Electronic Supplementary Information

Novel cone-like ZnO mesocrystal with coexposed $(10\bar{1}1)$ and $(000\bar{1})$ facets and enhanced photocatalytic activity

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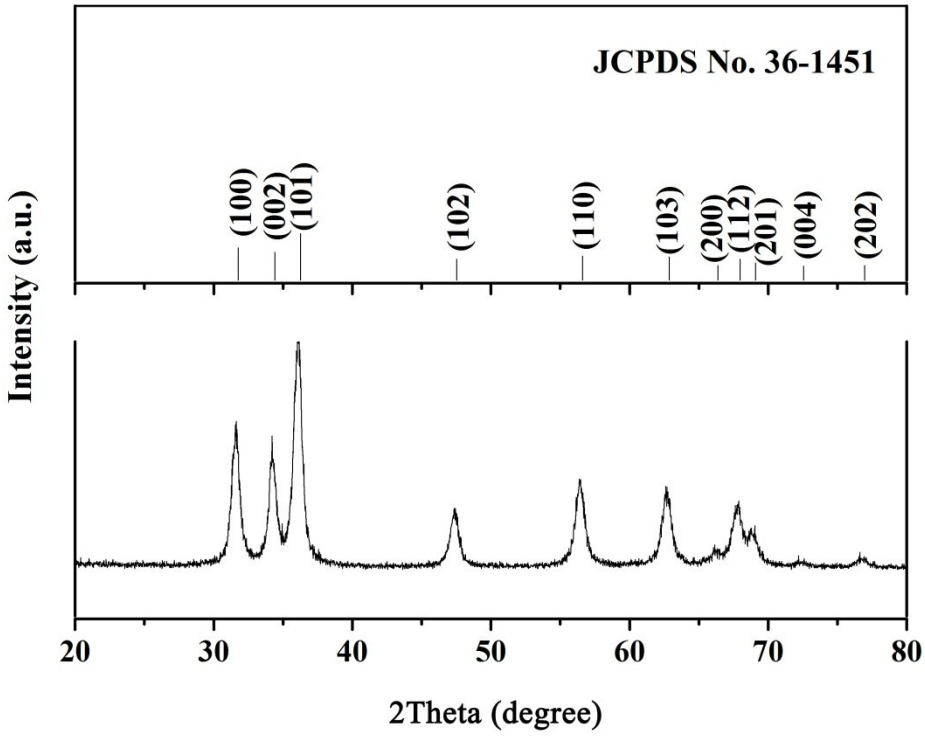

Figure S1. XRD pattern of as-prepared cone-like ZnO mesocrystals (Sample A).

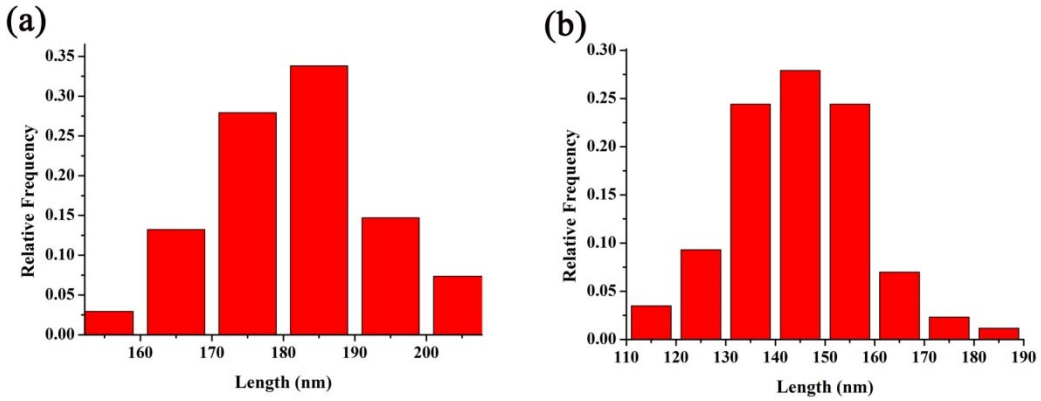

Figure S2. The size distribution diagrams of cone-like ZnO mesocrystals (Sample A).

