Design of Highly Active Perovskite Oxides for Oxygen Evolution Reaction by Combining Experimental and ab Initio Studies

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Perovskite oxides (ABO3) have recently attracted attention since tailoring their chemical compositions has resulted in remarkable activity toward oxygen evolution reaction (OER) which governs rechargeability of recently spotlighted metal–air batteries and regenerative fuel cells. For further development of highly OER active perovskite oxides, however, the exact mechanism the OER should be well understood. Herein, we introduce investigation of the OER mechanism of perovskite oxides by ab initio analysis based on well-defined model systems of LaMnO3 (LMO), LaCoO3 (LCO), and La0.5Sr0.5CoO3 (LSCO). In addition, we have systematically conducted electrochemical experiments from which we have observed an increasing trend in the OER activity in the order of LSCO > LCO > LMO. To validate the experimental results, free-energy diagrams have been constructed for oxygen intermediates on the surface of the defined models to find the limiting step by changing the B site atom (e.g., Mn and Co) and the partial displacement of Sr atoms in La site. (B6-2425)