Doctoral Dissertation Defense

Xue Rui

Wednesday, August 28th, 2019 at 2:00 pm in SES 2214

Committee Chair: Robert F. Klie

Committee Members: Serdar Öğüt, W. Andreas Schroeder, Fengyuan Shi, Jeremiah Abiade

Atomic-scale study of oxygen vacancies in transition metal perovskite oxides

Oxygen vacancies in transition metal perovskite oxides (ABO_3) play the key role in controlling the functional properties of materials, such as conductivity, ferromagnetic/antiferromagnetic and electrocatalytic performance. In particular, the presence of ordered oxygen vacancies, oxygen tetrahedral/square-planer (BO_4) layers, are capable of introducing crystal-chemical factors to break the initial equilibrium in the structure and highly influence those remarkable properties. During my PhD research, utilizing aberration-corrected scanning transmission electron microscopy accompanied with in-situ cooling/heating as well as ex-situ electrochemical cycling technique, I investigate the effects of ordered oxygen vacancies at the atomic scale in perovskite oxide. The crystal/electronic structure of ordered oxygen vacancies in oxygen deficient $La_{0.5}Sr_{0.5}CoO_{3-\delta}$ thin film is demonstrated to couple with substrate $SrTiO_3$ low temperature phase transition. The atomic arrangement of ordered oxygen vacancy domains in $LaNiO_{3-\delta}$ is shown to determine the ferromagnetic/antiferromagnetic property. The formation of oxygen vacancy orderings in $La_{1-x}Sr_xCoO_3$ oxygen evolution reaction catalysts is found to facilitate the surface decomposition/corrosion, creating highly active surfaces with increase interactions with Fe impurities. The dynamics of oxygen vacancy ordering in $La_{1-x}Sr_xCoO_3$ are studied during in-situ heating in the electron microscope column to simulate the oxygen reduction evolution, serving as important reference for analyzing surface decomposition in electrochemical cycling process. Based on all the in-situ/ex-situ observation, my research advances the understanding of structure-property relationship in oxygen deficient transition metal perovskite oxides, opening up pathways for controlling the functional properties of metal oxide device and catalyst via tuning oxygen vacancies.