Self-healing Polymers for Lithium Metal Batteries

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Abstract

Lithium ion batteries (LIBs) are the best options for energy devices, transportation and renewable energy application. However, the ever-increasing demand in the field of energy storage and electrical vehicles requires future batteries with increased performances. In particular, researchers have been focused on batteries with higher energy density. The substitution of the graphitic anode with metallic lithium fabricated lithium metal batteries (LMBs). LMBs are a valid alternative to commercial LIBs, because of their high energy density and high theoretic capacity. However, lithium anode has several safety issues, in particular due to the formation of dendrites. Several options have been proposed for limiting dendrites growth. Gel polymer electrolytes (GPEs) have been investigated for suppressing the dendrite growth and, as a consequence, increase the safety of the cell. Moreover, the insertion of self-capability in gel polymer electrolyte is a valid strategy for new lithium batteries able to have longer life. The self-healing properties is mainly given due to spontaneous reaction inside the polymer structure. Different are the chemical bonds involved in self-healing (es. Diels-Alder, ROMP, etc.) However, H-bond interaction is mainly used in lithium metal batteries, because it doesn't require an external stimulus and it is easily inserted inside the chains of the polymer due to an additive.

In this work, ureidopyrimidinone methacrylate (UpyMa) molecule is investigated as a self-healing additive for poly (ethylene glycol) methyl ether methacrylate polymers. The molecule is synthesized by using a coupling organic reaction involving methyl isocytosine and 2-isocyanatoethyl methacrylate. The product of the reaction is demonstrated with different spectroscopies analyses, and possesses a yield of 92.3%

Furthermore, UpyMa-Membranes have been synthesized through a solvent free UV polymerization involving the oligomer poly(ethyleneglycol) methyl ether methacrylate, polyethyleneglycoldiacrylate, and 2-Hydroxy-2-methyl-1-phenyl-propan-1-one. Different polymers have been synthesized and investigated. Polymers with 5wt% and 10wt% of UpyMa demonstrate good thermal and electrochemical stability and high ionic conductivity. Moreover, they have the capability of self-recovery after being

damaged at 50 °C in 2 hours, and at room temperature in 24 hours. The membrane with 5wt% of UpyMa is also the best candidate as GPE for its good interfacial stability and high lithium ion transference. The full cell is able to work at 0.2 C rate at room temperature for 300 cycles, with an initial discharge capacity of 143 mAh g^{-1} and a capacity retention of 80%. The self-healing properties of GPE are demonstrating opening the cell and damaged it with a cutter, and the assembled another time. The electrochemical performances of the cell are restored after a rest time, thanks to the H-bond interaction given by UpyMa additive inside the polymeric structure.

In conclusion, self-healing polymers in lithium metal batteries could be synthesized through a green UV-polymerization and used as gel polymer electrolytes in lithium metal batteries. The work demonstrates the importance of smart functionalities as self-healing in lithium batteries and the possible use of the synthesized polymer in LMBs .