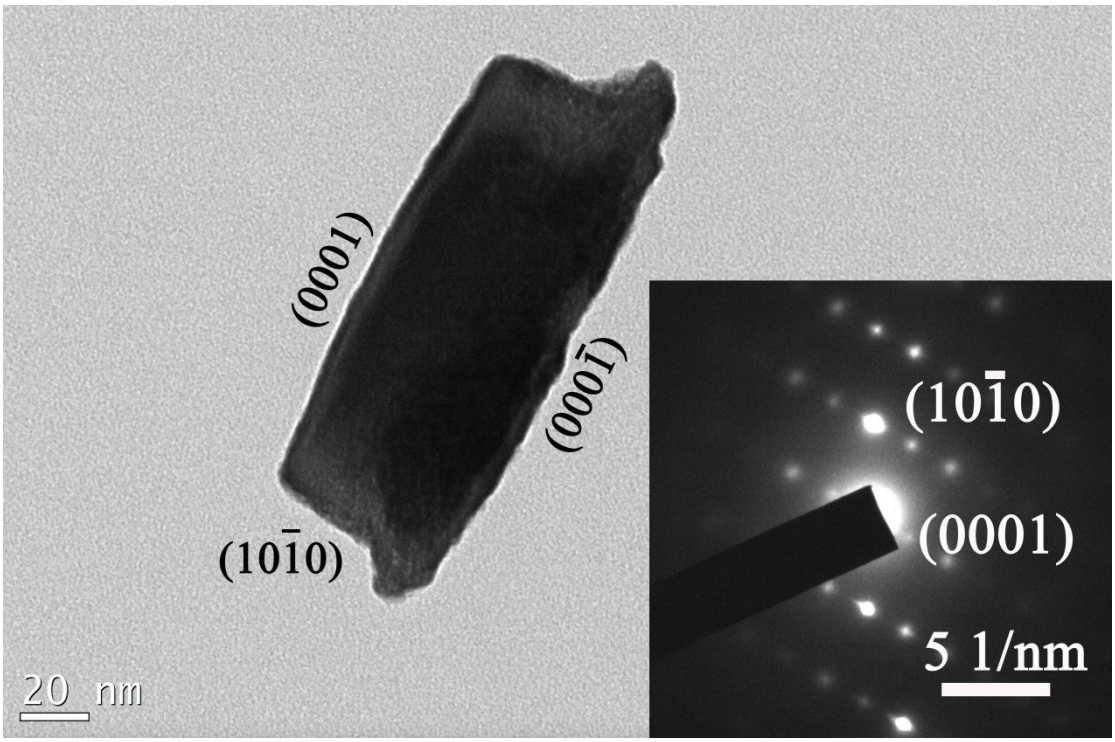

Figure S3. TEM image and SAED pattern of the bolt-like ZnO architecture (Volume of water = 5 mL).

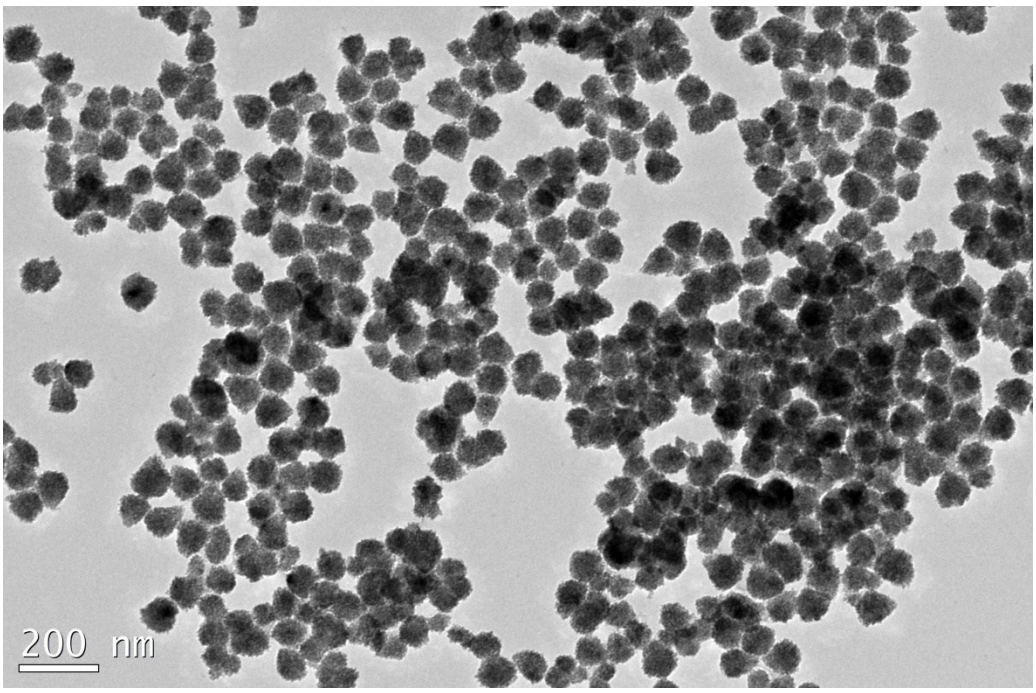

Figure S4. TEM image of ZnO synthesized in pure ethanol system.

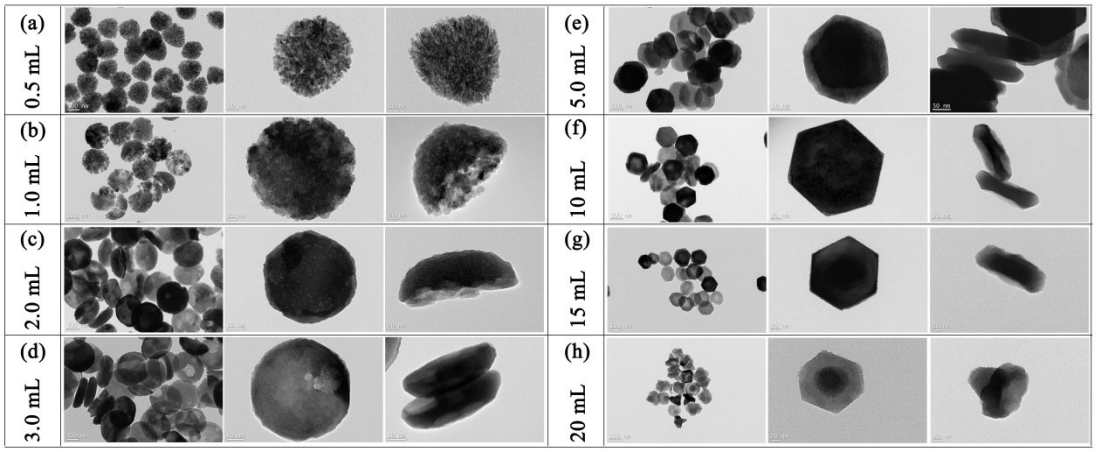

Figure S5. TEM images of the products synthesized in different amount of water (Volume of ethanol = 30 mL) at 70 ^{o}C.

