Solar-driven hydrogen production from water splitting

December 9 2021

Credit: Pixabay/CC0 Public Domain

For the sustainable development of humanity, future efforts are necessary to develop effective technologies to reduce fossil fuels. Solar-driven hydrogen production from water splitting can be an attractive way to supply clean energy. However, the efficiency of the water splitting is limited by the reaction at the anode. Therefore Qiuhua Liang investigated some promising anode materials that may help improve the efficiency of the water splitting.

The reaction that takes place at the anode is called oxygen evolution reaction (OER), which is often regarded as the main bottleneck in water splitting because it is a so-called four-electron transfer process. The efficiency of the OER relies heavily on the anode material. Qiuhua Liang found some anode materials that may increase the efficiency of the OER.

Traditional anode materials in water splitting

Over the last few decades, in order to increase the efficiency of the water splitting, oxides and nitrides of earth-abundant metals such as Fe2O3, TiO2, and GaN, have been widely studied as anode materials. However, these materials cannot boost the efficiency of the water-splitting further.

One of the main reasons is that they have a large overpotential. The OER at the anode includes four reaction steps, and it takes the total energy of 4.92 eV for the four reaction steps to proceed. The energy required for each step should ideally be one fourth of 4.92 eV. However, in reality, the energies involved in each step are usually not equally large, and the largest step with the free energy excess one fourth of 4.92 eV will define the overpotential.

The overpotential is used as the quantity determining the electrochemical activity. The smaller the overpotential value, the better the OER performance of the catalyst. This is similar to cooking. For example, if you cook four bowls of the same soup for four guests, the amount of salt given to you is certain. The salt that you put in each soup should be the same. Otherwise, if one bowl of soup is given too much salt, it is too salty, which is bad.

Alternatives

Qiuhua investigated some alternatives for the anode materials by molecular modeling. She found that by doping, the material has high overpotential can be tuned into low overpotential material. Doping can decrease the overpotential of the host and increase the water splitting activity. Similar to cooking, doping is like adding spices, such as basil or rosemary, which can make the soup tastier.

Qiuhua has investigated the transition metal (TM) doped 2D AlN/GaN and bulk ZnO for the OER by density function theory calculations (DFT). DFT is a computational quantum mechanical modeling method using functionals of the electron density, and it allowed her to give atomic-scale insight into the materials. The TM doped 2D AlN/GaN and bulk ZnO show much lower overpotentials than the undoped materials. Besides, RuO2 is one of the benchmark materials for OER, and is studied in detail to investigate the basis of its success for the OER.

In short, Qihuhua aimed to develop some alternatives to increase the efficiency of the water splitting catalysts and explain in detail why the materials show low overpotentials from atomic-scale insights.

Qiuhua Liang defended her thesis "First-principles study of electrode materials for oxygen evolution" on Wednesday 1st of December.

More information: Liang, Q. (2021). First-Principles Study of Electrode Materials for Oxygen Evolution. Eindhoven University of Technology. pure.tue.nl/ws/portalfiles/por … 0211201_Liang_hf.pdf

Provided by Eindhoven University of Technology