Computational Materials Design for Developing High Performance Solid Oxide Fuel Cell Electrodes

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Abstract

Solid oxide fuel cells (SOFCs) operated at high temperature have received much interests as prospective device due to their high efficiency and fuel flexibility. For enhancing the SOFC performance, however, there are critical issues to be resolved. First, oxygen reduction kinetics and its transport are drastically suppressed at reduced temperature. Second, severe degradation observed in electrode deteriorates long-term stability. To tackle these problems, it is essential to rationally develop the materials of SOFC components. Unfortunately, it is not easy to completely achieve it by depending only on conventional experimental methods. In this presentation, we therefore introduce computational approaches to design SOFC electrode materials mainly based on density functional theory calculations. We believe that our computational study will play an important role in improving SOFC performance by guiding or complementing the relevant experiments.

Keywords: *Solid oxide fuel cell, Segregation, Exsolution, Alloys, Density functional theory*

Biography

Professor Han is an associate professor of chemical engineering at Pohang University of Science and Technology (POSTECH). He is also an editor of Molecular Catalysis, Elsevier. His research area is Computational Catalysis and Energy Materials, especially focusing on solid oxide fuel cell materials, electrocatalysts, automotive catalysts, and liquid organic hydrogen carrier. He has published ~100 papers including JACS, Nat. Commun, Energy Environ. Sci., and so on.