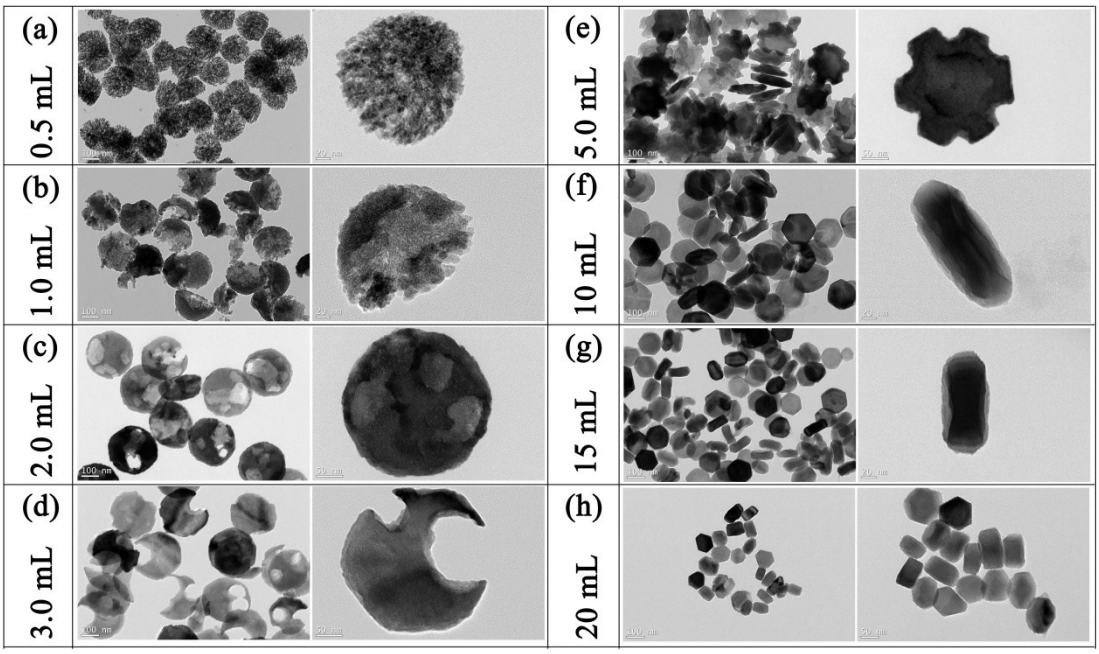

Figure S6. TEM images of the products synthesized in different amount of water (Volume of ethanol = 30 mL) at 65 ^{o}C.

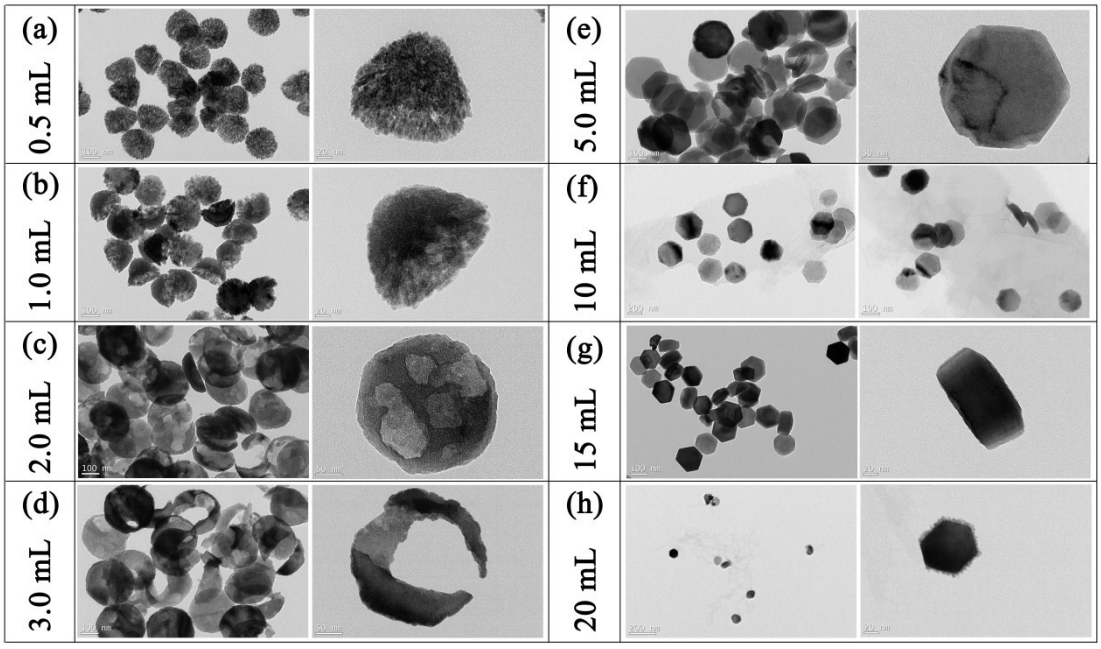

Figure S7. TEM images of the products synthesized in different amount of water (Volume of ethanol = 30 mL) at 60 ^{o}C.

