CHAPTER 1

INTRODUCTION

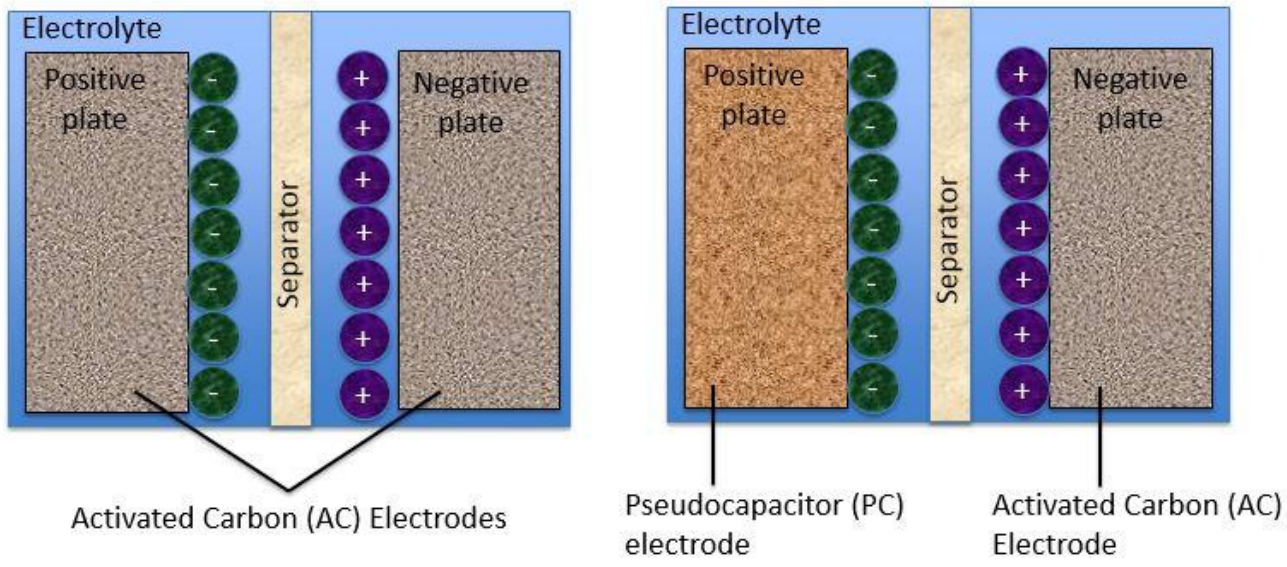
1.1 BACKGROUND OF THE PROBLEM

In our electric-powered era, electricity is essential to humankind. One of the problems in energy storage devices is the capacity of the storage and charging time. Batteries could hold a large amount of power, however takes hours to charge up. Capacitors, on the contrary, charge almost instantly; nonetheless store small amount of power. Supercapacitor have been explored to present a combination of high power, and fast charging features of battery and capacitor respectively.

Supercapacitor is an energy storage device known as electrochemical capacitor (EC); store the energy electric field of electrochemical double-layer. Supercapacitor accept and deliver charges faster than batteries, and tolerates high number of charge and discharge cycles (ca. 100,000 cycles) than rechargeable batteries (ca. 2,000 cycles).

Supercapacitor could be classified into three groups i.e., electrochemical double layer capacitor (EDLC), pseudocapacitor (PC), and hybrid supercapacitor. PC store electrical energy faradaically by electron charge transfer between electrode and electrolyte; involving mechanism of (i) adsorptions, (ii) reduction-oxidation reactions (redox reactions), and (iii) intercalation processes. These Faradaic processes allow PCs to achieve greater capacitance and energy density than that of the EDLCs.

Subsequently, supercapacitor could be classified into another two groups i.e., symmetric supercapacitor (SSC), and asymmetric supercapacitor (ASC).



(a) (b)

Figure 1.1 Symmetric supercapacitor (a), and asymmetric supercapacitor (b)

Basically, symmetric supercapacitors were fabricated using two activated carbon (AC) electrodes, and asymmetric supercapacitors, which one of the AC electrodes is replaced by a pseudocapacitor (PC)-type electrode. The electrodes in both device structures are separated by aqueous electrolyte.

1.2 PROBLEM STATEMENT

Selection of material for the electrode of the supercapacitor is necessary to get the best performance; could be in perspective of availability and economy. The importance of this research is to investigate the correlation between electronic structure and electron conductivity in MoX_2 (X = S, Se, and Te) to determine the most effective material as the electrode.

1.3 OBJECTIVES OF RESEARCH

The objectives of this study are:

i. To build the models of basic crystal of MoX_2 (X = S, Se and Te) using Gaussian 09W software.

ii. To simulate the realistic models of MoX_2 (X = S, Se and Te) using Gaussian 09W software.

iii. To observe the overlapping site of the realistic models of MoX_2 (X = S, Se and Te).

1.4 SCOPE OF THE STUDY

1. To build the models of basic crystal of MoX_2 (X = S, Se and Te) using Gaussian 09W software.
    a. Finding the MoX_2 (X = S, Se and Te) CIF file from www.crystallography.net, published from the previous researchers.
    b. Create the first smallest model of the nanocrystal.