

*Supplementary Material*

**Hydrogen and propane production from butyric acid photoreforming  
over Pt-TiO<sub>2</sub>**

**Gabriele Scandura<sup>1,2</sup>, Jorge Rodríguez<sup>1</sup>, Giovanni Palmisano<sup>1,2\*</sup>**

<sup>1</sup>Department of Chemical Engineering, Khalifa University, Masdar Institute Campus , PO Box 54224, Abu Dhabi, United Arab Emirates.

<sup>2</sup>Research and Innovation Center on CO<sub>2</sub> and H<sub>2</sub> (RICH), Khalifa University, P.O. Box 127788, Abu Dhabi, United Arab Emirates.

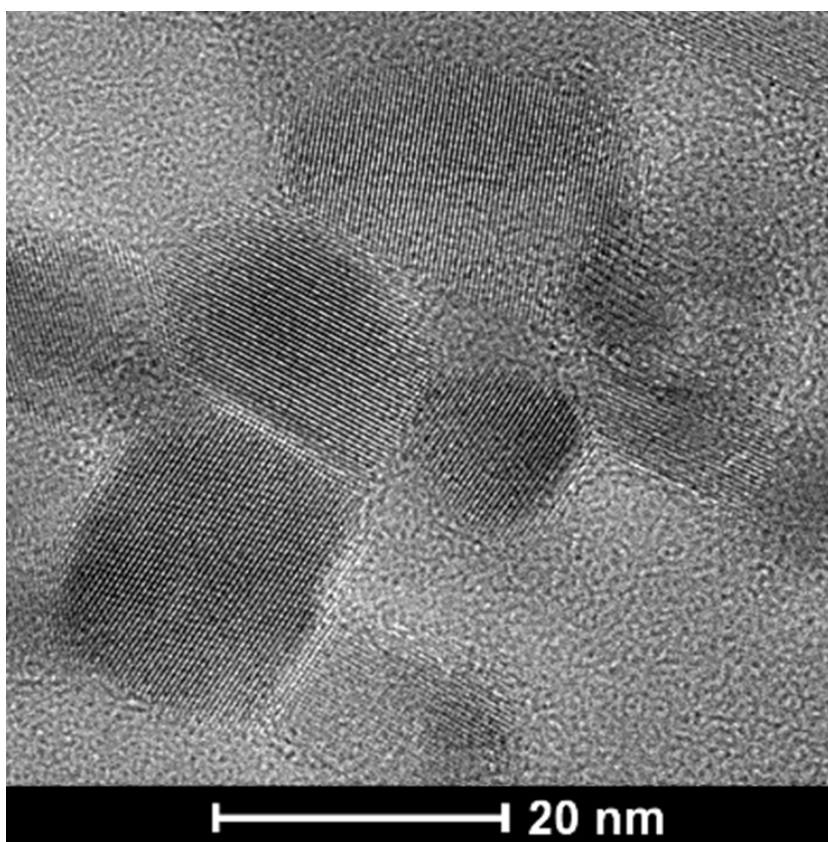
**\* Correspondence:**

Giovanni Palmisano

giovanni.palmisano@ku.ac.ae

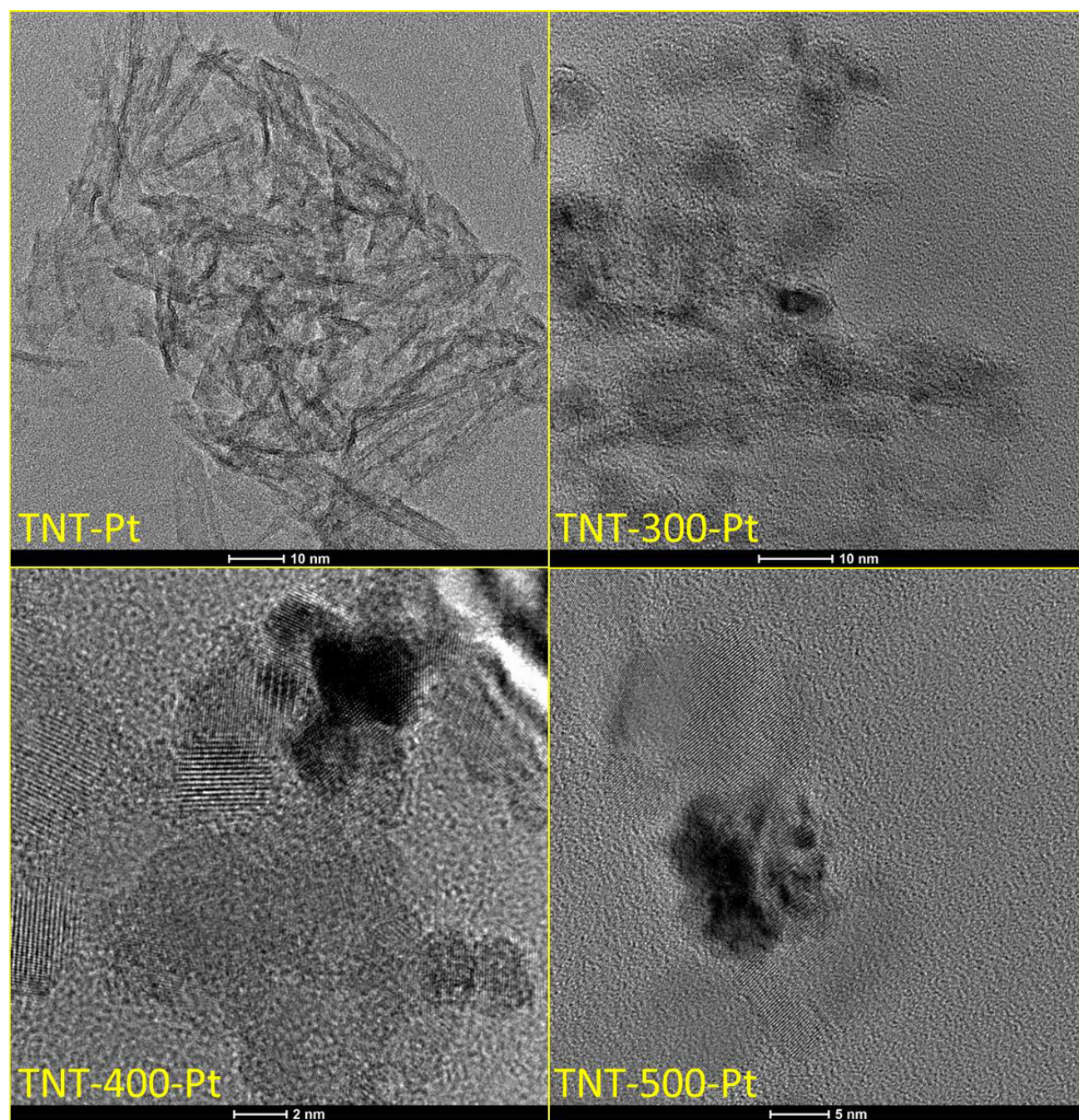


**Supplementary Figure 1.** Picture of the reaction system used for the photocatalytic runs.

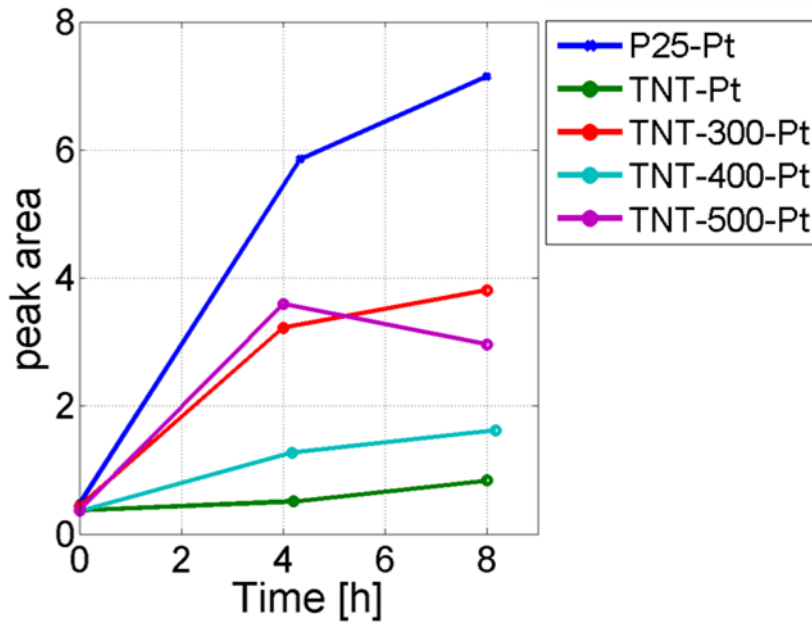


**Supplementary Figure 2.** TEM image at high magnification of TNT-400.





**Supplementary Figure 3.** TEM images of TNT and TNT calcined at different temperature and decorated with platinum.



