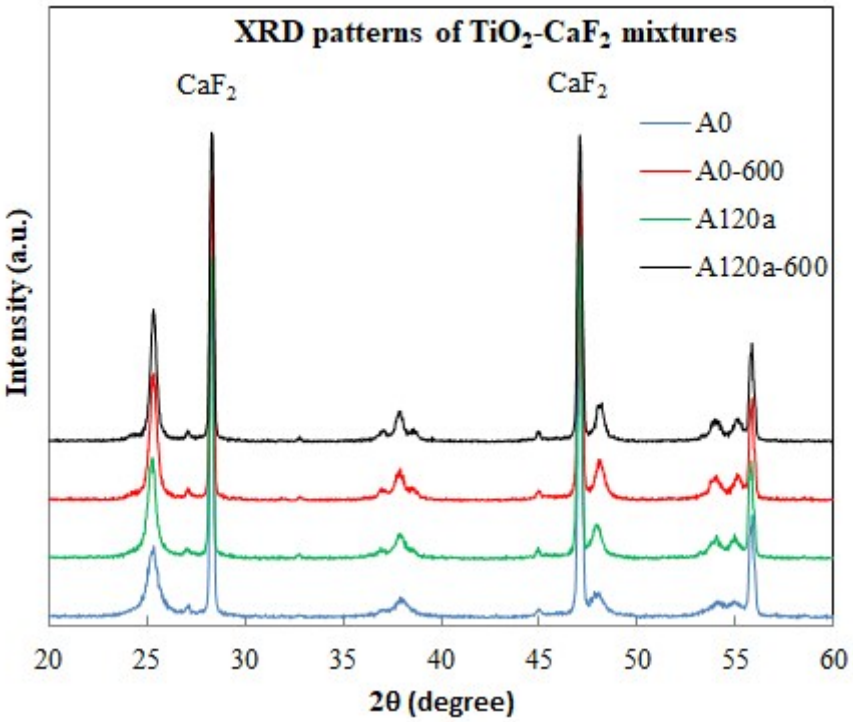
Electronic Supplementary Material (ESI) for Catalysis Science & Technology.


# Supplementary Information

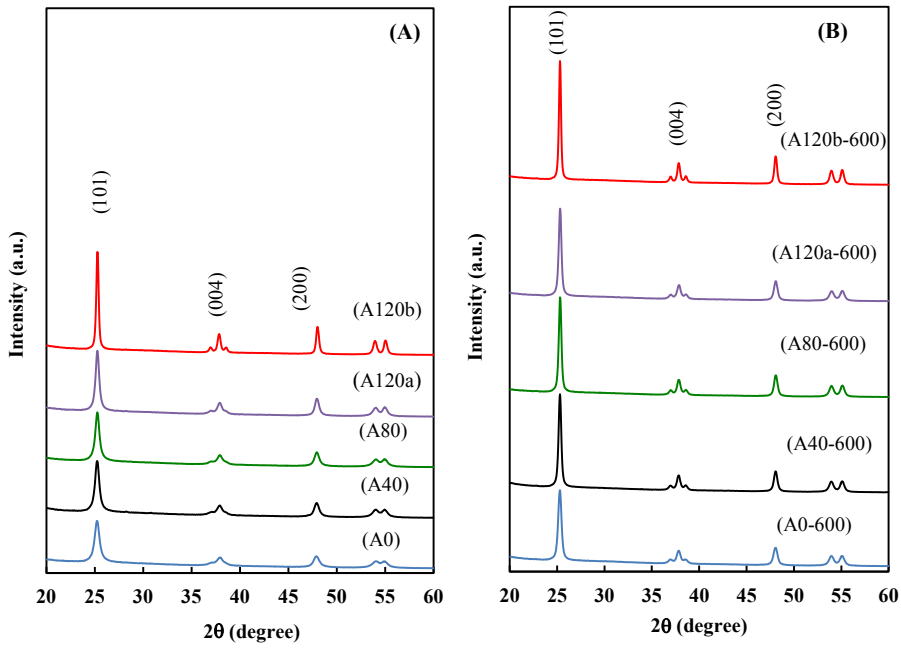
Manuscript ID: CY-ART-11-2017-002382.R1

Influence of fluorine in the synthesis of anatase $TiO_2$ for photocatalytic partial oxidation: are exposed facets the main actors?