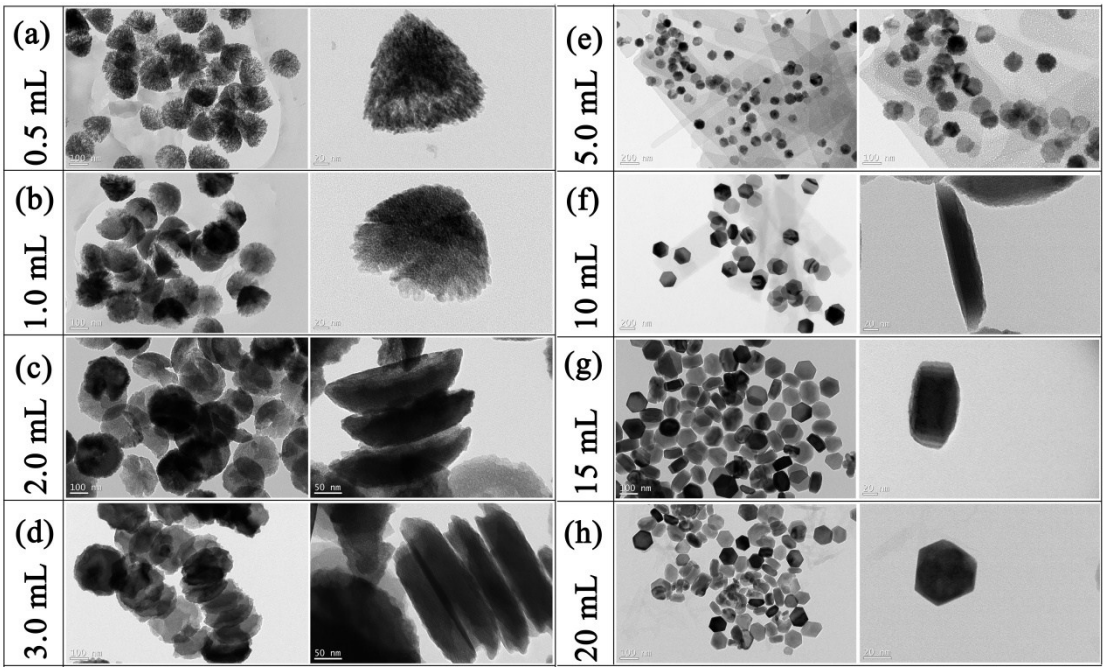

Figure S8. TEM images of the products synthesized in different amount of water (Volume of ethanol = 30 mL) at 55 °C.

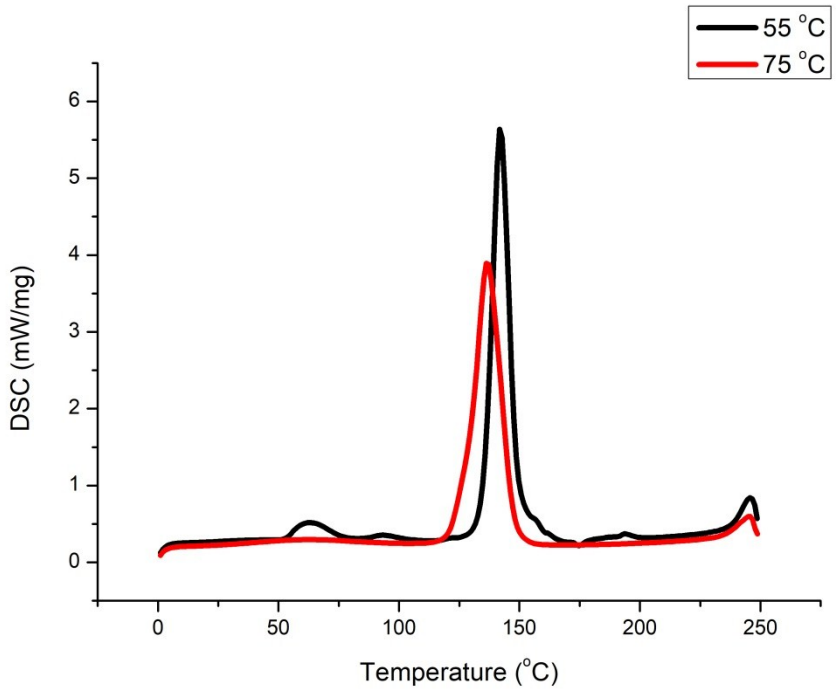

Figure S9. DSC results of ZnO products (water = 0.5 mL, ethanol = 30 mL) synthesized at different temperature.

