Theoretical study on interfacial properties for PEC electrode: improving STH efficiency and corrosion resistance

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PEC H_2 production is one of the most promising renewable energy solutions that address the issue of intermittent nature of solar energy. After the first demonstration by Fujishima and Honda in 1972 using the TiO_2 electrode,[1] extensive amount of researches have been performed in order to find the optimal electrode, which lead to the significant improvement in Solar-To-Hydrogen (STH) conversion efficiency based on the multi junction semiconductor cells whose surfaces are decorated with co-catalysts.[2,3] However, no electrode material tested to date has shown a satisfactory level of STH efficiency and of corrosion resistance simultaneously.

From the viewpoint of basic science, one of the challenging aspects of this problem, perhaps, is complex and dynamical nature of electrode-electrolyte interface: emersion of electrode to electrolyte itself would naturally oxidize the electrode surface, for which intended and/or un-intended impurities may or may not come into play. The chemical reactions of our interests, hydrogen evolution and corrosion, take place at the electrode-electrolyte interface, and therefore, it is extremely challenging to obtain the information on the microscopic mechanisms of these reactions by experiments or by theory.

The DOE/EERE PEC H_2 Production Working Group, Surface Validation Team, consisting of NREL, UNLV and LLNL sub teams, has been tackling this problem by combining the experimental characterization techniques using the state-of-art X-ray spectroscopy and large-scale ab-initio computer simulations using the high-performance computers: the electrodes used for H_2 production by the NREL team are characterized by the UNLV team and compared directly to simulation results provided by the LLNL team.

At the presentation, we will discuss on the recent findings on the interfacial properties and its potential implication to STH conversion efficiency and/or corrosion resistance.[4] We will also discuss on the interpretation of spectroscopic data for the $GaInP_2$ samples treated with nitrogen,[5] the method developed by the NREL team that has proved to improve the corrosion resistance significantly.[6]

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