Supplementary information

Photocatalytic and Electrically Conductive Transparent Cl-doped ZnO thin films *via* Aerosol Assisted Chemical Vapour Deposition

Arreerat Jiamprasertboon,[a,b] Michael J. Powell,[b] Sebastian C. Dixon,[b] Raul Quesada-Cabrera,[b]Abdullah M. Alotaibi,[b] Yao Lu,[c] Aoyun Zhuang,[b] Sanjayan Sathasivam,[b] Theeranun Siritanon,[a] Ivan P. Parkin[b] and Claire J. Carmalt[b,*]

[a] School of Chemistry, Institute of Science, Suranaree University of Technology, 111 University Avenue, Muang, Nakhon Ratchasima, 30000, Thailand

[b] Material Chemistry Centre, Department of Chemistry, University College London, 20 Gordon Street, London, WC1H 0AJ, UK

[c] Department of Mechanical Engineering, University College London, London, WC1E 7JE, United Kingdom

Film synthesis

All Cl-doped ZnO films were obtained as present in Figure 1. More details were described in main text.

Figure 1 The photographs of all synthesised films: undoped ZnO film (a) and Cl-doped ZnO films with corresponding mol% $FeCl_3$ of 1 (b), 3 (c), 5 (d), 7 (e), 10 (f) and 15 (g).

XPS analysis for at.%Cl in films

To obtain the at.%Cl, the fitting analysis of $Cl2p_{3/2}$ and $Zn2p_{3/2}$ were performed and the obtained peak areas of both peaks were used for the calculation as:

$$\text{at.\%Cl} = \left[\frac{corrected\ area\ of\ Cl\ 2p_{3/2}}{(corrected\ area\ of\ Cl\ 2p_{3/2} + \ corrected\ area\ of\ Zn\ 2p_{3/2})}\right] x\ 100$$

where corrected peak area = peak area × R.S.F. (relative sensitivity factor).

Table 1 shows the at.%Cl both at surface and in the bulk from depth profile XPS (500-2500 s). Note that the signal to noise ratio in the film with 1 mol% $FeCl_3$ added is very weak which are not allowed to make a proper fitting. Figure 2 shows the Cl 2p XPS spectra of all films from the surface and depth profiling. The absence of Fe was detected in doped samples at both surface and depth profiling. Figure 3 is shown as a representative for Fe 2p XPS spectra of the film prepared using 10 mol% $FeCl_3$.

