

Some reflections on the appropriate materials for PEC

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Photoelectrochemical decomposition of water for the generation of hydrogen has been studied for the past five decades in an intense manner without much success. Various authors have brought forth many governing principles for the selection of materials. The predominant view is the so called band gap engineering wherein the band gap of the semiconductor employed is modulated in a variety of ways like doping, coupling of the semiconductors or other methods of sensitization. In spite of this intense research, the necessary levels of percentage of decomposition of water for the process to be economically viable appear to elude the search. This situation has to be remedied soon since humanity is worried for the availability of appropriate energy conversion fuels.

It has been proposed that the ionicity of the metal oxygen bond in the case of oxide semiconductors is one of the parameters that has to be modulated which will facilitate the activation by visible light. However all the available semiconducting oxides possible to be used in water decomposition has ionic character above 60% or less than 20% and there are no materials so far tried which have percentage ionic character in the range 30-50%.

It is possible that the constructed system like semiconductors on graphene layers or on carbon substrates may be one of the ways of modulating ionic character of the semiconductor. However the available data especially the XPS data on the binding energy of the metal ion or oxide ion have not provided any clue in this direction. It may be worthwhile to revisit all these data from this point of view to find if this postulate has any relevance at all.

Essentially all surfaces are non native configuration of the bulk native configuration. This can be considered in the frame work of core shell model. The possibility of modulating the shell with respect to the thickness of the shell is another way of modulating the bonding characteristics of metal and oxygen.

This will be an worthwhile exercise if the available data in the literature are evaluated to test this hypothesis to carry it forward or to throw it away.