

## Photo-anode Nanostructure Design and Electron Transport Mechanism of Photoelectrochemical Cells

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This research employs the density functional theory (DFT) to analyze the different anode designs of photoelectrochemical biofuel cells[1] and to study the electron transport mechanism between the electrode, the sensitizers and the electrolytes. The major objective is to design different nanostructures of zinc oxide semiconductors, which have a great potential in many ways including cost reduction, higher dye absorption efficiency and practical applications in industry. We built up the ZnO nanowires, nanotubes, the combination of both ZnO and TiO<sub>2</sub> structures as shown in Figure 1, and the molecular models of dyes as well as the electrolytes. Simulation results have found that the ZnO nanowires exhibit the smallest band gap as shown in Figure 2. The band gap increases as the diameter decreases, showing the quantum confinement effect. It is concluded that we can successfully transfer electrons by using ZnO nanotubes with different dyes such as chlorophyll-a and cyanidin as shown in Figures 3. In addition, the combined structure of ZnO and TiO<sub>2</sub> is also studied, and was found that the electrons can transfer from the oxygen atoms to zinc atoms in ZnO nanowires (shown in Figure 4). In conclusion, this research is able to determine the optoelectric properties of photoelectrochemical biofuel cells and it is envisioned that this will expand the green energy applications in the industry [2].

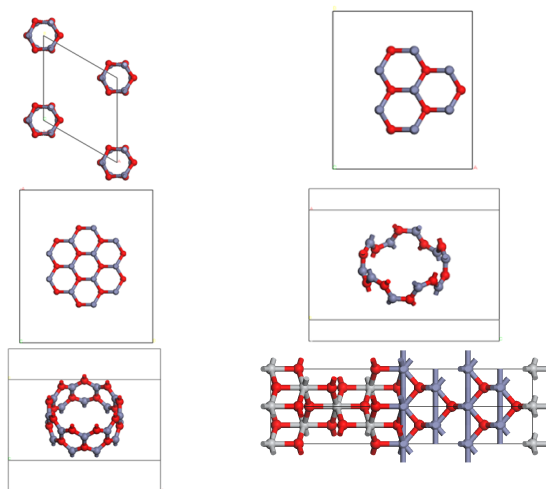


Figure 1 Different designs of the ZnO (+TiO<sub>2</sub>) nanostructures

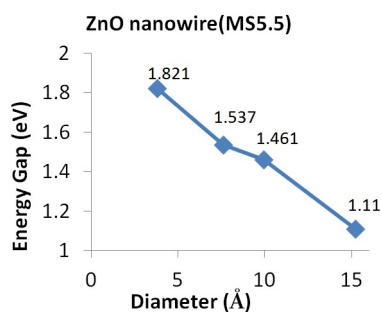


Figure 2 The band gap of ZnO with different diameters

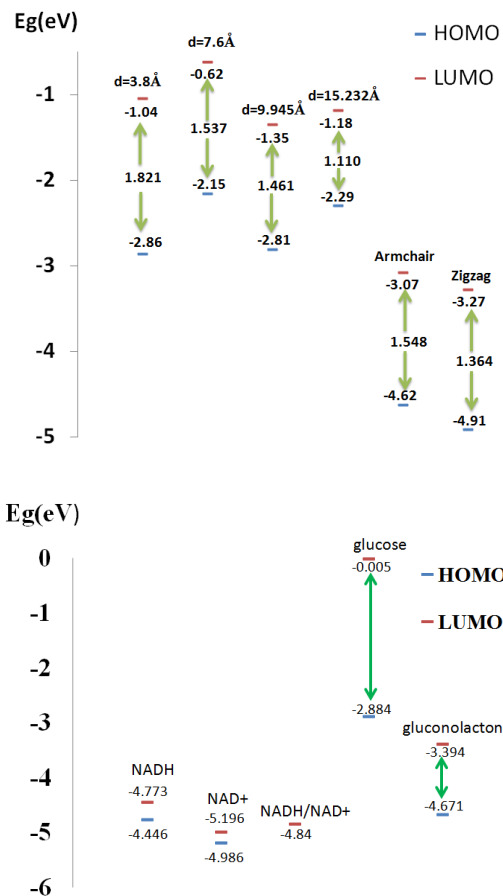


Figure 3 The energy diagrams of electrodes and electrolytes using CASTEP and DMol<sup>3</sup> calculations

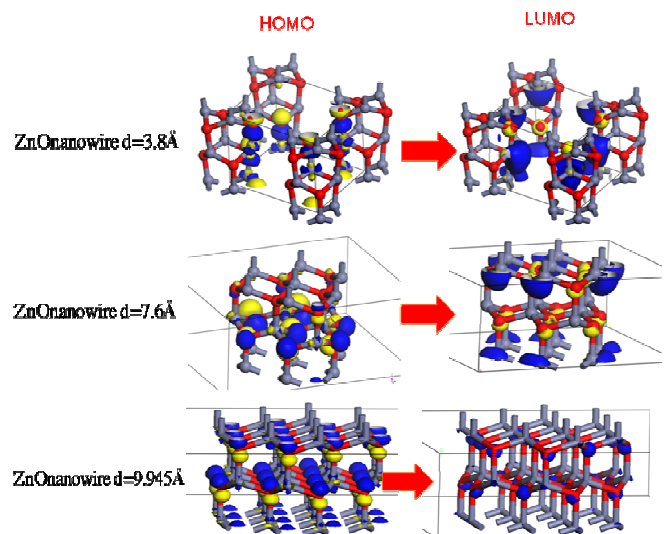


Figure 4 Electron orbital configuration of ZnO nanowires

## REFERENCES

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- [2] Liu, C.T. (supervised by Prof. C.W. Hong), Nanostructure design of the photo-anode of a photoelectrochemical biofuel cell, MSc. Thesis, National Tsing Hua University, 7/2012.