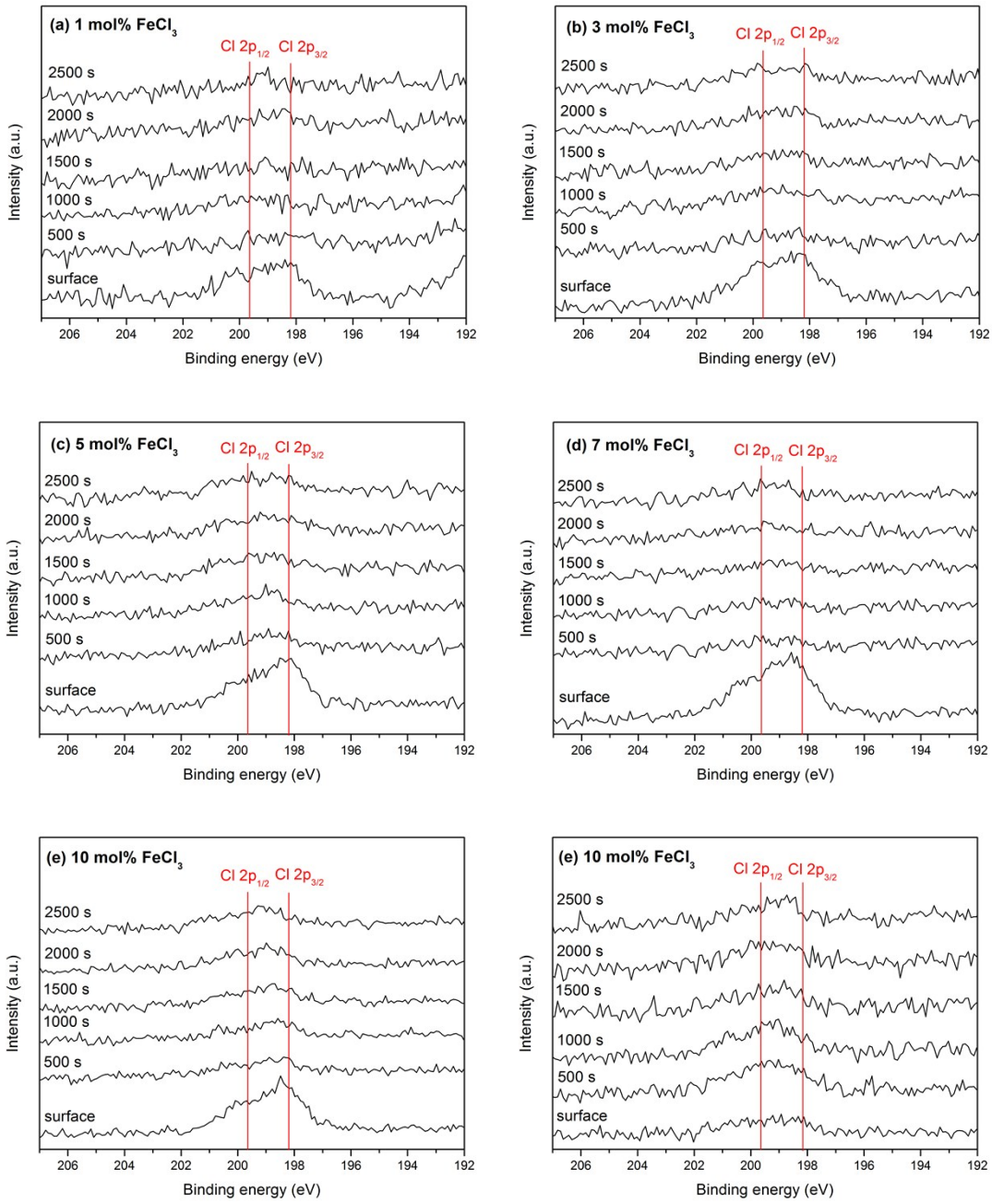

Figure 2 Surface and depth-profile Cl 2p XPS spectra of ZnO:Cl films prepared using $FeCl_3$ (a) 1 mol%, (b) 3 mol%, (c) 5 mol%, (d) 7 mol% and (e) 10 mol%.

