Available online 8 October 2020, 127250
Chemical Engineering Journal
PREPRINT

Supporting Information

A novel gas flow-through photocatalytic reactor based on copper-functionalized nanomembranes for the photoreduction of CO_2 to C1-C2 carboxylic acids and C1-C3 alcohols

Daniele Giusi[a], Claudio Ampelli[a,*], Chiara Genovese[b], Siglinda Perathoner[a] and Gabriele Centi[b]

[a] *University of Messina, ERIC aisbl and CASPE/INSTM, Dpt. ChiBioFarAm, viale F. Stagno d'Alcontres 31, 98166 Messina, Italy*

[b] *University of Messina, ERIC aisbl and CASPE/INSTM, Dpt. MIFT, viale F. Stagno d'Alcontres 31, 98166 Messina, Italy*

[*] ampellic@unime.it

https://www.sciencedirect.com/science/article/pii/S1385894720333751
https://doi.org/10.1016/j.cej.2020.127250

Calculation of Apparent Quantum Yield (AQY)

The Apparent quantum yield (AQY) is defined as the ratio of number of reacted electrons to the number of incident photons.

It can be calculated by the following equation:

$$AQY\% = \frac{Number\ of\ reacted\ electrons}{Number\ of\ incident\ photons}\ x\ 100$$

The number of incident photons is given by:

$$Number\ of\ incident\ photons = \frac{Light\ absorbed\ by\ the\ photocatalyst}{Average\ photon\ energy} x\ t$$

where

Light absorbed by the photocatalyst = 0.064 W cm^{-2}

t = 5 h (reaction time)

$$Average\ photon\ energy = \frac{hc}{\lambda}$$

with

h (Planck's constant) = 6.626 10^{-34} J s

c = 3 10^{8} m s^{-1}

The value of λ has been calculated as the average wavelength of the broadband light source (335 10^{-9} m)

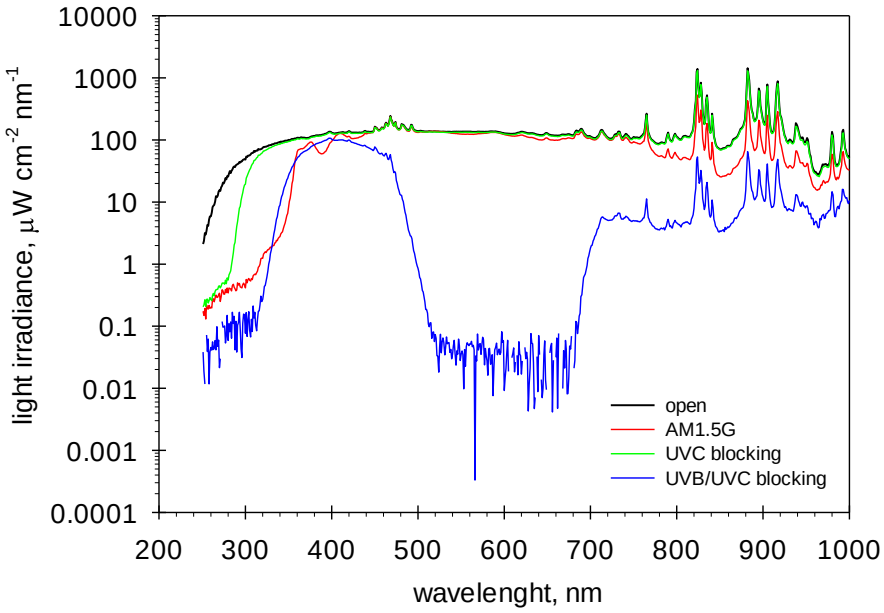

Figure S1: Light spectral irradiance vs. wavelength with different cut-off light filters by using a 300 W Xe-arc lamp.

