

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Dissociation of Water on Ti-Decorated C nanostructures¹ YANG

LEI, Queen Mary, University of London, WENGUANG ZHU, Harvard University, SHENG MENG, University of Texas & ORNL, ZHENYU ZHANG, University of Tennessee & ORNL, ZHENGXIAO GUO, Queen Mary, University of London — Direct thermal splitting of water produces pure hydrogen but requires exceptionally high temperatures, making practical implementation challenging. Here we use first-principles simulations to show that water can dissociate on Ti decorated carbon nanostructures, such as graphenes and nanotubes. The behavior of water molecules approaching a Ti adatom is investigated. A single water molecule dissociates freely on a Ti-decorated graphene layer. A small energy barrier has to be overcome to dissociate a second water molecule, with the released H atoms readily combining to form H₂. As the number of water molecules further increases, the Ti adatom will dissociate from the graphene layer. We find similar results for when a Ti atom is adsorbed on a carbon nanotube. When more Ti atoms are adsorbed on the outside of the carbon nanotube, the energy barrier against dissociating water molecules is greatly decreased. We also explore the effects of replacing Ti by other potential catalytic elements.

¹Supported by UCDOE, USNSF, & EPSRC/UK-SHEC.

Yang Lei
Queen Mary, University of London

Date submitted: 21 Dec 2005

Electronic form version 1.4