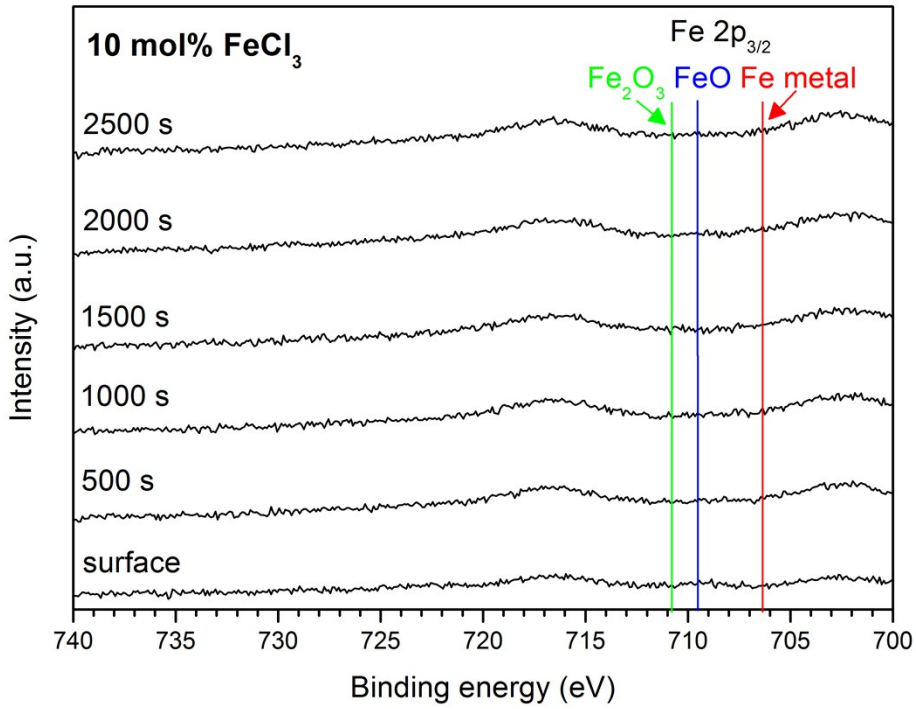

Figure 3 Surface and depth-profile Fe 2p XPS spectra of ZnO:Cl films prepared using 10 mol% $FeCl_3$. The lines refer to the expected peak position according to each form of Fe at Fe $2p_{3/2}$ region.

Table 1 at.%Cl in Cl-doped ZnO films considered at surface and in the bulk from depth profile XPS

mol% $FeCl_3$ added	at.% at surface	Average at.% in the bulk	Average at.% in the whole film
1 mol%	4.32	N/A	N/A
3 mol%	3.36	0.60	1.32
5 mol%	4.61	0.63	1.30
7 mol%	3.03	0.35	0.79
10 mol%	4.47	0.84	1.45
15 mol%	12.61	1.07	2.99

Stearic acid degradation

Stearic acid degradation was investigated from the corrected area of FTIR absorbance spectra collected in the range of 2700-3000 cm^{-1} as shown in Figure 4. The linear regression of the initial 30-40% degradation steps (zero-order kinetics) with a conversion factor (1 cm^{-1} ≈ 9.7 x 10^{15} molecule of stearic acid/cm^2)[1] was utilized to determine the photocatalytic activity rates as formal quantum efficiency (FQE) value.

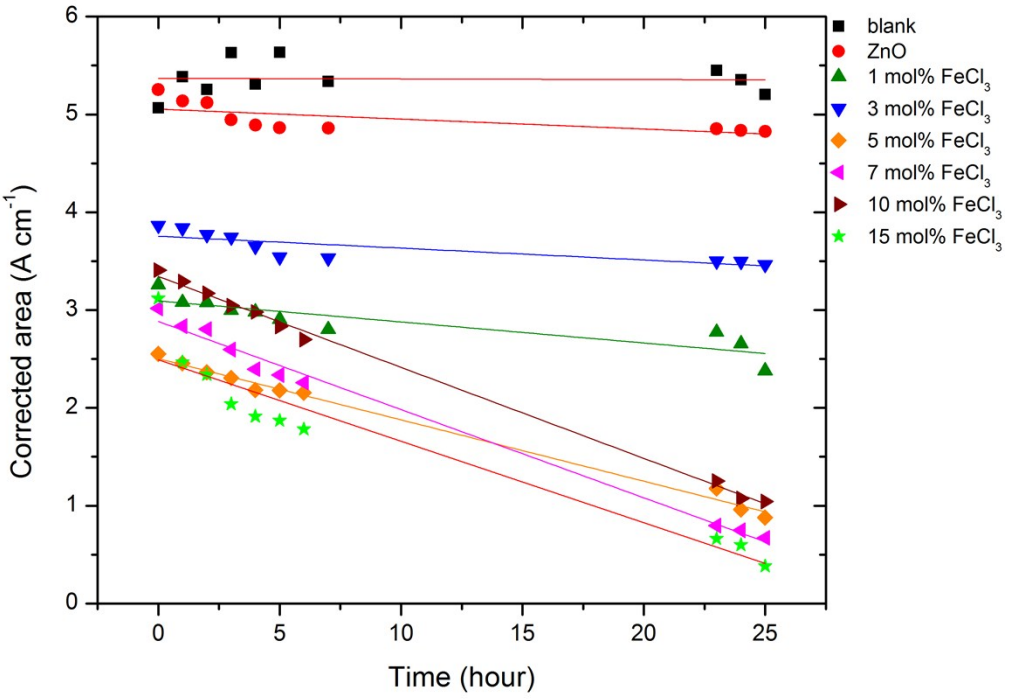

Figure 4 Plot of corrected area under FTIR spectra collected in the range of 2700-3000 cm^{-1}

