

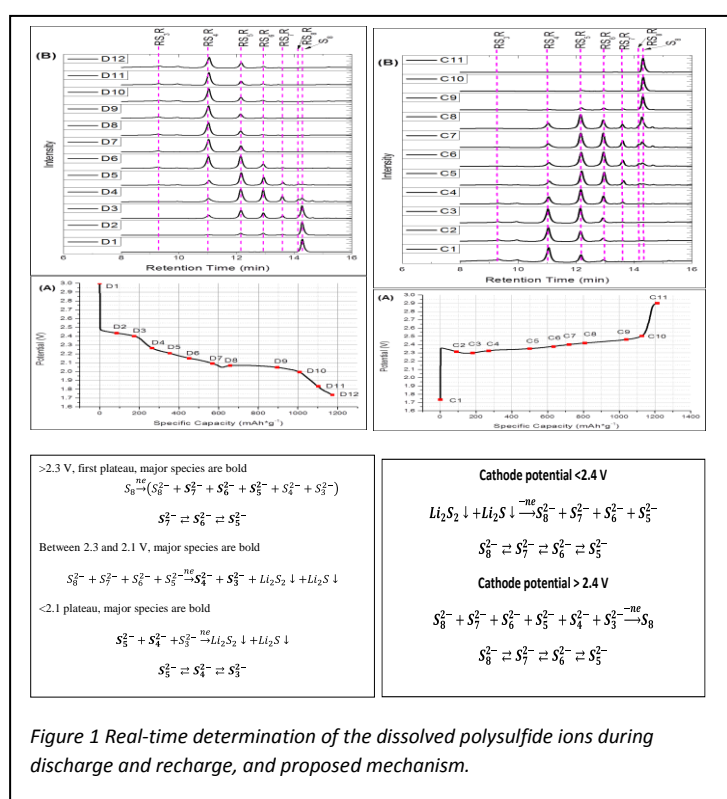
## Mechanism Panel Abstract & Speaker Biography

### Investigation of the Sulfur Redox Reaction Mechanism by the Quantitative and Qualitative Measurement of Dissolved Polysulfide Ions

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The challenge of searching for a battery system with an energy density beyond Li-ion promotes the acceleration of research of Li-Sulfur system. The significant advantage of the system is not only its high energy density, but also the low cost of sulfur material. However, even after the extensive studies, the mechanism of Li-S battery is still not clear. It is mainly due to the fact that quantitative and qualitative measurement of the soluble polysulfides



are very difficult, due to the fact that pure polysulfide standard solution does not exist. We have developed a method which can accurately identify each polysulfide ion and determine the concentration of each polysulfide ion using HPLC-MS technique.

The mechanism of the sulfur cathode in Li-S batteries has been proposed. It was revealed by the real-time quantitative determination of polysulfide species and elemental sulfur by means of the high performance liquid chromatography in the course of the discharge and

recharge of a Li-S battery. A three-step reduction mechanism including two chemical equilibrium reactions was proposed for the sulfur cathode discharge. The typical two-plateau discharge curve for sulfur cathode can be explained. A two-step oxidation mechanism for the  $Li_2S$  and  $Li_2S_2$  with a single chemical equilibrium among soluble polysulfide ions was proposed. The chemical equilibrium among  $S_5^{2-}$ ,  $S_6^{2-}$ ,  $S_7^{2-}$  and  $S_8^{2-}$  throughout the entire oxidation process resulted for the single flat recharge curve in Li-S batteries.

We also developed a rapid derivatization method to capture the polysulfide ions as soon as they formed electrochemically on the interface of the sulfur electrode, so any subsequent fast chemical reactions between the polysulfides and sulfur were avoided. It was found that the major polysulfide ions formed at the first reduction wave of elemental sulfur were the  $S_4^{2-}$  and  $S_5^{2-}$  species, while the widely accepted reduction products of  $S_8^{2-}$  and  $S_6^{2-}$  for the first reduction wave were in low abundance. The electrochemically produced  $S_4^{2-}$  and  $S_5^{2-}$  species then reacted with elemental sulfur forming other long chain polysulfide ions to establish the first chemical equilibrium in the reduction reaction.

### Speaker Biography:

Prof. Deyang Qu graduated with a B.Sc. in Electrochemistry with honors from the Department of Chemistry, Wuhan University, China in 1986. He continued his graduate studies at University of Ottawa in Canada with Professor B.E. Conway and earned his Ph.D. in electrochemistry in 1994. Right after graduation, Prof. Qu started his career in the battery industry. Before joining the faculty of UMass Boston in the spring of 2005, he had spent twelve years in the battery industry. In 2015, he was named as Johnson Controls Endowed Chair Professor in University of Wisconsin Milwaukee. Prof. Qu has developed research programs in the area of Li-air, Zn-air batteries, Li-S, Li-ion battery, advanced lead acid batteries, fuel cells, supercapacitors and hydrogen storage.