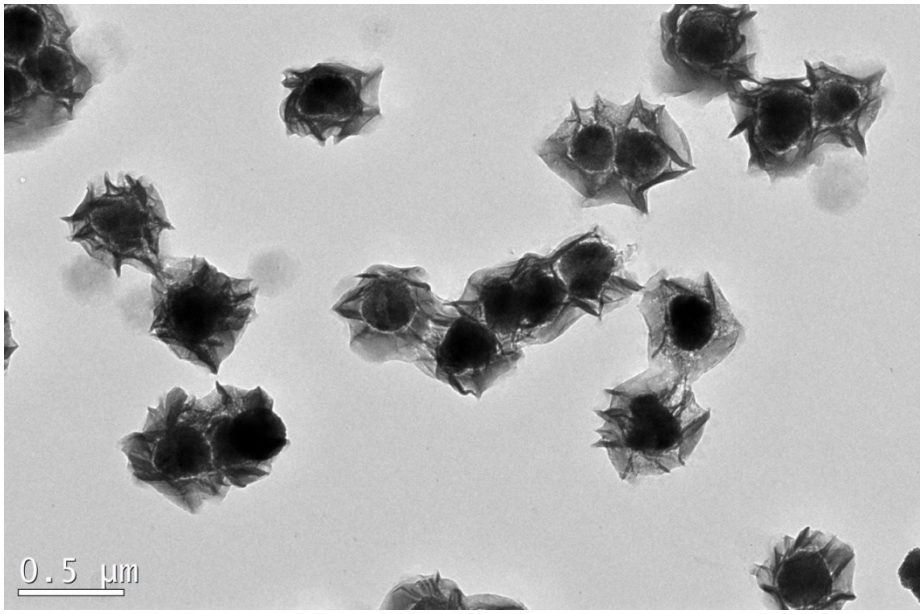

Figure S10. TEM image of the products synthesized in different amount of water (Volume of ethanol = 30 mL, Temperature = 75 °C) at short reaction time (1 min).

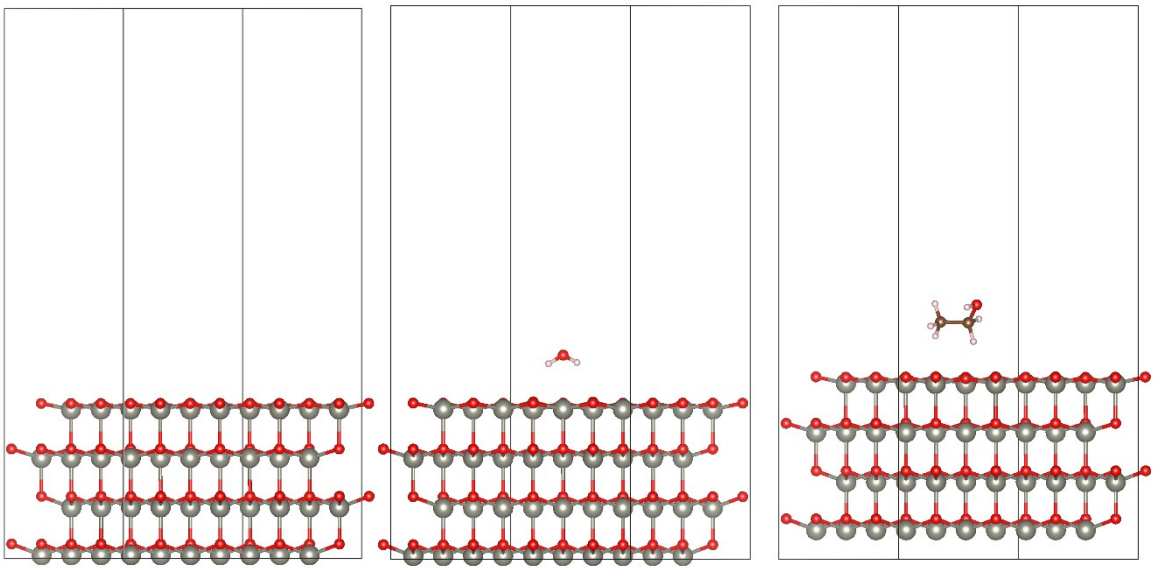

Figure S11. The models of the isolated ZnO (0001) surface (a) and the relaxed ZnO (0001) surface with the molecules of H_2O (b) and C_2H_5OH (c) adsorbed to it.

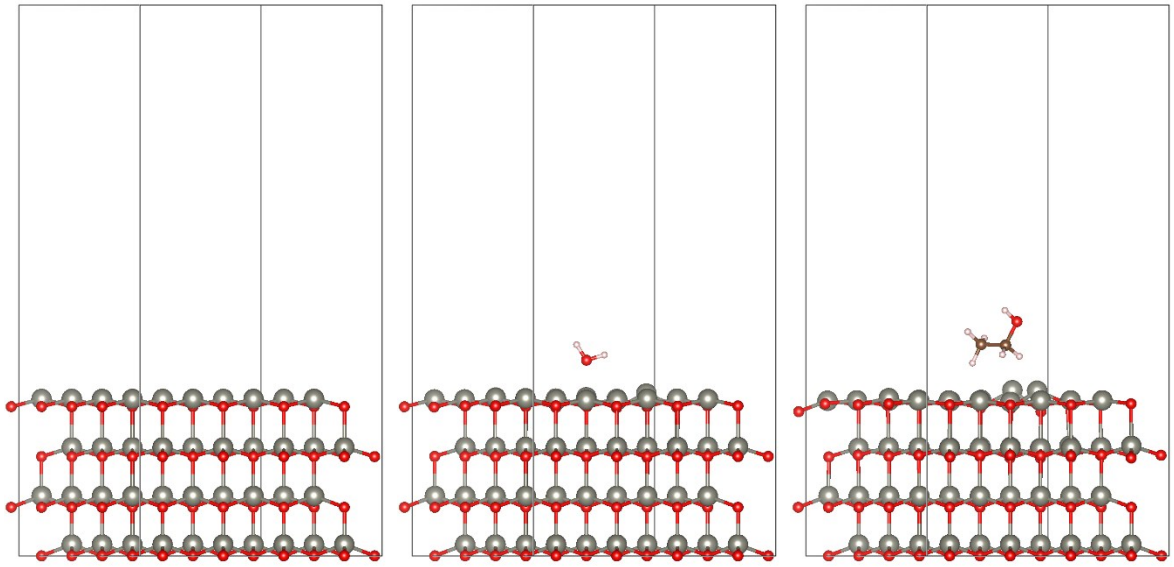

Figure S12. The models of the isolated ZnO $(000\bar{1})$ surface (a) and the relaxed ZnO $(000\bar{1})$ surface with the molecules of H_2O (b) and C_2H_5OH (c) adsorbed to it.

