# ABSTRACT

With the rapid increase in population, the world's energy demand also expected to increase. Solar energy is an ideal energy source and can be used all over the world, as it is readily available globally for presumably the entirety of human existence, which made it the most promising renewable energy source that will fulfil the world energy demand.

Dye-sensitized solar cells (DSSCs) are photoelectrochemical solar cells manufactured by using dyes and mimic photosynthesis in plants. Their efficiency reached up to 13% by optimizing material and structural properties. However, there are still some challenges that need to be improved before DSSCs successfully enters the photovoltaic market for application. The main two issues are low cell performance and long-term stability.

There are three main processes summarized the path of charges in DSSCs, charge generation, charge collection and charge recombination, which significantly affects the cell performance. Different components are used in manufacturing DSSC, and each one of them plays an essential role in influencing the interface. Studying the structure of the $TiO_2$/dye and $TiO_2$/dye/electrolyte interfaces and understanding their effect on the charge transportation process will be the aim of this dissertation.

Using specific surface sensitive techniques, photoelectron spectroscopy (PES) including, X-ray photoelectron spectroscopy (XPS), ultra-violet photoelectron spectroscopy (UPS) and metastable induced electron spectroscopy (MIES) to observe the changes in the dye/ $TiO_2$ and $TiO_2$/dye/electrolyte interface from both molecular and electronic perspective. While neutral impact collision ion scattering spectroscopy (NICISS) used to measure the molecular coverage and concentration depth profiling of the dye.

In chapter 4, two different processes were applied on the $TiO_2$ substrate, heating with four ascending temperatures and heating-sputtering with different doses using Argon projectiles ($Ar^+$) were used to investigate the dye adsorption and configuration on $TiO_2$ surface. The heating process was more effective in removing the surface contaminations, while in the heating-sputtering processes, contaminations were removed, and surface defects such as the oxygen vacancies ($Ti^{3+}$) were created on $TiO_2$ surface. An observation of an increase in the dye adsorption was obtained using the heating process, while a decrease in the dye adsorption

resulted from the heating-sputtering process. Furthermore, both processes show different dye configuration of $TiO_2$ substrate.

Two different functional groups were used during a study investigating the addition of co-adsorbents in repressing dye aggregation on $TiO_2$. In chapters 5 and 6, the phosphonic acid decylphosphonic acid (DPA) and the carboxylic acid chenodeoxycholic Acid (CDCA) were used, respectively. Different concentrations of these co-adsorbents were used. It was shown that both types of co-adsorbents suppressed the formation of dye thicker layers. However, they behave differently concerning the type of dye that has been used.
The results show that the incorporation of co-adsorbent within the dye solution affected the dye adsorption and configuration on the $TiO_2$ surface. When co-adsorbents are adsorbed on the $TiO_2$ surface, they work as a buffer layer and replacing the weakly interacting and undesirable dye molecules that not involved in charge generation.

In chapter 7, a 1000 h stability test was conducted in three different conditions to investigate the degradation mechanisms of DSSC performance using DPA as a co-adsorbent. Light exposed condition, heat condition, and dark condition. The changes of the dye and electrolyte components on the $TiO_2$ /dye/electrolyte interface as cell ages were investigated using PES and NICISS for a better understanding of the process at the molecular level. The results show that the DSSCs containing co-adsorbent have more stabilized cell performance. Co-adsorbents remove the weakly dye molecule leading to better adsorbent of the electrolyte and additives, resulting in stabilizing the open-circuit voltage as the cell ages.

PES and NICISS are powerful surface sensitive techniques that have been used in this work to gain an insight into the DSSC interfaces at a molecular level as the cell ages.