

3<sup>rd</sup> International Conference on

# ELECTROCHEMISTRY

July 10-11, 2017 Berlin, Germany

## Modeling and simulation of Li-air battery operated with high temperature ionic liquid electrolyte

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Li-air cell operated with ionic liquid electrolytes is a very promising energy storage technology for electric vehicle and plug-in hybrid electric vehicle due to several favorable characteristics of ionic liquids. However, Li-air cells that employ room temperature ionic liquid (RTIL) electrolytes exhibit poor performance due to limited oxygen solubility and low reactant species mobility. To circumvent these aforementioned drawbacks, we investigated the electrical performance of a Li-air cell with ionic liquid electrolytes operating at high temperature. A continuum based model developed for ternary electrolyte system is used to quantify the performance of the Li-air cell, with an ionic liquid (MPPY-TFSI) electrolyte, as a function of operating temperature. Key parameters of ionic liquid electrolytes are obtained from atomistic simulations, such as molecular dynamics (MD) and density functional theory (DFT) calculations. The continuum based cell level simulation results show that the battery performance can be improved significantly by increasing operating temperature. For instance, specific capacity as high as 3000 mAh/g can be achieved at 110°C operating temperature, which is almost 25 times higher than its counterpart at room temperature. Simulation results also reveal that by increasing the operating temperature, the specific capacity can be improved significantly for high load current density, which is one of the most critical drawbacks in RTIL based Li-air battery. We also studied the effect of cathode thickness on the performance of Li-air battery at different operating temperature. The transport limitation of oxygen and lithium ions can be alleviated at higher operating temperature suggesting that even thicker cathode materials can be used to enhance the cell capacity at elevated temperature.

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## Preparation and properties of immobilized redox active ionic liquids and polymer ionic liquids

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Recently, we have developed a new family of ionic liquids that exhibit well-defined redox properties. Herein, we will report the surface modification of carbon materials by means of electrografting. Electrochemical processes based on oxidative or reductive grafting have been used for the attachment of organic molecules, such as redox active ionic liquids, onto various electrode surfaces providing new and special properties to the interfaces. The immobilization of redox active poly(ionic liquid) by surface-initiated atom transfer radical polymerization (SI-ATRP) process onto electrode surfaces has been investigated. The surface and electrochemical properties of these modified surfaces were investigated by combining different techniques (XPS, AFM, ellipsometry and contact angle). The nanostructured redox active poly(ionic liquid) exhibits high heterogeneous electron transfer rate about 150 s<sup>-1</sup>. We will show the use of redox active poly(ionic liquid) polymer brush as electrochemically reversible tunable surface wettability system and as electrochemical sensors.

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