

European Chemistry Congress

June 16-18, 2016 Rome, Italy

Design of active and durable catalysts with non-precious materials for oxygen reduction and evolution reactions: First principles prediction and experimental validation

Byungchan Han

Yonsei University, Korea

Using first-principles density functional theory (DFT) calculations and experimental materialization, we design highly active and durable catalysts toward oxygen reduction reaction (ORR) with nonprecious Cu@N-C materials. DFT calculations indicate that encapsulated Cu metal by N-doped carbon shells is a promising electrocatalyst for ORR. To validate the prediction we synthesize three different types of catalysts with various applied processes: (i) hydrothermally treated “Cu@N-C(hydro)”, (ii) “Cu@N-C(heat)” heat-treated at $T = 1000\text{ }^{\circ}\text{C}$ for 2 h, and (iii) “Cu@N-C(CO₂)” oxidized by CO₂ for 15 min at $T = 1000\text{ }^{\circ}\text{C}$. It is shown that applying the CO₂ treatment can be a key process controlling electronic structures and shell thickness of the materials leading the high ORR catalytic performance. To alleviate the substantial overpotential problem in water splitting process storing the energy in fuels of O₂ and H₂ we develop hexagonal perovskite oxide with a transition metal of mixed oxidation states. Both computational prediction and experimental measurements consistently show that its performance is better than IrO₂.

Biography

Byungchan Han has completed his PhD in 2007 from MIT and Postdoctoral studies from Stanford University at Mechanical Engineering. He is an Associate Professor at Department of Chemical and Biomolecular Engineering in Yonsei University. His research interests are multi-scale computational design of emerging materials for renewable energy devices, and Materials Genome Project, and Machine Learning. He was chosen amongst 10 most leading young scientists in Korea and has published more than 40 SCI papers in reputed journals and has been serving as an Editorial Board Member of reputed journals.

bchan@yonsei.ac.kr

Notes: