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3D structured porous transition-metals poly-phosphides nano-needle arrays as an efficient bifunctional electrocatalyst for the evolution reaction of hydrogen and oxygen

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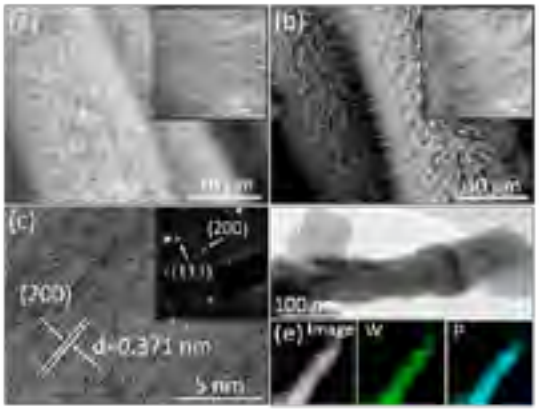
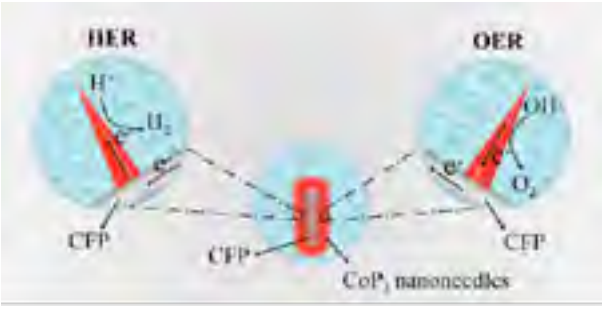
The design and development of high-efficiency and non-noble metal hydrogen evolution reaction (HER) electrocatalysts with optimized nanostructures for human clean and sustainable energy systems has attracted significant research interest over the past years. Herein, self-supported transition-metals poly-phosphides (TMP) (such as CoP3, WP2) nanoneedle arrays on carbon cloth were topotactically fabricated by *in situ* phosphidation of a transition-metals oxides nanoneedle arrays precursor. Such a binder-free flexible HER electrocatalysts with integrated three-dimensional nanostructures can not only provide a large surface area to expose abundant active sites, but also facilitate electrolyte penetration for electrons and electrolyte ions, which exhibit superior bifunctional electrocatalytic activity and durability for both the HER and OER. In addition, density functional theory (DFT) calculations indicate a low kinetic energy barrier for H atom adsorption on the TMP surface which guarantees the excellent catalytic activity of the catalyst. The excellent electrocatalytic activity makes the present 3D structured TMP electrocatalysts promising catalysts for large scale highly pure hydrogen evolution by electrochemical water splitting.





Biography

Shijian Chen is a Professor at Chongqing University. His research areas are wide-band-gap semiconductor based materials and devices; new energy materials and material design from the first-principles computational. His current research specifically focuses on new materials for production of hydrogen fuel from water. He has done his Post-doctoral Fellowship from Monash University from 2008 to 2012, and as an Alexander von Humboldt Research Fellow at University of Hannover from 2007-2008. He is the author of over 50 peer-reviewed publications with more than 1000 citations. He received his PhD from Chinese Academy of Sciences in 2006.

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