$Na-O_2$ Batteries: In-situ soft X-ray absorption spectroscopy studies

Mohammad N. Banis[1,2], Hossein Yadegari[2], Qian Sun[2], Tom Regier[3], Teak Boyko[3], Jigang Zhou[3], Yun M. Yiu[2], Ruying Li[2], Yongfeng Hu[3], Tsun K. Sham[1,2], Xueliang Sun[2]

1. Soochow-Western Centre for Synchrotron Radiation Research, Western University, London Ontario, Canada
2. Western University, London, Ontario, Canada
3. Canadian Light Source, Saskatoon, Saskatchewan, Canada
mohammad.norouzi.b@gmail.com

The search for new energy storage systems has intensified the research on metal-air batteries such as sodium-oxygen ($Na-O_2$) batteries. This is mainly due to their high theoretical energy density and deceptively simple underlying cell reactions. The oxygen is used to form insoluble oxides in non-aqueous electrolytes during discharge process, which ideally should decompose during charging. Although the general mechanism of $Na-O_2$ has been established, some aspects of the cell chemistry remains ambiguous. Various compounds have been reported as the discharge products in $Na-O_2$ system. The diversity of discharge products in $Na-O_2$ cells mainly originates from the relative instability of NaO_2 in the cell environment. However, the mechanism behind the degradation process of the discharge products is not clear. Meanwhile, ex-situ analysis of the highly sensitive discharge products is generally affected by contamination from surrounding environment. Thus, effective in-situ characterization techniques are required to provide an accurate understanding of the decomposition mechanisms involved in $Na-O_2$ cells.

Soft X-ray absorption spectroscopy (XAS) at the O K-edge, provides appropriate selectivity and sensitivity required for the analytical tracing of the products in $Na-O_2$ cells. In the present work, we developed an in-situ soft XAS technique to study the degradation mechanism of discharge products in non-aqueous Na-O2 cells. The ultra-high vacuum condition employed in this technique eliminates any potential source of contamination, providing accurate and reliable chemical information on the electrochemical mechanism of the cells.

We tracked the formation and decomposition of discharge products in a working $Na-O_2$ cell by monitoring the O K-edge XAS spectrum at the positive electrode of the cell. The results indicated reversible formation and decomposition of irregular structures, and conformal film-like NaO_2 on the surface of Au air electrode during the discharge/charge cycles, respectively. Using in-situ soft XAS (mapping) measurements in conjunction with electrochemical characterization and ex-situ electron microscopy, we showed that a progressive degradation reaction occurs at the products/electrolyte interface. The present study illustrates the capability of in-situ soft XAS technique in illuminating the underlaying mechanisms of charge/discharge processes in metal-O_2 batteries. It is expected that the developed in-situ soft XAS cell can be further modified for other types of metal-O_2 batteries, metal-ion batteries and fuel cells studies.

This research was supported by National Science and Engineering Research Council of Canada, Canada Research Chair, the Interdisciplinary Initiative (IDI) of Western University and Soochow-Western Centre for Synchrotron Radiation Research. The research described in the paper was performed at the Canadian Light Source which is supported by CFI, NSERC, CHIR, NRC, and the University of Saskatchewan.