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Understanding underlying chemistry for renewable energy materials and environmental remedies using first principles-based computational modelings

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First principles-based computational modelings propose key dscriptors and design concepts for discovering highly active materials in renewable energy system application. Density functional thoery calculations combined with statistical mechanical formalism identify optimum catalysts for oxygen (hydrogen) reduction (oxifation) and evolution reactions beyond concentional Pt used in fuel cell and Li-ion batteries. In this talk, the author will present the reaction mechanism of environmentally toxic gases with water and suggest how to remove them by designing efficient filters. Organic iodine and POCl3 are introduced as the examples.

Biography

Byungchan Han obtained his PhD degree in MIT at the Department of Material Science and Engineering. He was a Research Associate in MIT and Stanford University for four years. From 2015, he has been working at Yonsei University as an Associate Professor. His research interests are developing emerging energy materials for renewable energy devices. He was introduced as 10 most leading young scientists in the Korean newspaper. He was awarded a medal from International Advanced Association of Materials in 2016. He is an Associater Editor of *Scientific Reports*.

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