate nano-powder was characterized extensively using X-ray diffraction for structural properties and phase evolution was studied against different calcination temperatures. Optical characterization techniques like UV-Vis spectroscopy and FTIR spectroscopy were utilized for evaluation of optical transitions and vibration spectra. Prepared zinc titanate nano-powder was utilized for preparation of mesoporous electrode using Dr. blade method.

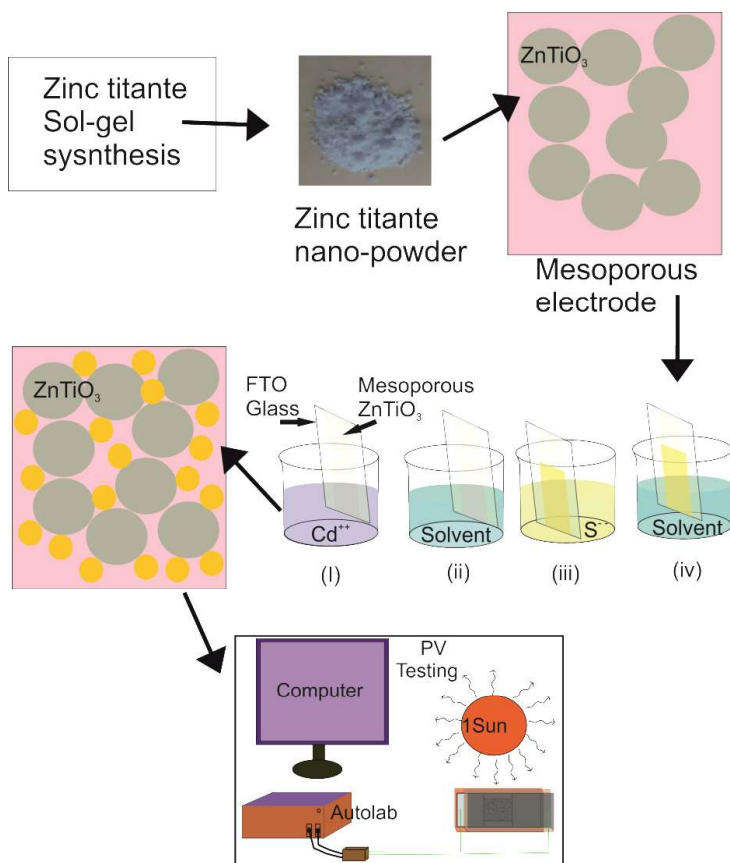


Figure 3.4 Process flow for zinc titanate photoelectrode material preparation, photoelectrode preparation, sensitization and PV performance evaluation.

These prepared mesoporous electrodes were sensitized using CdS quantum dots with successive ionic layer adsorption and reaction (SILAR) technique. Sensitized photovoltaic electrodes were characterized extensively using structural and optical characterization techniques. Prepared sensitized photoelectrodes were utilized to prepare QDSSCs which were further characterized for their photovoltaic performance using Autolab potentiostat under 1 Sun illumination. Prepared QDSSCs were also characterized using impedance spectroscopy by making use of FRA 32 module of Autolab PGSTAT302N.

### 3.4 Detailed Balance Efficiency Calculation for QDSSCs

Klimov performed detailed balance calculation for quantum dot solar cell using ideal electrode conditions and provided theoretical detailed balance photovoltaic efficiencies against absorber's bandgap. However, lab scale efficiencies still lag far more behind for quantum dot solar cell as compared to the theoretical efficiencies predicted by Klimov. Klimov considered ideal electron and hole transport materials, which are perfectly matched with excitonic absorber i.e. QDs electronic energy states in calculation. However, in practical conditions conduction band minima of electron transport material and red-ox level of widely used polysulfide electrolyte plays deciding role in estimation of open circuit potential of solar cells. In this study, this condition is named as limited open circuit voltage condition. The detailed balance efficiency calculations were performed for quantum dot sensitized solar cell considering  $\text{TiO}_2$  as electron transport material and polysulfide electrolyte as hole transport material. Ultimate efficiency for quantum dots sensitized solar cells was also estimated for limited open circuit voltage condition. MATLAB code was written for computing theoretical efficiencies using detailed balance calculations and is provided in annexure A.

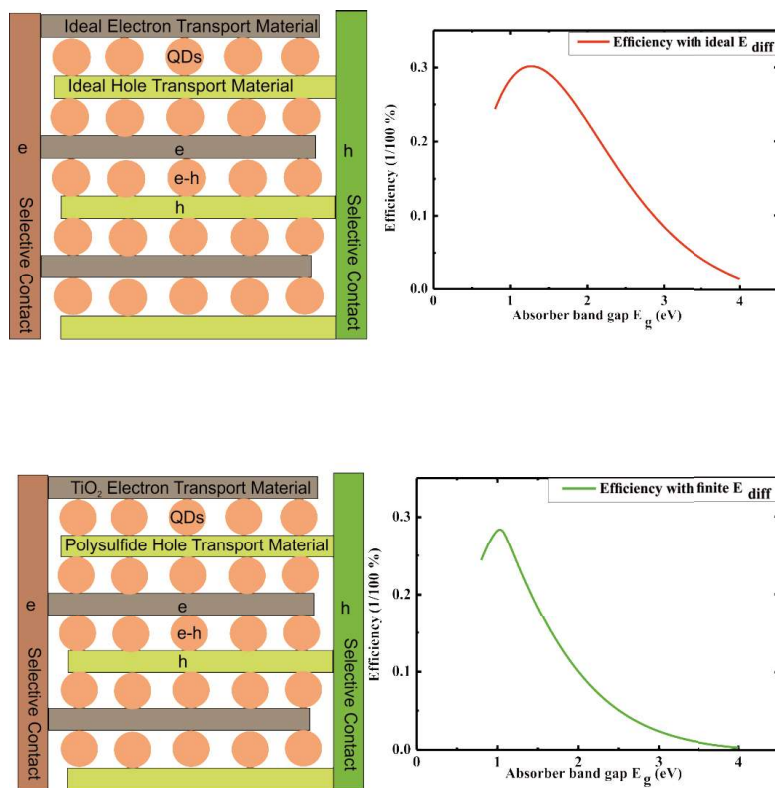


Figure 3.5 Detailed balance efficiency calculation with ideal and limited open circuit potential conditions.

Figure 3.5 shows schematic diagram of device with ideal electron transport material and hole transport material and corresponding detailed balance efficiency.

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