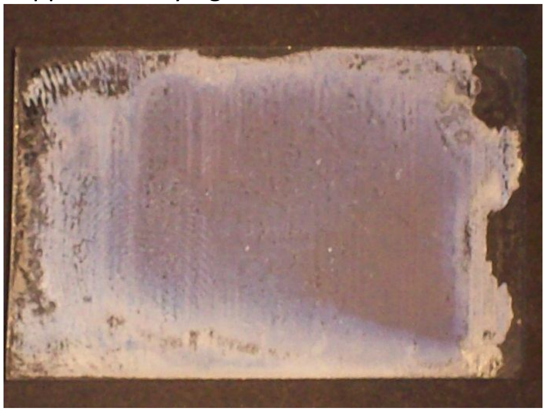
Hydrogen production by Tuning the Photonic Band Gap with the Electronic Band Gap of TiO_2

G.I.N. Waterhouse[a], A.K. Wahab[c], M. Al-Oufi[c], V. Jovic[a], D. Sun-Waterhouse[a], D.H. Anjum[d], J. Llorca[b] and H. Idriss[c]*

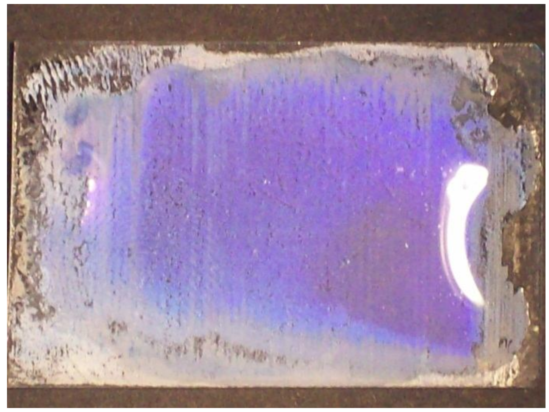
[a] School of Chemical Sciences, University of Auckland, New Zealand.
[b] Institute of Energy Technologies and Centre for Research in NanoEngineering, Technical University of Catalonia, Barcelona, Spain.
[c,]*SABIC Research Centres, Riyadh and KAUST, Saudi Arabia and the University of Aberdeen (UK).
[d] KAUST, Thuwal, Saudi Arabia