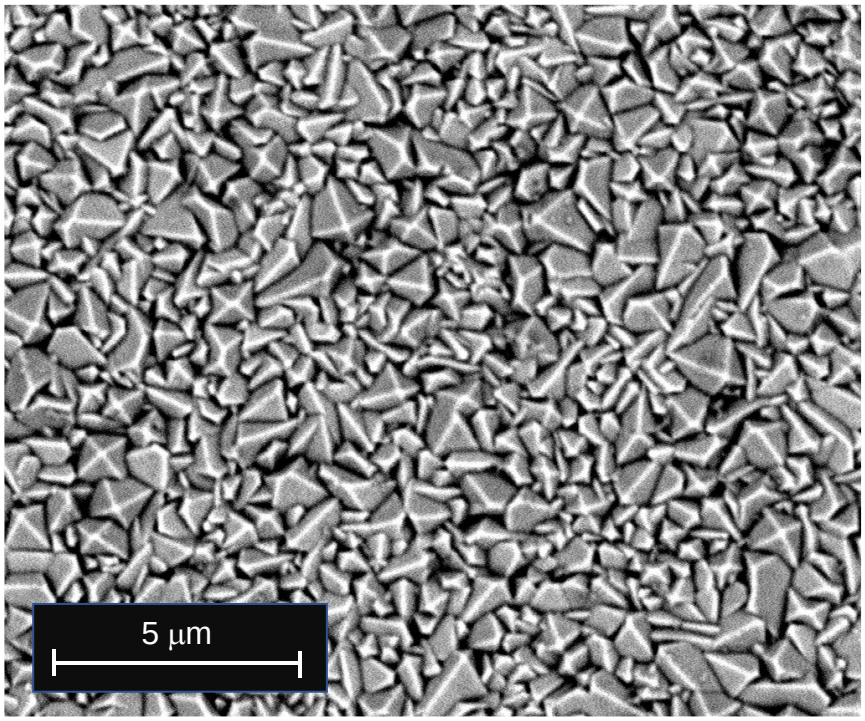

Figure S2: SEM images of *p*-type Cu_2O layer grown on metallic Ti layer (*Cu_2O/Ti p-type*).

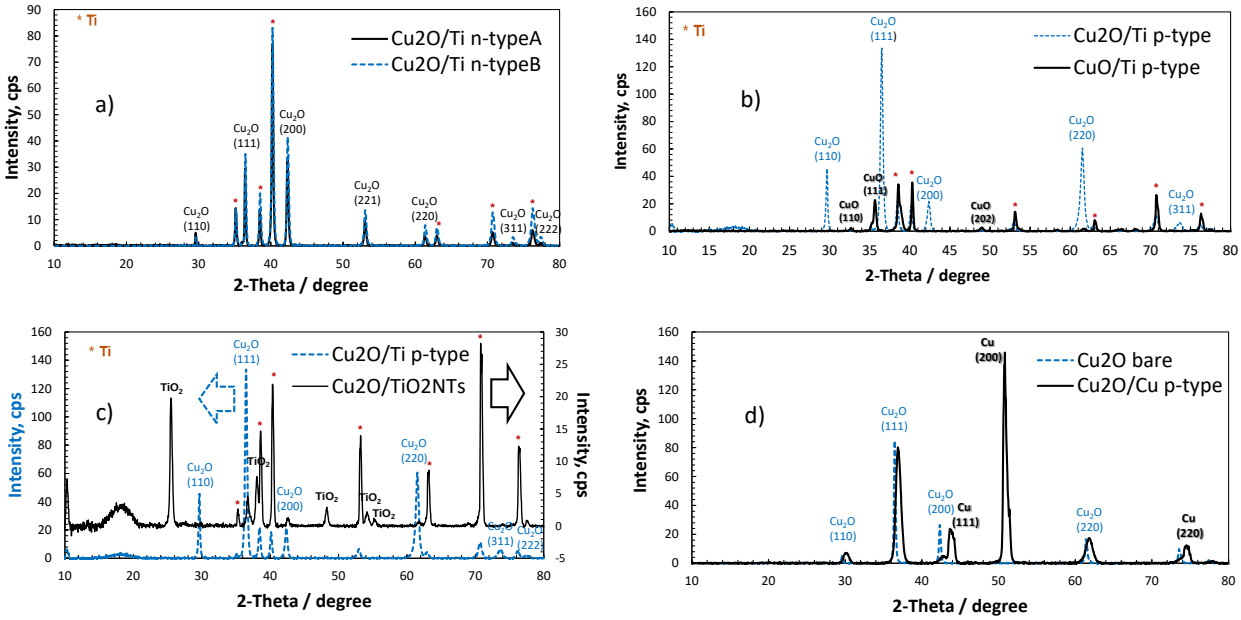

Figure S3: Comparison of X-ray diffraction patterns between: a) *Cu_2O/Ti n-typeA* and *Cu_2O/Ti n-typeB*, b) *Cu_2O/Ti p-type* and *CuO/Ti p-type*, c) *Cu_2O/Ti p-type* and *Cu_2O/TiO_2NTs p-n*, and d) *Cu_2O/Cu p-type* and *bare Cu*.

