Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Surface Hydroxyl Groups of Anodized TiO2 Nanotube for More Efficient Photoenergy Conversion[1] CHIUNG-YUAN LIN, JING-NENG YAO, National Chiao Tung University, Department of Electronics Engineering — Experimentalists can apply a hydrothermal crystallization method to the anodized TiO_2 nanotube-array. Structural transformation of the nanotubes is easily induced if the tubes are treated by hydrothermal solutions of different pH levels. Such transformation under the treatment of basic solutions, if not damaging the nanotubes, will in turn strongly enhance the anchoring of the carboxyls to the tube surface, and consequently improve the performance of the dye-sensitized solar cells with the TiO2 nanotubes being the photoelectrodes. In this work, we perform density-functional calculations of such nanotubes with different H^+ and OH^- attaching to the tube surface. The results provide a great deal of additional details of the tube morphology that is not accessible by the experiments, and reproduce the stability observed experimentally under the attachment of different functional groups.

[1]Supported by Taiwan National Science Council

Chiung-Yuan Lin
National Chiao Tung University, Department of Electronics Engineering

Date submitted: 08 Nov 2012 Electronic form version 1.4