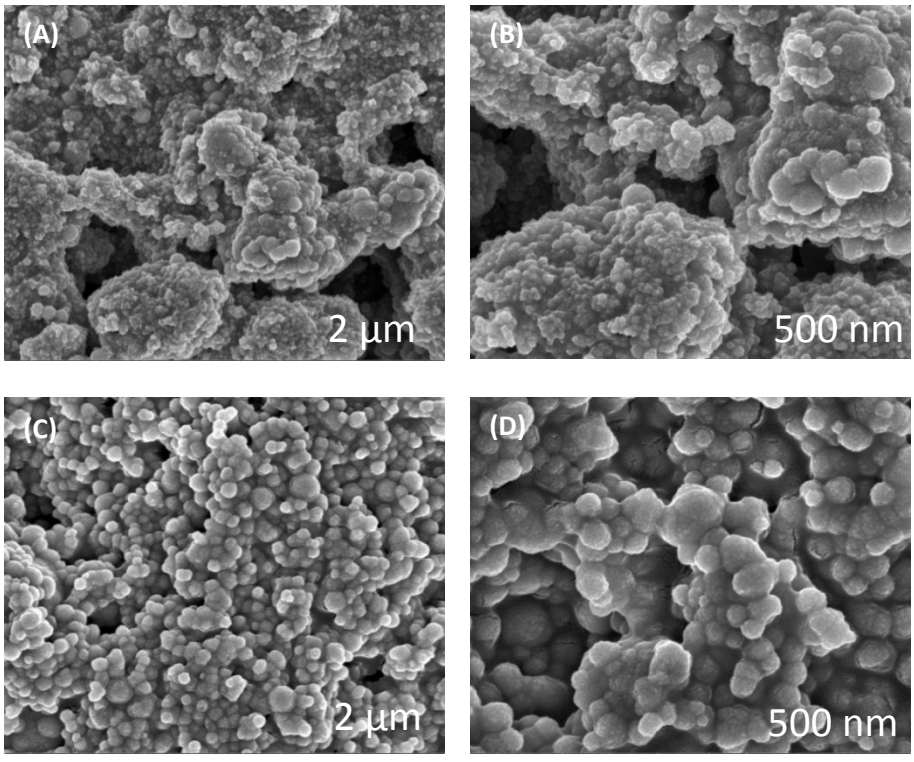

S1: XRD patterns of some representative $TiO_2$-$CaF_2$ mixtures.

All of the prepared samples (S2) consisted of pure anatase $TiO_2$.