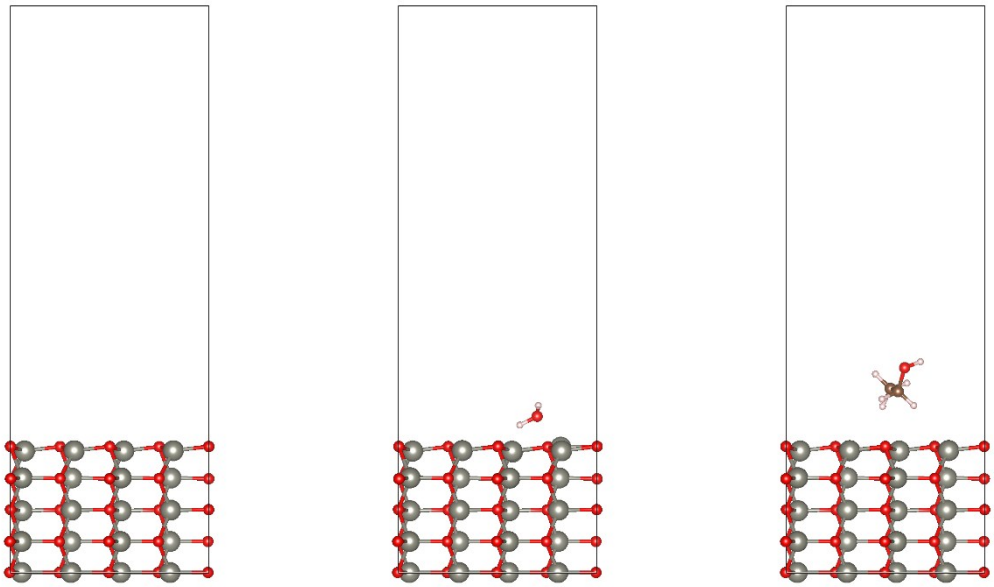

Figure S13. The models of the isolated ZnO $(10\bar{1}0)$ surface (a) and the relaxed ZnO $(10\bar{1}0)$ surface with the molecules of H_2O (b) and C_2H_5OH (c) adsorbed to it.

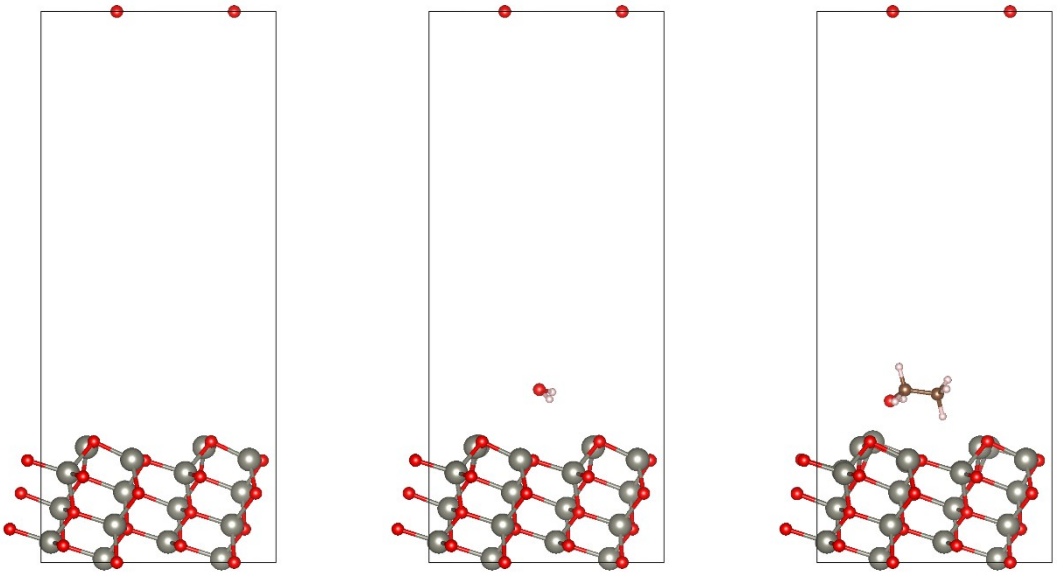

Figure S14. The models of the isolated ZnO $(10\bar{1}1)$ surface (a) and the relaxed ZnO $(10\bar{1}1)$ surface with the molecules of H_2O (b) and C_2H_5OH (c) adsorbed to it.