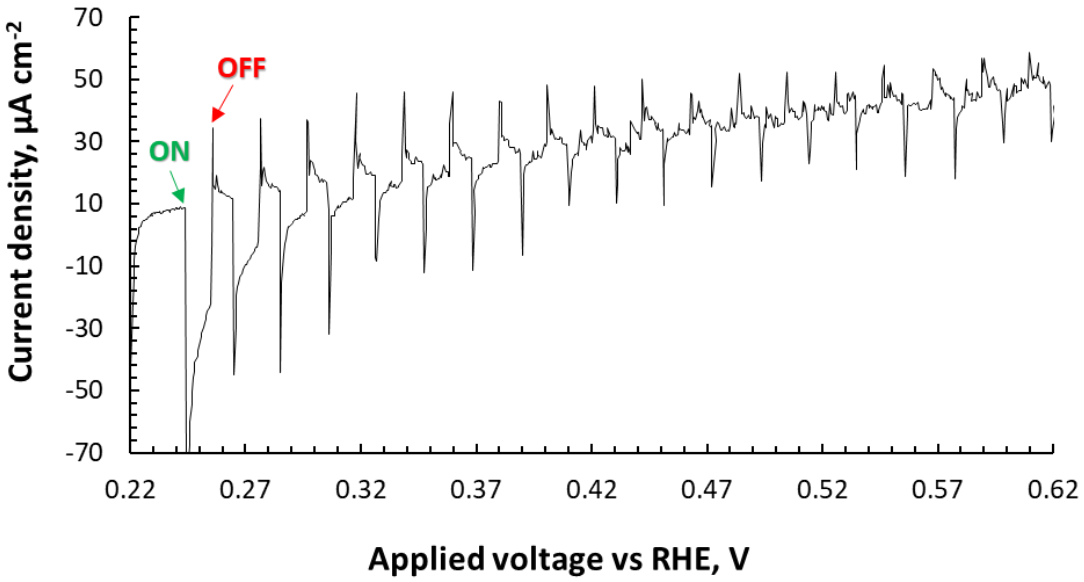

Figure S4: Current density vs. applied voltage for *Cu_2O/Cu p-type* layer under ON/OFF pulsing cycles of light irradiation (scan rate: 10 mV s^{-1}).

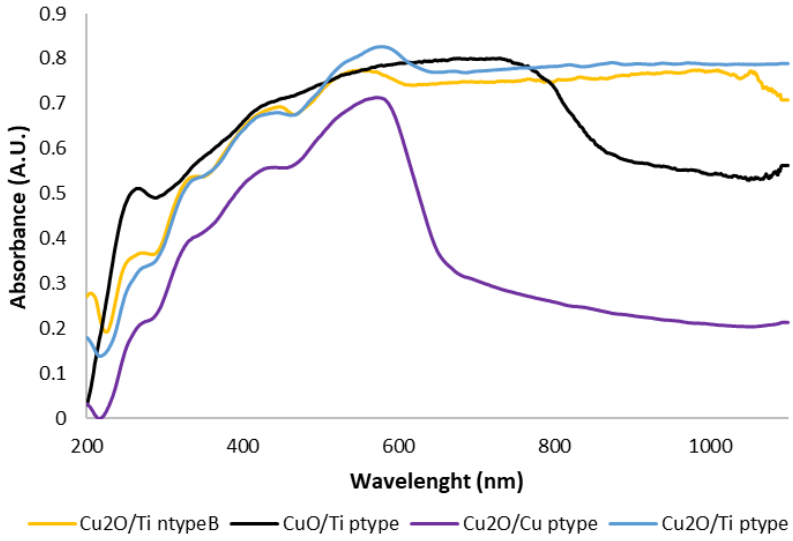

Figure S5: UV-visible diffuse reflectance spectra of *Cu_2O/Ti n-typeB*, *Cu_2O/Ti p-type*, *Cu_2O/Cu p-type* and *CuO/Ti p-type* samples.