*Email: idrissh@sabic.com; h.idriss@abdn.ac.uk

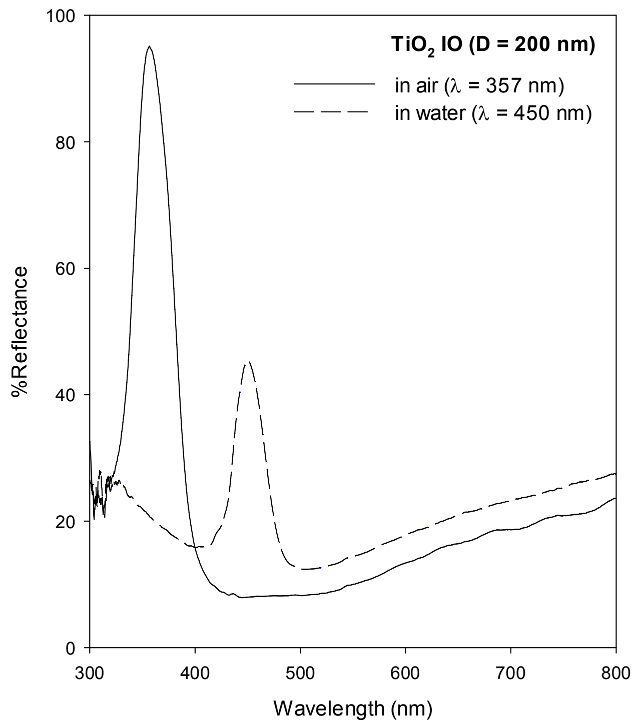
Supplementary figures



TiO_2 inverse opal (D = 200 nm) in air

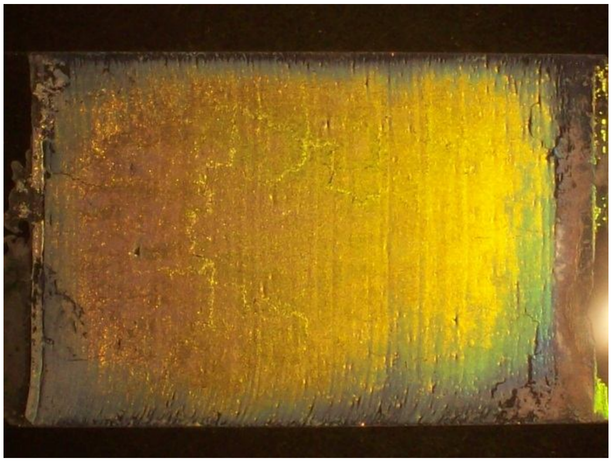


TiO_2 inverse opal (D = 200 nm) in water

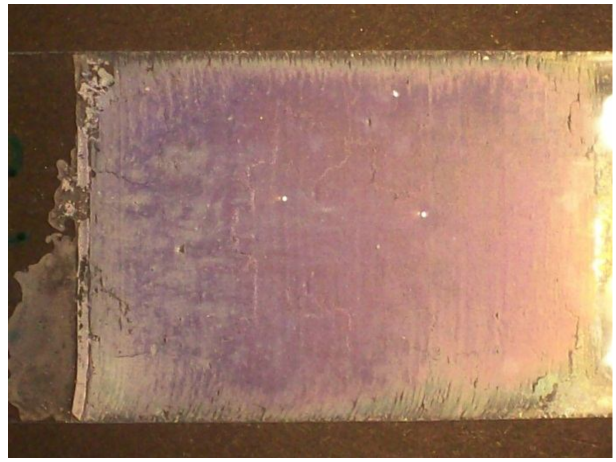


S1

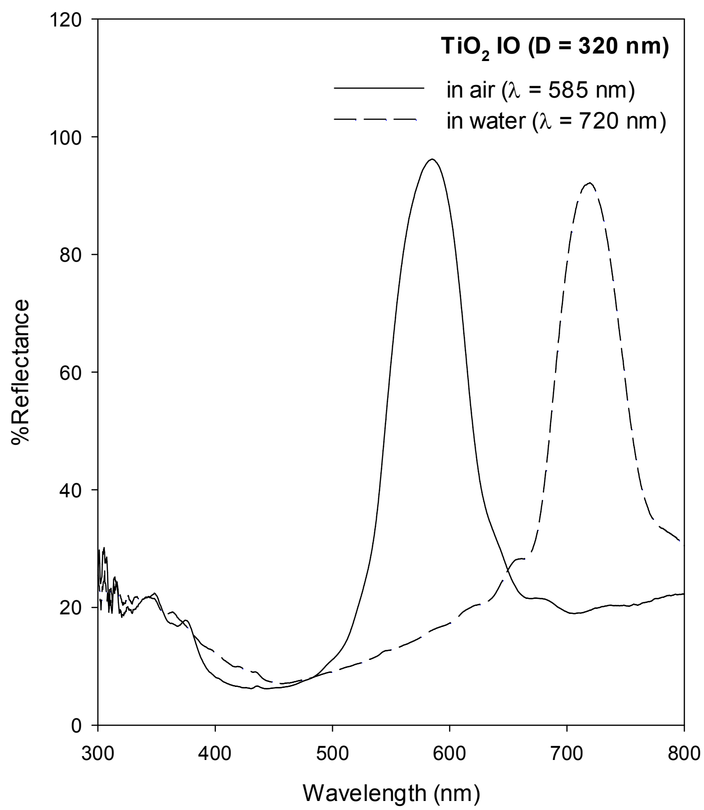
UV-Vis reflectance spectra for a TiO_2 inverse opal with macropore diameter (D) = 200 nm in air (n = 1.00) and in water (n = 1.34). The spectra were collected along the [111] direction of a TiO_2 inverse opal thin film. The PBG for Bragg diffraction on f.c.c. (111) planes is observed at 357 nm in air, and 450 nm in water. The shift in the PBG on immersion of the inverse opal in water results from an increase in the average refractive index of the photonic crystal when it is filled with water. The attenuation of the reflectance peak in water is due to increased scattering of light and a decrease in refractive index contrast between titania (n = 2.1-2.3 for sol-gel derived anatase) and the medium filling the macropores.