**Supplementary Figure 4.** Peak area from the HPLC chromatogram of a significant unknown reaction by-product.

### Material balances details

The concentration of methane ( $[CH_4]$ ), ethane ( $[C_2H_6]$ ), propane ( $[C_3H_8]$ ) and  $CO_2$  in gas phase were obtained through GC analysis and multiplied by the total gas volume in the reactor. Similarly, the concentration of butyric acid ( $[BA]$ ), given by HPLC, was multiplied by the total liquid volume in the reactor. The amount of  $CO_2$  dissolved in water ( $[CO_2]_L$ ) was calculated by means of Henry's law, knowing the concentration of  $CO_2$  in the reactor headspace ( $[CO_2]_G$ ), the room temperature and the pH of the solution (3.61).

The quantities in table 5 (in the manuscript) were computed as follows:

$$C_{BA,R} = ([BA]_0 - [BA]_f) * V_L * 4$$

$$TOC_R = (TOC_0 - TOC_f) * V_L / AW_C$$

$$C_{BA,R} = C_{KT} + C_{UT}$$

$$C_{KT} = C_{KL} + C_{KG}$$

$$C_{UT} = C_{UL} + C_{UG}$$

$$C_{KL} = [CO_2]_L$$

$$C_{KG} = ([CH_4] + [C_2H_6] * 2 + [C_3H_8] * 3 + [CO_2]_G) * V_G$$

$$C_{UL} = TOC_{BA,R} - TOC_R$$

$$C_{UG} = TOC_R - C_{KG} - [CO_2]_L$$

where:

$AW_C$  = carbon atomic weight

$V_L$  = total liquid volume in the reactor

$V_G$  = total gas volume in the reactor

$C_{BA,R}$  = carbon as BA reacted (mol C)

$TOC_0$  = initial total organic carbon in liquid phase (mg/L)

$TOC_f$  = final total organic carbon in liquid phase (mg/L)

$TOC_R$  = TOC reacted (mol C)

$C_{KT}$  = total carbon as known product (mol C)

$C_{UT}$  = total carbon as unknown products (mol C)

$C_{KL}$  = carbon known products in liquid phase (mol C)

$C_{KG}$  = carbon as methane+ethane+propane+CO<sub>2</sub> in gaseous phase (mol C)

$C_{UL}$  = carbon as unknown products in liquid phase (mol C)

$C_{UG}$  = carbon as unknown products in gaseous phase (mol C)

$C_{KT}$ ,  $C_{KL}$ ,  $C_{KG}$ ,  $C_{UT}$ ,  $C_{UL}$ ,  $C_{UG}$  can also be given as fraction (%) of  $C_{BA,R}$ .