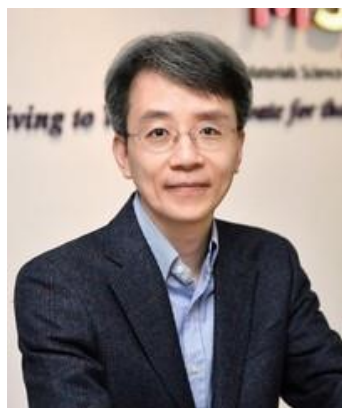


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## Correlation between Symmetry-Broken Atom Configurations and Electronic Structure Variations in Oxides for Oxygen Electrocatalysis

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### Abstract

A great deal of research has been carried out over the last two decades to achieve better efficiency in energy storage and conversion. As many actual devices based on electrochemical reactions for energy conversion and production operate at room temperature, the utilization of adequate electrocatalysts is imperative to significantly lower the activation barrier during the redox reactions and thereby enhance the overall storage and conversion performance. Hydrogen-evolution/oxygen-evolution reactions (HER/OER) are key electrochemical processes at the cathode and anode sides, respectively, in electrolyzers for hydrogen production *via* water splitting. It is generally accepted that the activation barrier of the OER associated with transfer of multiple electrons and protons is larger than that of the HER, resulting in a comparatively higher anodic overpotential to split water. Therefore, the OER is a predominant pathway that can notably affect the overall efficiency of electrolysis. Furthermore, as acidic solutions are utilized in proton-exchange-membrane (PEM) electrolyzers usually showing high OER current at lower overpotentials, the stability of catalysts at the anode side is another significant issue in addition to the high catalytic activity. In this presentation, we focus on recent breakthroughs in OER electrocatalysts on the basis of atomic-scale surface structure and composition variations along with the electronic structure changes. To this end, we highlight the critical roles of atomic-level defects, including ionic vacancies and grain boundaries, and lattice distortion, encompassing oxygen octahedral displacements, in oxides, many of which are largely utilized for OER catalysis in alkaline electrolytes under strong anodic potentials. The issues of surface instability and subsequent element dissolution at the nanoscale in both acid and alkaline electrolytes are also covered and thereupon exploiting such instability in alternative methods toward surface modification for better catalytic properties is suggested.