TiO_2 inverse opal (D = 320 nm) in air

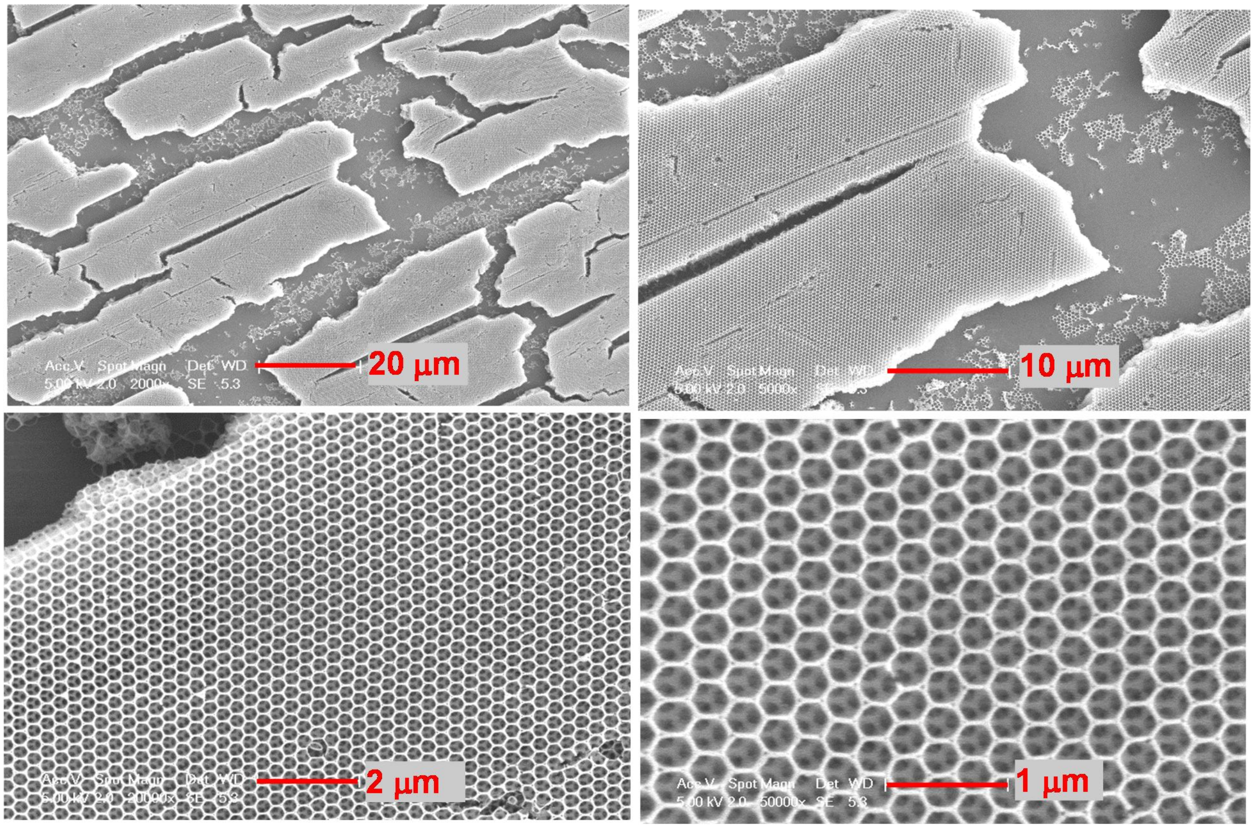


TiO_2 inverse opal (D = 320 nm) in water



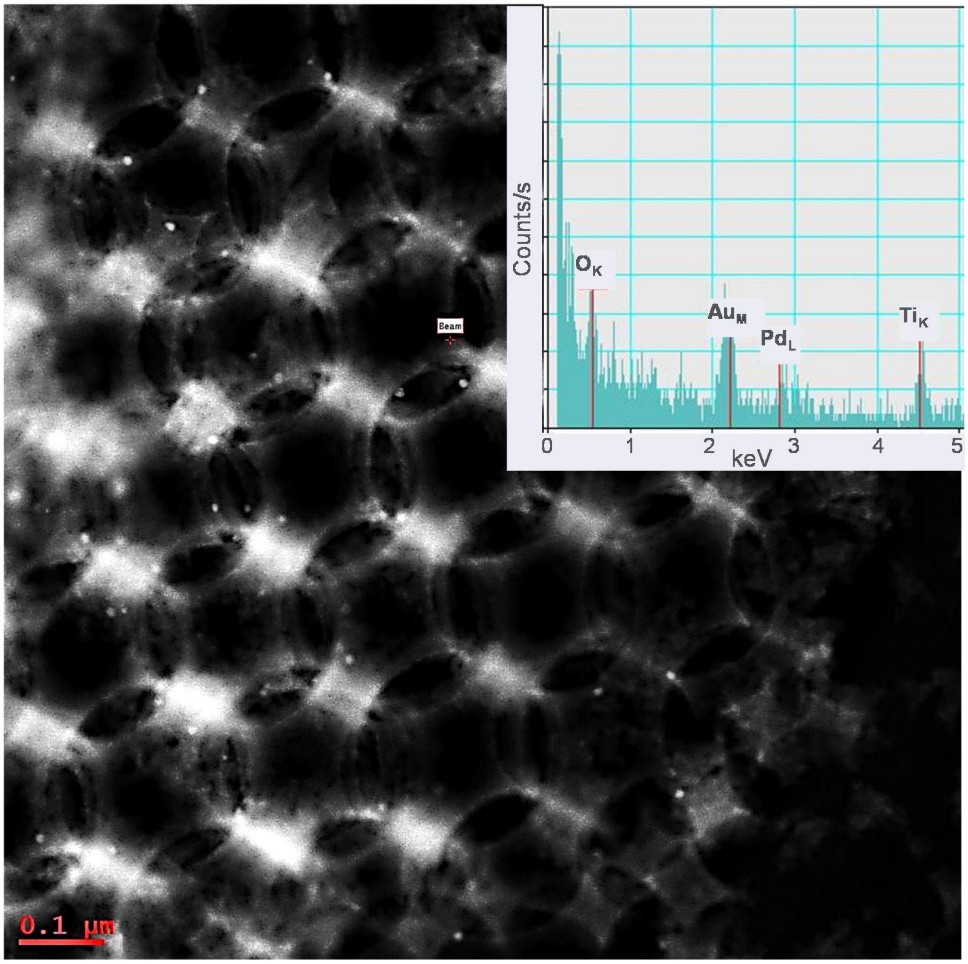
S2

UV-Vis reflectance spectra for a TiO_2 inverse opal with macropore diameter (D) = 320 nm in air (n = 1.00) and in water (n = 1.34). The spectra were collected along the [111] direction of a TiO_2 inverse opal thin film. The PBG for Bragg diffraction on f.c.c. (111) planes is observed at 585 nm in air, and 721 nm in water. The shift in the PBG on immersion of the inverse opal in water results from an increase in the average refractive index of the photonic crystal when it is filled with water.