Mass Spectra of the red precipitate

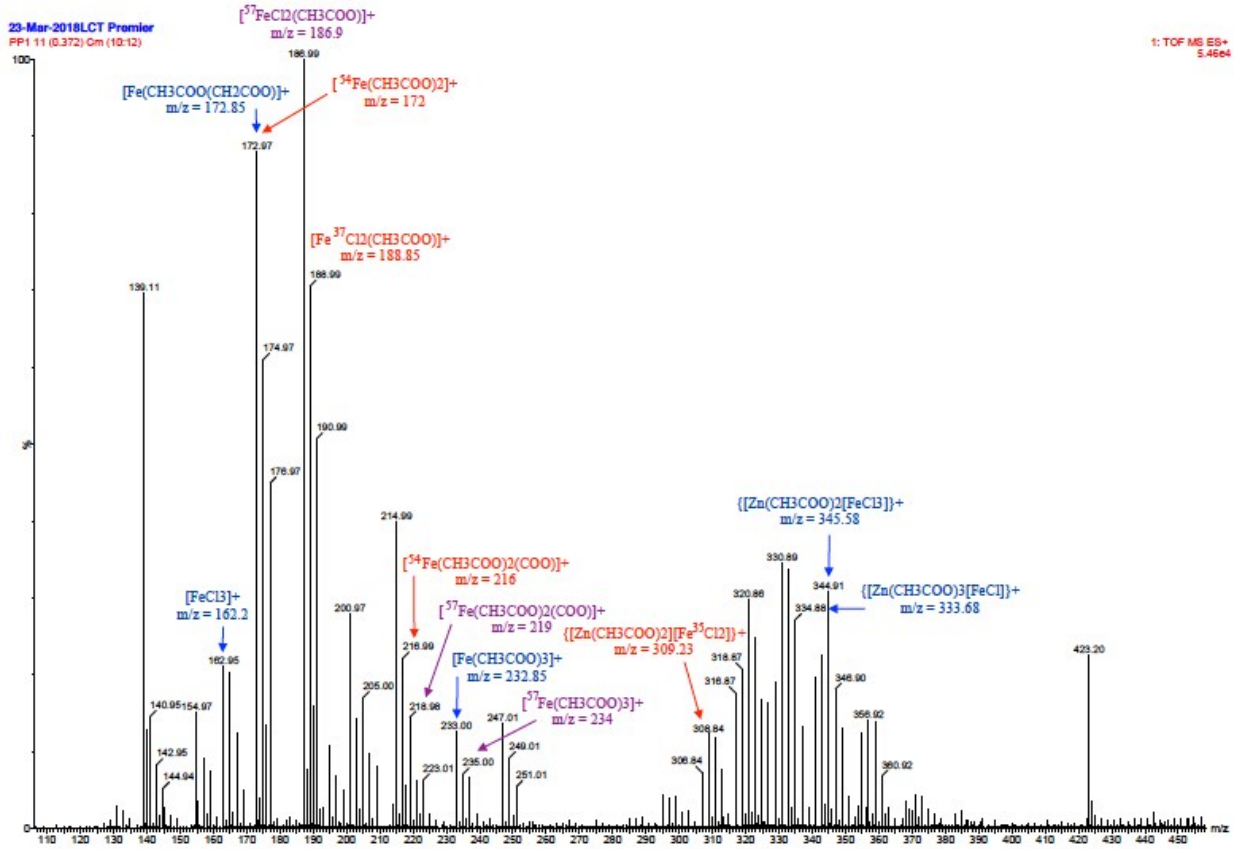

Figure 5 Mass spectra of the red precipitate observed in the bubbler of precursor solution after aerosol assisted CVD procedure of Cl-doped ZnO films.

References

1 A. Mills and J. Wang, *J. Photochem. Photobiol. A Chem.*, 2006, **182**, 181–186.