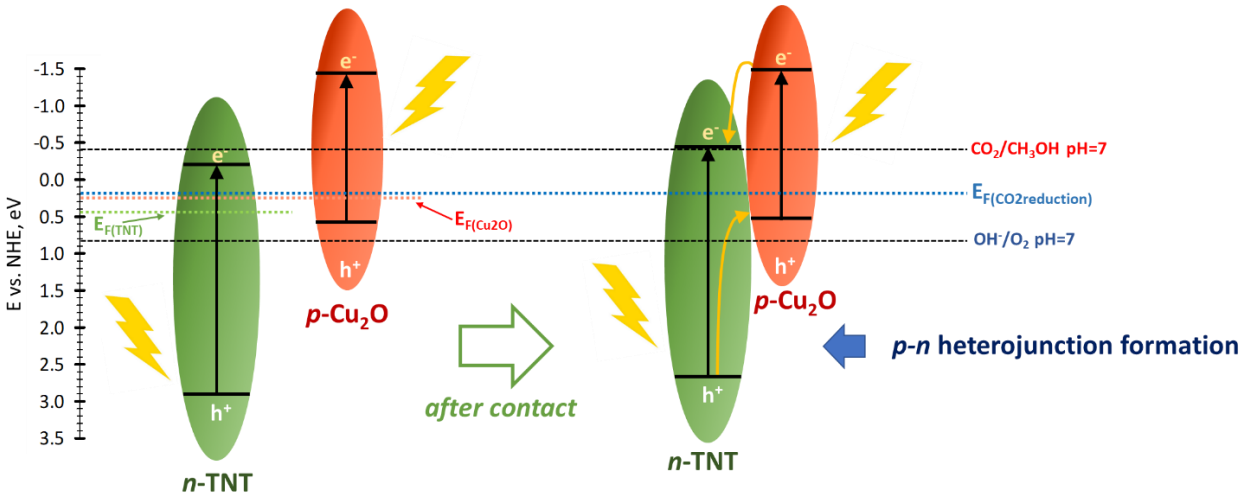

Figure S6: Band alignment of TNT and Cu_2O bands after contact with formation of a *p-n* heterojunction.