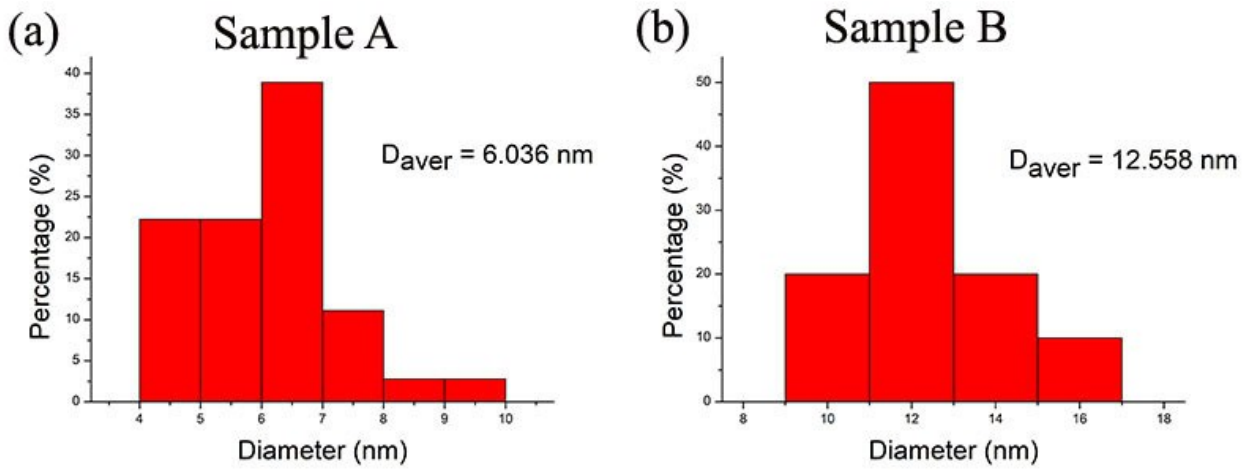

Figure S15. The size distribution diagrams of Sample A (a) and Sample B (b).

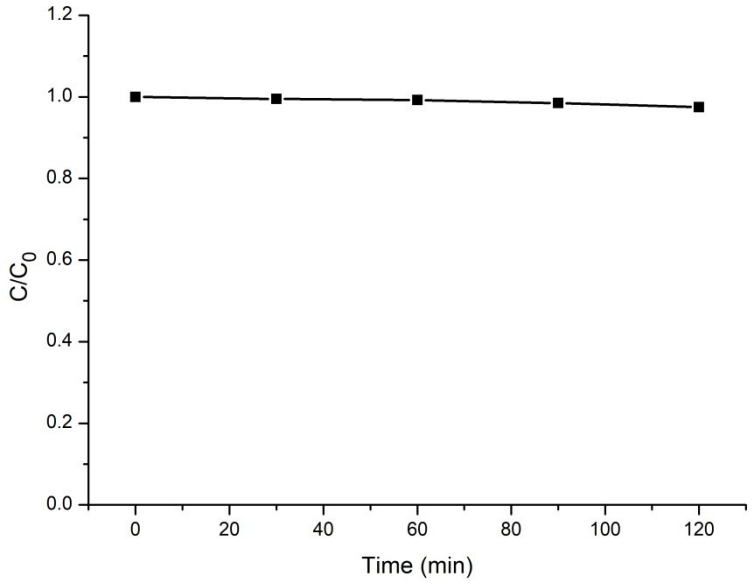

Figure S16. A blank experiment under UV light irradiation.

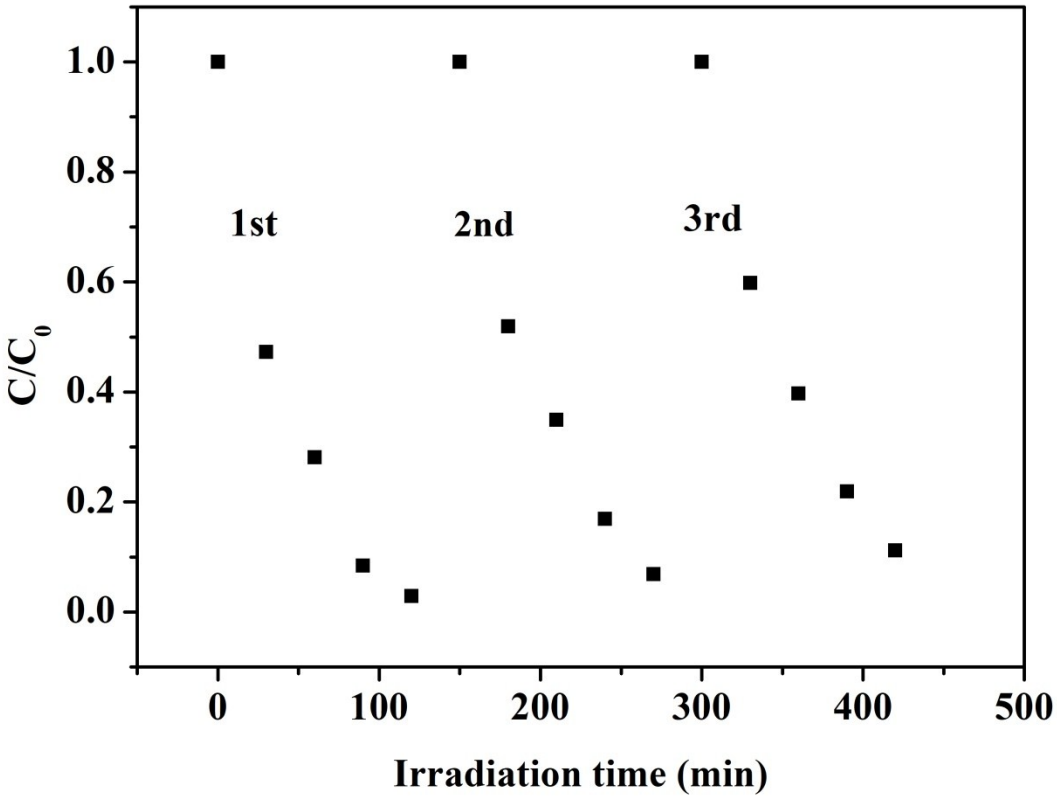

Figure S17. The cycle experiment of Sample A.

