# STUDIES ON CORRELATION BETWEEN ELECTRONIC STRUCTURE AND ELECTRONIC CONDUCTIVITY IN $MoX_2$ (X = S, Se and Te)

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## ABSTRACT

A successful research have been conducted to investigate the molybdenum dichalcogenides, $MoX_2$ (X = S, Se, and Te) as the electrode materials in electrochemical cells. The relationship between number of layer and bandgap of the materials has been studied by many researcher in the past. They hardly stated that, the properties such as speed of storage and amount of chargers that could be stored within the cells will be answered as soon as the correlation been studied. In this study, fundamental parameters such as size-offset between a monolayer and exciton Bohr radius of $MoX_2$ and ground and excited state electron density have been investigate. In this study also, realistic monolayer models of $MoX_2$ were identified using quantum chemical calculations which also explain a correlation between size-offset and charge storage properties. We conclude that as the size-offset decreases, the higher possibility of wave functions overlap between the excited state, and ground state electrons; therefore the higher the electron mobility, and conductivity of the $MoX_2$ would be.

## ABSTRAK

Satu kajian yang berjaya telah dijalankan untuk mengkaji dichalcogenides molibdenum, MoX2 (X = S, Se, dan Te) sebagai bahan elektrod dalam sel elektrokimia. Hubungan antara beberapa lapisan dan nilai jurang jalur bahan telah dikaji oleh ramai penyelidik pada masa lalu. Mereka kuat menyatakan bahawa, sifat-sifat seperti kelajuan penyimpanan dan jumlah pengecas yang boleh disimpan dalam sel-sel akan terjawab setelah hubungan tersebut dikaji. Dalam kajian ini, parameter asas seperti saiz "offset" antara lapisan mono dan jejari exciton Bohr kepada $MoX_2$ dan electron pada keadaan asas dan ketumpatan elektron keadaan teruja telah disiasat. Dalam kajian ini juga, model realistik lapisan mono $MoX_2$ telah dikenal pasti menggunakan pengiraan kimia kuantum yang juga menjelaskan hubung kait antara saiz mengimbangi dan sifat penyimpanan caj. Kami menyimpulkan bahawa semakin rendah penurunan saiz "offset", kemungkinan yang lebih tinggi fungsi gelombang bertindih antara electron pada keadaan teruja, dan electron pada keadaan asas; oleh itu pergerakan electron yang lebih tinggi, dan kekonduksian daripada $MoX_2$ akan terhasil.