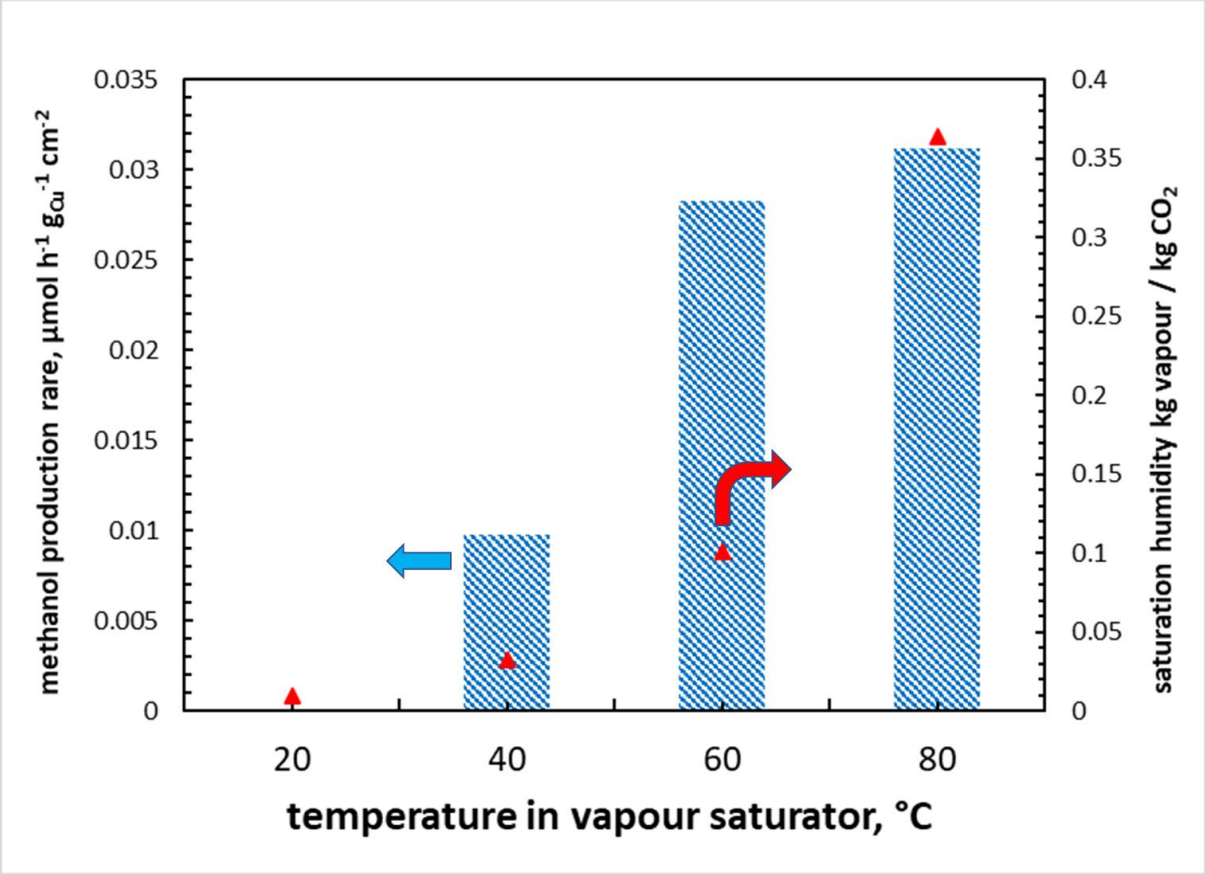

Figure S7: Methanol production rate vs. temperature in the vapour saturator for *Cu_2O/Ti p-type* sample. Saturation humidity values in the inlet gas flow are also reported.

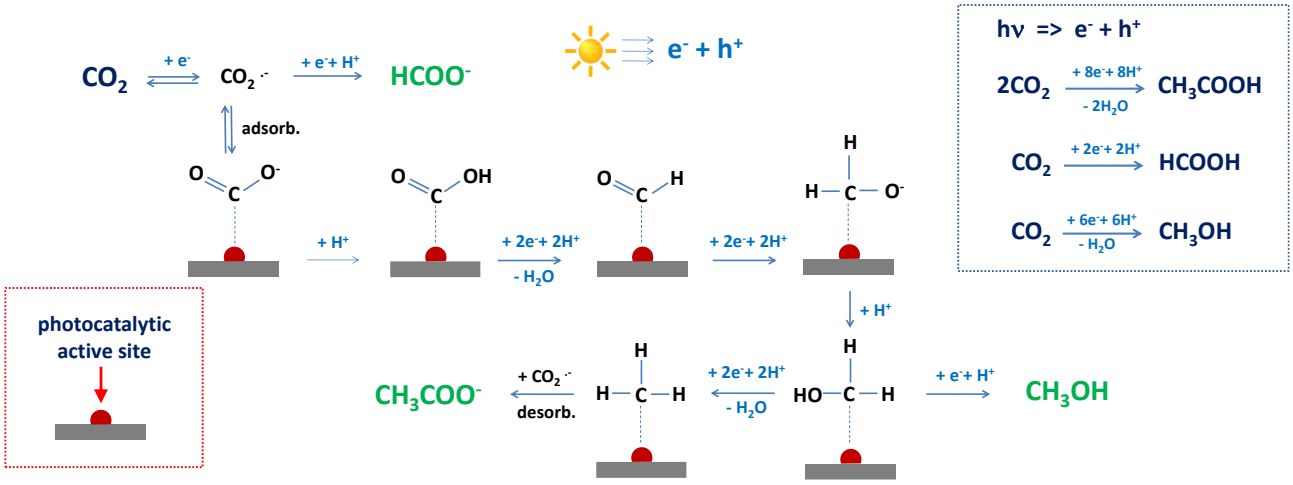

Figure S8: Schematic mechanistic pathway for the photocatalytic production of formic acid, acetic acid and methanol on Cu_xO-TNT electrodes. Adapted from [1].

