Development of Catalytic Systems for Rechargeable Li-O₂ Batteries

<u>Eduard Nasybulin</u>,^a Wu Xu,^{a,*} Mark H. Engelhard,^b Jianming Zheng,^a Priyanka Bhattacharya,^a Yuyan Shao,^c Zimin Nie,^a Ji-Guang Zhang^{a,*}

^{a.} Energy & Environment Directorate

^{b.} Environmental Molecular Science Laboratory

^{c.} Fundamental and Computational Sciences Directorate Pacific Northwest National Laboratory, Richland, WA 99354, USA

Li-O₂ batteries are promising for high energy density storage applications. Rechargeability of Li-O2 batteries is based on the reversible formation/oxidation of Li2O2. Despite high capacity values achieved for mesoporous carbon-based air cathodes, cycling on such electrodes suffers from poor reversibility and high discharge-charge voltage hysteresis. Resent reports have demonstrated that the formation of Li2O2 is accompanied by the decomposition of both electrolyte and carbon-based electrode. Also, there is a concern about anodic stability of the carbon-based electrode during the charging process above 3.5 V vs. Li/Li⁺. The decomposition products mainly represent insulating carbonate-based species which accumulate with cycling and cause fast capacity fading. The high discharge-charge voltage hysteresis is another issue limiting the development of practical Li-O₂ batteries. Slow kinetics of Li2O2 formation/oxidation is responsible for the large overpotentials.

Efficient catalytic system may not only improve the electron transfer in the air cathode (decrease overpotentials) but also suppress formation of the side products (prolong cycle life). Therefore, the concept of catalysis in Li-O2 batteries is broadened from the traditional electrocatalysis. A number of materials including metals, metal oxides, and organic compounds are evaluated in the present study. It is demonstrated that some of the materials have a pronounced effect on the discharge and/or charge voltages while others improve the cycling performance without significant changes in the voltage profiles. The electrochemical performance of various catalic materials in Li-O2 batteries and O2-rich environment is demonstrated with the support from product analyses. Details will be reported in the presentation.

Acknowledgement

This work was sponsored by the Vehicle Technologies Program of the U.S. Department of Energy.