# EFFECTS OF ADDITIVES ON ELECTROCHEMICAL PERFORMANCE OF ANODE MATERIALS IN PC-BASED ELECTROLYTES

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We have developed a high throughput virtual screening technique, based on quantum chemical calculations, to identify potential electrolyte additives for PC-based electrolytes. This screening method is cost effective, time saving and can be used for all additive applications. Based on high throughput screening, 11 compounds were selected as potential lead structures from the first Pareto front and crucial properties were examined and compared using DFT calculations. Among these compounds, two additives were selected, synthesized and experimentally tested to illustrate the potential of the selected additives and hence the screening technique. The additives were tested using 1M $LiPF_6$ /PC and 1M $LiPF_6$ /PC: dimethyl carbonate (DMC) (1:1 v/v). The CV of 1 M $LiPF_6$/PC:DMC (1:1) and 1 M $LiPF_6$/PC, with and without, different additive concentrations are carried out in this work.The cell without the additive cannot be cycled which is consistent with the charge/discharge test. No reduction peak is observed in the potential region above 1 V; however, a broad feature starts to appear below 0.8 V, in the region where reduction of PC occurs. However, lithium intercalation and deintercalation is not observed which can be related to the exfoliation of the MCMB electrode. The cells with different additive concentrations all show a peak, due to additive reduction, in the potential region between 1.8-1.4 V centered at 1.7 V for CMDO and at 1.6 V for BCMDO. This observation is consistent with the calculated reduction potential and the charge/discharge profile. The intensity of the peak increases as the additive concentration increases. In the lower potential region (below 0.8 V), the broad feature observed for the cells without the additives, correlated with the decomposition and cointercalation of PC, disappears with the addition of the additives. This result suggests that the additive can suppress the cointercalation and decomposition of PC, while lithium intercalation and deintercalation can be maintained. The mesocarbon microbead electrode showed an excellent electrochemical performance in a PC based electrolyte with 2% additives. The first cycle coulombic efficiency of the proposed additives was >84%, increasing to 99% after the second cycle. When compared with previously reported sulfur or halogen containing additives, the computationally designed additives resulted in better coulombic efficiency. The MCMB electrode's electrochemical performance improvement is therefore attributed to addditive decomposition products.