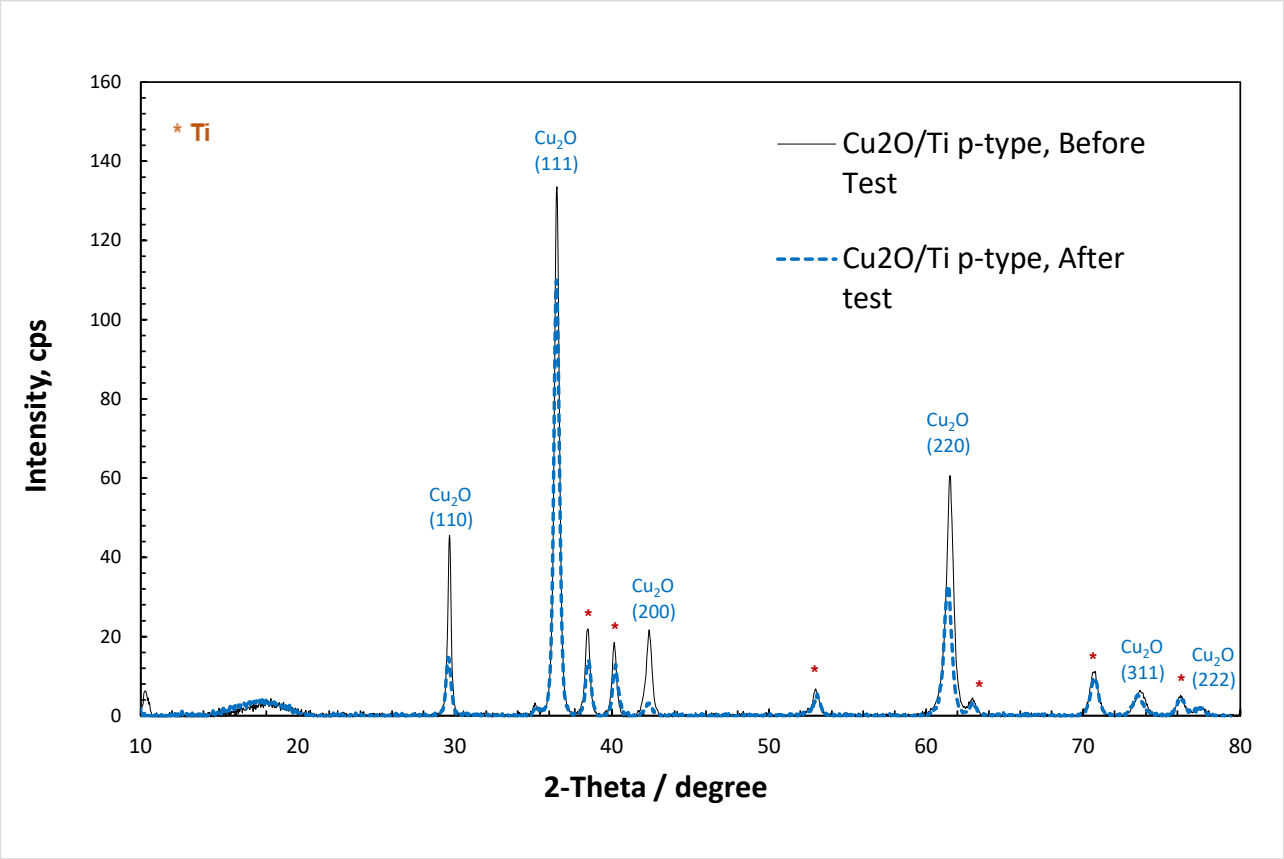

Figure S9: Comparison of X-ray diffraction patterns of fresh and used *Cu_2O/Ti p-type* photocatalyst.

References

[1] C. Genovese, C. Ampelli, S. Perathoner, G. Centi, Mechanism of C–C bond formation in the electrocatalytic reduction of CO_2 to acetic acid. A challenging reaction to use renewable energy with chemistry, Green Chem., 19 (2017) 2406-2415.