

## **Modelling Panel Abstract & Speaker Biography**

### **Minutiae of Thermodynamics and Transport Phenomena in Li-S Battery Electrolytes**

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Lithium-sulfur technology might finally realize a battery beyond intercalation with a much higher energy density and cheaper price. Unfortunately, the maturation of this promising technology is impeded to a high extent by the undesirable release and freedom of the polysulfide species in the bulk of electrolyte. There is a consensus among the battery researchers that these species feature a fast mobility in the electrolyte. Surprisingly but, to date, there is a very limited quantitative insight about the modifications lent to the Thermodynamics and Transport parameters of the electrolyte in the presence of alien polysulfide species. The experimental/theoretical understanding of the polysulfides movement and their interactions with the primary ions in the electrolyte has been neglected due to the complexity of analysis in the multicomponent systems.

In our recent paper<sup>1</sup>, we communicated a model-based measure of the polysulfides mobility in a typical Li-sulfur battery electrolyte (i.e., LiTFSI in DOL/DME). Here, a general discussion of the complexities involved in the theoretical/experimental account of the Thermodynamics and transport (charge/mass) in Li-S batteries will be presented.

#### **References**

1. M. Safari, C.Y. Kwok, L. F. Nazar, 'Transport Properties of Polysulfide Species in Lithium-Sulfur Battery Electrolytes: Coupling of Experiment and Theory,' ACS Central Science 2 (8) (2016) 560-568.

#### **Speaker Biography:**

Momo Safari is an Associate Professor in 'Battery Technology' at University of Hasselt in Belgium. He received his PhD degree in Electrochemical Engineering from Universite de Picardie Jules Verne, Amiens, in 2011, working with Dr. C. Delacourt and Prof. Jean-Marie Tarascon. He was a postdoctoral Fellow in the group of Prof. L. F. Nazar at University of Waterloo before joining the Hasselt University. Momo is interested in advanced batteries and most of his research centers around experimental/theoretical investigation of parasitic reactions and aging phenomena in porous electrodes and electrolytes.

Applications of his research include optimization of the electrode/electrolyte formulations, end-of-life tests and simulations, and development of physics-based macroscopic models/ algorithms for SOC and SOH estimations.

