## Mechanisms Panel Abstract & Speaker Biography

## A Quantitative Tool to Predict the Phase Composition of Lithium-Sulfur Batteries

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Lithium-sulfur batteries are one of the most promising candidates for the next generation electrical energy storage. They are made of cheap and abundant elements and they have a theoretical specific energy of ca. 2600 Wh kg<sup>-1</sup>, which is much higher than that of lithium-ion batteries. However, the development of lithium-sulfur batteries is hampered by their complicated reaction mechanism. In order to reach their full potential, lithium-sulfur batteries should achieve the complete reduction of solid sulfur into solid Li<sub>2</sub>S, and this reaction occurs via a multistep reaction pathway involving a range of soluble polysulfides. In order to achieve a high specific energy, the battery should run with the minimum amount of electrolyte required, and this corresponds to a situation where all polysulfide species should reach saturation. The corresponding equilibrium voltage profile during charge and discharge will be given by the saturation concentration of polysulfides (Nernst equation) and the capacity will depend on the efficiency in the conversion from solid sulfur to liquid polysulfides and to solid Li<sub>2</sub>S, and the reverse reactions. Here we report the first phase diagram of system S-Li<sub>2</sub>S-electrolyte, and we demonstrate that the phase diagram is a practical tool to predict the equilibrium polysulfide concentration at any composition, the formation of solid phases, and to develop a quantitative understanding of the effect of solvent on battery performance.



Figure 1. Suggested ternary phase diagram of a S-Li2S-electrolyte system.

## Speaker Biography:

James received a first-class Master's degree in Chemistry (MChem) in 2014 from the University of Southampton, where he continued studying for my Ph.D. under the supervision of Dr. Nuria Garcia-Araez and Prof. John Owen in collaboration with OXIS Energy.

His Ph.D. focuses on fundamental studies of lithiumsulfur batteries and in particular, on understanding the lithium polysulfide intermediate composition through the development of methods to construct the first



experimental ternary phase diagram for lithium-sulfur batteries.