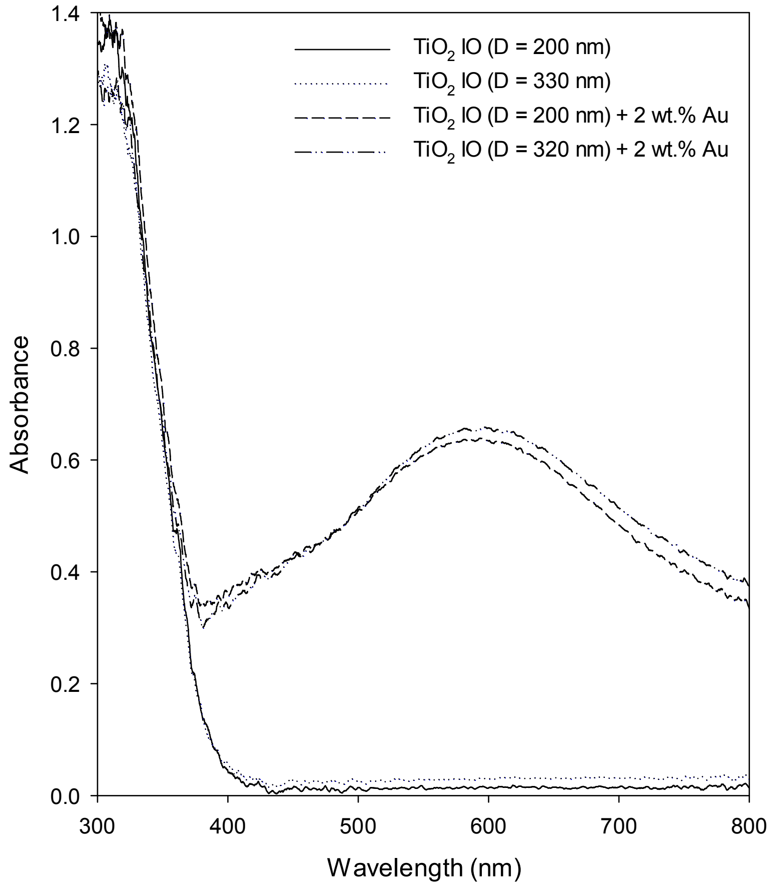
S3

SEM images of PBG 585 nm Inverse Opal TiO_2 a the indicated magnification.



S-4

Dark Field Transmission Electron Microscopy of 0.5 wt% Au-0.5 wt.% Pd/TiO_2. The bright dots are those of Au and Pd metals. Inset: EDS analysis indicating the presence of both Au and Pd.



S5

UV-Vis absorbance spectra for TiO_2 inverse opal powders with macropore diameters of 200 nm and 320 nm in air. The spectra show strong absorption below 400 nm due to anatase TiO_2. PBGs are not seen in the spectra because the lattice planes are randomly oriented and the PBGs are broad due to the high refractive index of TiO_2. Deposition of gold nanoparticles on the TiO_2 supports gives rise to intense absorption bands at ~580 nm due to the gold surface plasmon resonance, which contributes to the high photocatalytic activity of these samples under direct sunlight.

Example of calculations of the photons conversion under direct sun light excitation.

S6

From figure 2 hydrogen production at about 500 minutes is ca. 5×10^{-4} mol/g of catalyst at a UV flux close to 0.5 mW/cm^2 (as upper limit). The flux converted to number of photons using Plank's equation (at a wavelength average of 360 nm) = 5.5×10^{14} photons per second hitting the area of the catalyst inside the reactor, at the maximum (catalyst amount 25 mg in 200 mL reactor). The amount of hydrogen produced per second is about 2.5×10^{14} molecules. Since each hydrogen molecule needs two electron to form two photons are involved. Therefore the total number of photons consumed is 5×10^{14}. Dividing the number of photons consumed by the number of photons hitting the catalyst gives about full conversion of the UV light.