

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Theoretical modification of WO_3 for water splitting PREDRAG LAZIC, MARIA K. CHAN, RICKARD ARMIENTO, YABI WU, GERBRAND CEDER, Massachusetts Institute Of Technology — Using the sun's energy to produce hydrogen from water through photocatalytic process has been a dream since its first demonstration by Fujishima and Honda 40 years ago. Since then significant effort has been made to find a suitable material for this purpose but so far efficiency of the available materials is too low to be commercially interesting. However there are some promising candidates that have some very desirable properties for solar water splitting and their other properties are believed to be improvable by some changes in the material. One of such candidates is WO_3 which shows a very good light absorption and very high stability in aqueous environment. Unfortunately it also has a position of conduction band minimum slightly too low to support H^+/H_2 reaction of hydrogen evolution and also has a relatively large gap which prevents it from using a large part of solar spectrum and thus yielding a low efficiency for water splitting. We have tried to remedy those two problems by substitutions and codoping in the pure WO_3 material within the density functional theory. For some of the modifications we see improved material properties.

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Date submitted: 08 Dec 2010

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