BANDGAP ENGINEERING OF FUNCTIONALIZED POLYETHYLENE OXIDE (PEO) ELECTROLYTE

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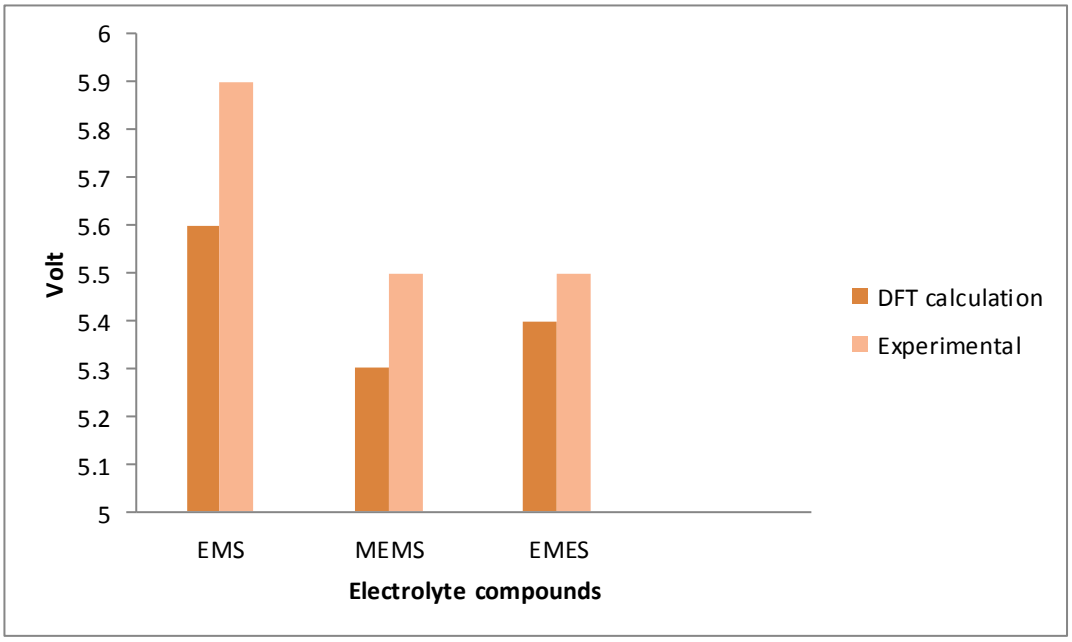
ABSTRACT

Electrolytes enable conduction of ions in a battery across the electrodes. One of the most important properties of an electrolyte material is its electrochemical window, which determines overall safety of the battery. Electrochemical window (also known as HOMO LUMO gap or bandgap) is calculated in the present work for polyethylene oxide (PEO) with different chemistries using a combination of Hartree-Fock and density functional theory (DFT) techniques. The aim is to study how the bandgap can be varied with different functional groups added to the polymer. The calculations are initially compared with the corresponding experimental values for various sulfone compounds. The following graph shows a close match between the two. Hence the method is further extended to PEO functionalized with groups like OH, COOH, NH_2,NP and$(CH_3)_3Si$ to study how the bandgap can be engineered by varying the chemistry of the material. These functional groups are added to the polymer in order to enhance ion diffusivity, however we find that all these groups resulted in lowering the bandgap by 0.5 to 2.5 V compared to non-functionalized PEO.



Comparison of electrochemical window (or bandgap) between experimental and calculated values for ethyl methyl sulfone (EMS), methoxy ethyl methyl sulfone (MEMS) and ethyl methoxy ethyl sulfone (EMES); a class of electrolytes.