Develop New Non-aqueous Electrolytes for Rechargeable Li-Air Battery Application

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Background and Introduction

Li-air cells can be considered as the ‘holy grail’ of lithium batteries because they offer, in principle, a significantly superior theoretical energy density to conventional lithium-ion systems. This lithium-ion cell chemistry, the best to data, would provide a theoretical specific energy of ~900 Wh/kg if the calculation is based on the masses of the anode and cathode materials alone; in practice, 150-200 Wh/kg has been accomplished at the cell level. In contrast, a lithium-air cell, when discharged to the peroxide composition Li2O2 at an average 3.1 V would provide a theoretical specific energy of 3623 Wh/kg, or when discharged to Li2O at the same voltage, 5240 Wh/kg.

Such larger theoretical energy density of Li-air battery is because the cell consists of lithium metal as an anode, and the cathode oxidant, oxygen, is stored externally since it can be readily obtained from the surrounding air. Figure 2 shows the schematic diagram of a typical lithium-air cell configuration, which consists of a porous carbon supported catalytic cathode designed to promote oxygen diffusion and reduction and a pure lithium metal anode. These two electrodes are separated by a lithium-ion conducting electrolyte. During discharge, lithium metal at the anode is oxidized to lithium ion and liberates electrons, while at cathode, oxygen is reduced in either a two-electron or four-electron process to form Li2O2 or Li2O, respectively, both of which are thermodynamically possible.

Figure 2 Li-air battery flow chart

There are still many challenges to be overcome, from finding suitable catalyst for cathode reactions (ORR and OER), to designing porous cathode structure for storing the oxygen reduction product, to optimizing the cell chemistry and identifying the reaction products. Predict ways to discover novel catalysts to facilitate the oxygen reduction/evolution reactions and to develop new electrolytes to achieve good round trip efficiency and rechargeability in Li-air cells.

Impact

Approach

Ideal reaction scheme (on the air cathode)

Figure 1 The gravimetric energy densities (Wh/kg) for various types of rechargeable batteries compared to gasoline.

2 Li+ + 2 e− + O2 (molecule) → Li2O2 (scarcely soluble)

Li2O (radical)

锂离子电池

Figure 6 HRTEM image of MnOx/C composite

Reactons with electrolyte

Figure 7 Voltage profile in 1M LiPF6/PC (on the air cathode)

Disproportionation

Figure 8 Comparison of the computed barriers (enthalpies) for activation of (A) PC decomposition and (B) 1NM1 decomposition by O2 anion radical, Li2O radical, Li2O anion, and Li2O2.

Develop novel catalysts to facilitate cathode reactions

Develop new electrolytes that can resist oxidation.

Preliminary Results

I. In-situ Synthesis of Catalytic Air Cathode Materials

Figure 3 Typical voltage profile of Li-air battery using PC as electrolyte

Figure 4 High-resolution XRD patterns of original SPL carbon and SPL carbon after being loaded with MnO2 catalyst.

Figure 5 SEM images of (a) original carbon and (b) as-prepared MnOx/C composite

II. Increase Stability Towards Oxygen Reduction Products with Oligoether-functionalized Silane Electrolytes

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Figure 8 Voltage profile in 1M LiPF6/PC

Figure 9 First charge and discharge cycles of a Li-air cell with propylene carbonate (PC) and 1NM3.

Figure 10 Comparison of the computed barriers (enthalpies) for activation of (A) PC decomposition and (B) 1NM1 decomposition by O2 anion radical, Li2O radical, Li2O anion, and Li2O2.

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Develop novel non-aqueous electrolytes, explore new approach to fabricate novel catalysts on carbon cathode and apply state-of-the-art characterization for Li-air batteries application.