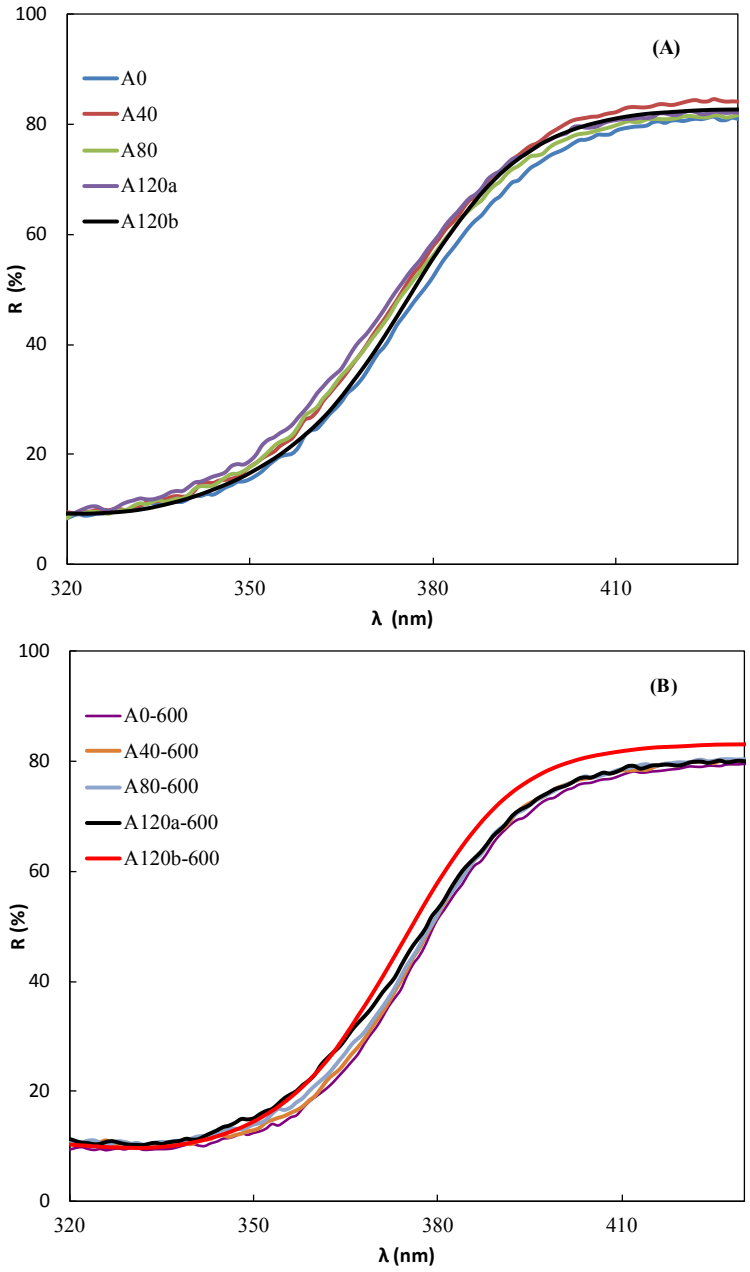



S2. XRD patterns of the used samples. The anatase (101), (004) and (200) main reflection peaks are indicated. Notably, the same scale was used in the two figures to highlight the different crystallinity of the different samples.

SEM observations, Figure S3 revealed that all the samples presented irregular shapes and consisted of aggregates of small roundish particles.

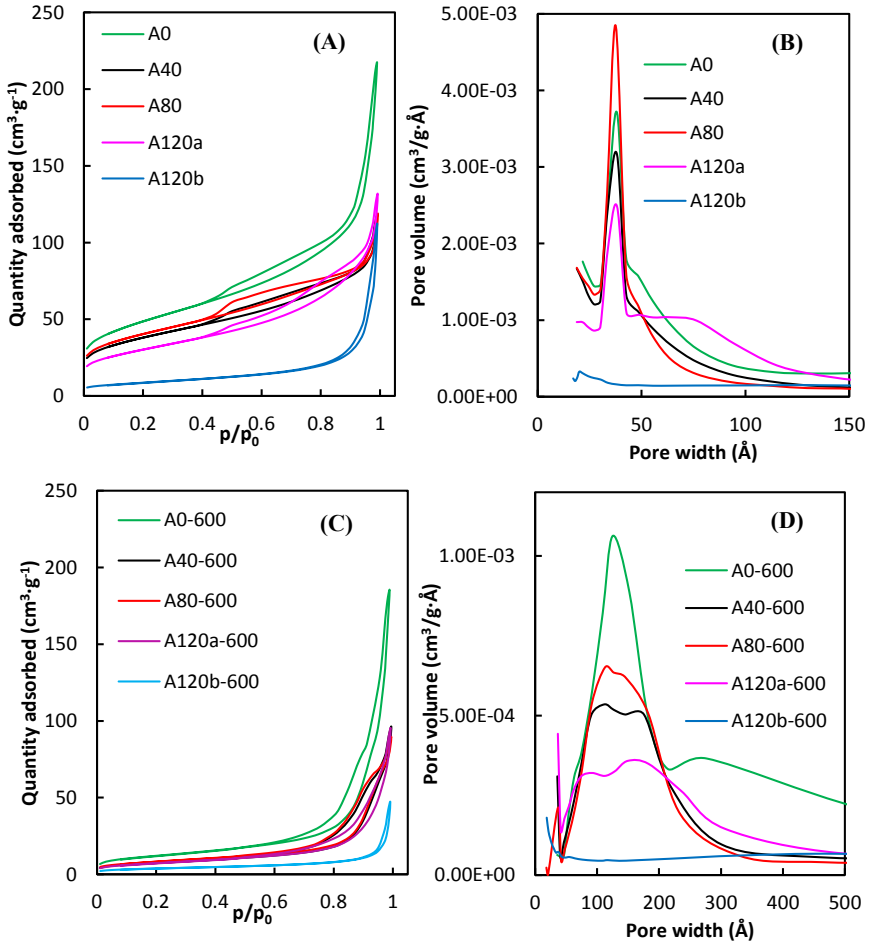



S3. SEM images of the samples: A0 (A) and (B); A120a (C) and (D).




