
Supporting Information

Correlation of crystal structures, electronic structures and photocatalytic properties in a series of Ag-based oxides, AgAlO_2 , AgCrO_2 and Ag_2CrO_4

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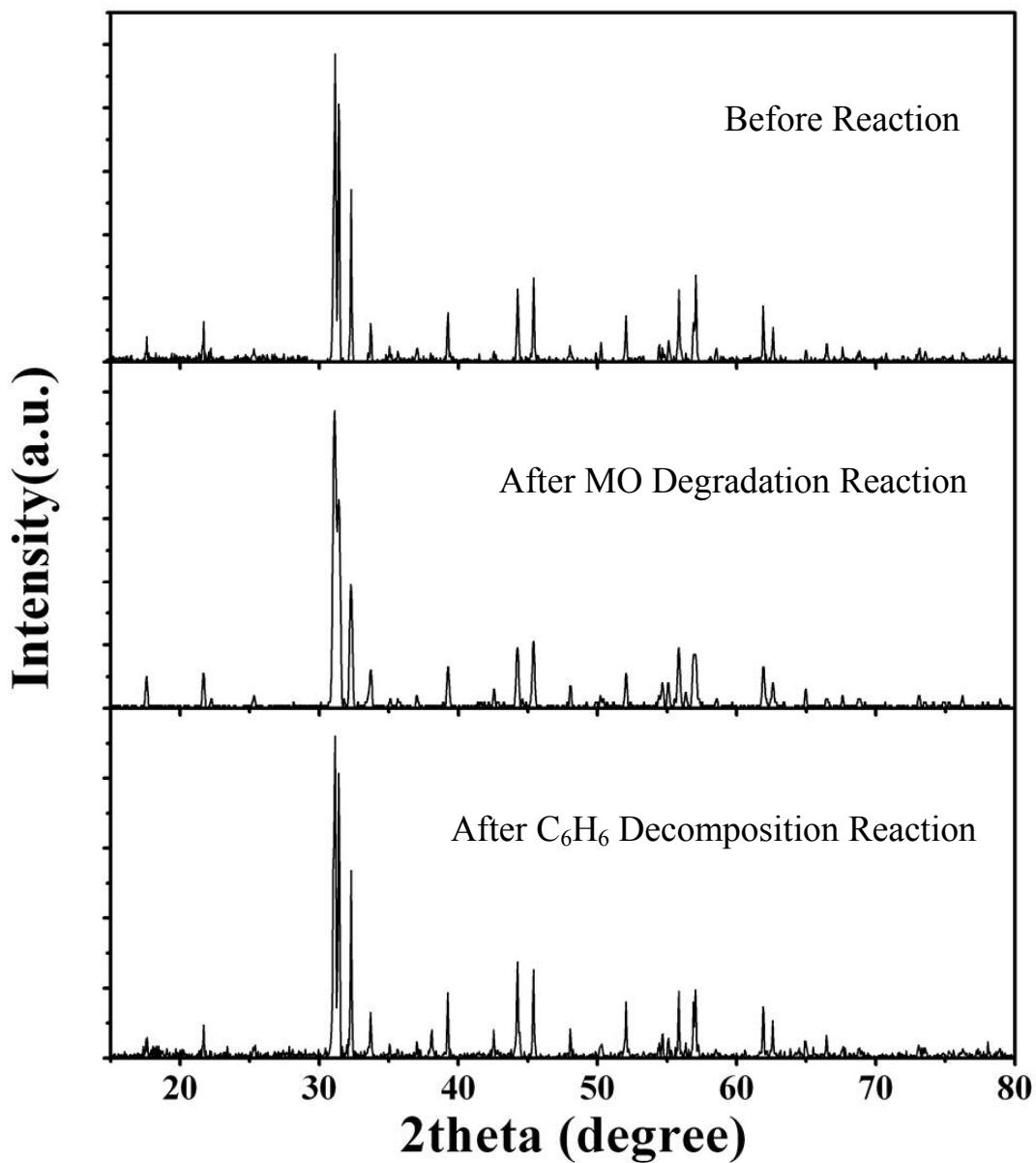
TABLE 1: The Lattice Parameters and the Atomic Coordinates in AgAlO_2 and Ag_2CrO_4 used in Calculation

Crystals	Lattice Parameters	Atoms	Wyckoff Site	Atomic Coordinates		
				x	y	z
AgAlO_2	$a = 5.2728 \text{ \AA}$	Ag	4a	0.0598	0.6427	1.0069
	$b = 6.7628 \text{ \AA}$	Al	4a	0.0706	0.1239	-0.0013
	$c = 5.3626 \text{ \AA}$	O1	4a	0.0342	0.0679	0.3119
	$\alpha = \beta = \gamma = 90^\circ$	O2	4a	0.1117	0.6681	0.4346
Ag_2CrO_4	$a = 10.6751 \text{ \AA}$	Ag1	4a	0.5000	0.5000	0.5000
	$b = 7.0542 \text{ \AA}$	Ag2	4c	0.1494	0.2500	0.4809
	$c = 5.7500 \text{ \AA}$	Cr	4c	0.3136	0.2500	0.9593
	$\alpha = \beta = \gamma = 90^\circ$	O1	4c	0.1583	0.2500	0.8933
		O2	4c	0.3348	0.2500	0.2441
		O3	8d	0.3813	0.4430	0.8464

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Figure 1

The XRD patterns of Ag_2CrO_4 samples



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Figure 2

Repeated photocatalytic decomposition of C₆H₆