S4: DRS spectra of uncalcined (A) and calcined samples (B).

In Figure S5 the nitrogen adsorption-desorption isotherms at −196 ◦C and the pore size distribution are reported for all of the samples. All of the curves can be classified as type IV isotherms with hysteresis loop associated to H3 type.




S5. $N_2$ adsorption-desorption isotherms and pores size distribution of the various samples.

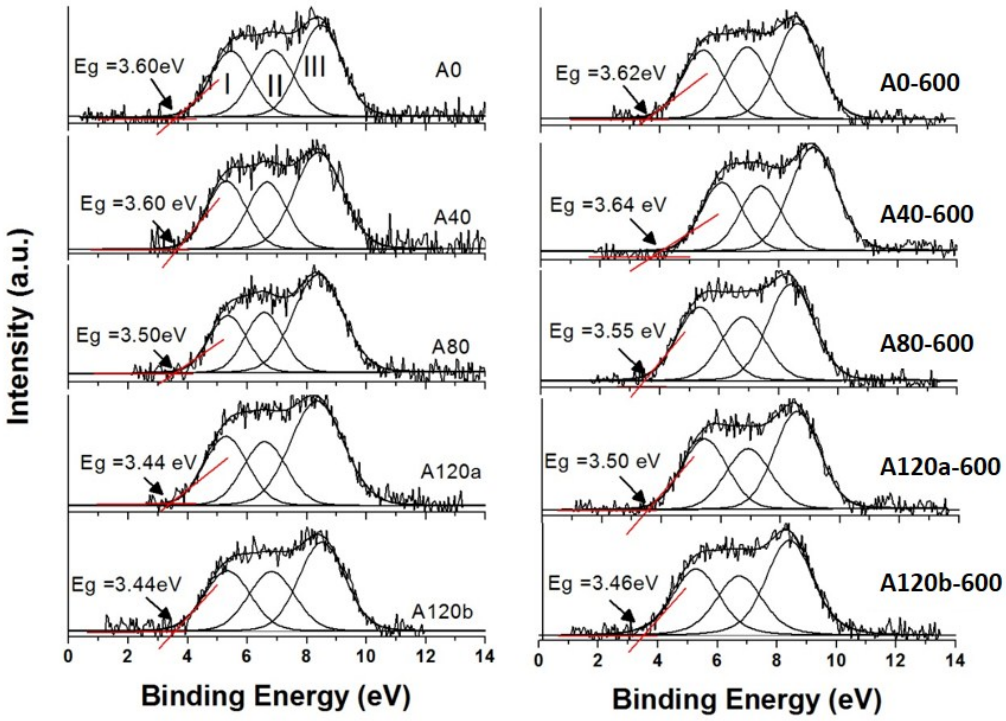



Figure S6. XPS valence band spectra excited by Al Kα radiation. The extrapolation of the VBE is indicated.

Table S1: Band-gap values and valence and conduction band edges of all the samples.

| Sample | Band-Gap (eV) | VBE(eV) | CBE (eV) |
|---|---|---|---|
| A0 | 3.16 | 3.6 | 0.44 |
| A40 | 3.18 | 3.6 | 0.42 |
| A80 | 3.19 | 3.5 | 0.31 |
| A120a | 3.2 | 3.44 | 0.24 |
| A120b | 3.18 | 3.44 | 0.26 |
| A0-600 | 3.18 | 3.62 | 0.44 |
| A40-600 | 3.18 | 3.64 | 0.46 |
| A80-600 | 3.18 | 3.55 | 0.37 |
| A120a-600 | 3.17 | 3.5 | 0.33 |
| A120b-600 | 3.21 | 3.46 | 0.25 |

Table S2: 4-MBA conversion and 4-MBAl selectivity after 240 min of irradiation in the presence of the sample A80.

| **Sample** | **Run** | **$X_{t=240}$ (%)** | **$S_{t=240}$ (%)** |
|---|---|---|---|
| A80 | 1st | 23.0 | 56.4 |
| A80 | 2nd | 25.4 | 55.3 |
| A80 | 3th | 25.5 | 51.1 |