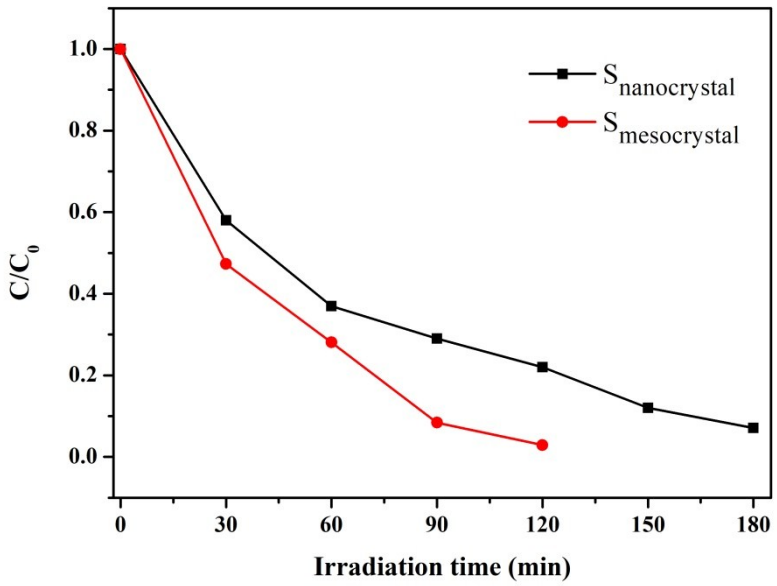

Figure S18. Photocaltalytic results of the Sample A ($S_{mesocrystal}$) and cone-like nanocrystals ($S_{nanocrystal}$).

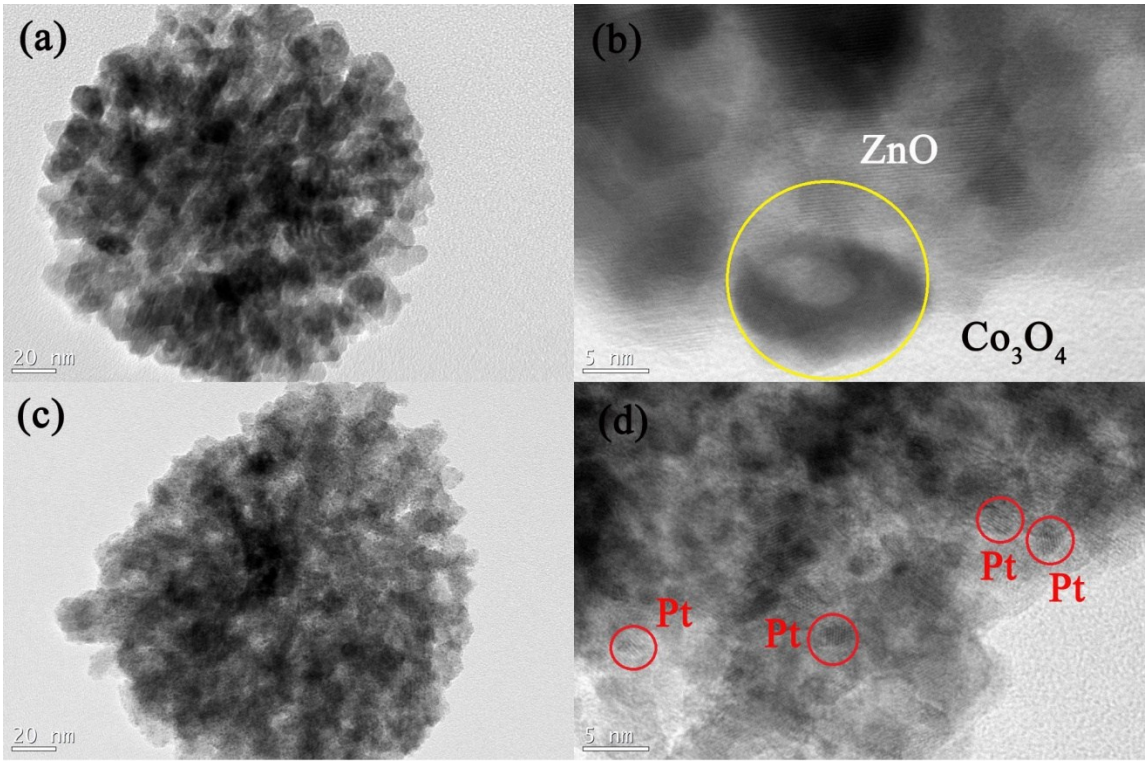

Figure S19. TEM images of the photodeposition products synthesized in H_2PtCl_6/ triethanolamine and $CoCl_2/NaIO_3$ solution, respectively.

Synthesis. 0.03 g ZnO powder and a calculated amount of metal precursors (5 wt%) were mixed in 50 mL deionized water. The suspension was then irradiated by a 300W Xe lamp under continuous stirring. After 3 h photo-deposition, the suspension was filtered, washed with deionized water and ethanol for more than three times, and finally dried at 60 ^{o}C for overnight.

Table S1. The detailed experimental conditions of the products synthesized at 70 °C.

Sample	Concentration of $Zn(CH_3COO)_2$	Reaction temperature	Reaction time	The volume of ethanol	The volume of water
A	0.15 mM	70 ℃	15 min	30 mL	0.5 mL
B	0.15 mM	70 ℃	15 min	30 mL	1.0 mL
C	0.15 mM	70 ℃	15 min	30 mL	2.0 mL
D	0.15 mM	70 ℃	15 min	30 mL	3.0 mL
E	0.15 mM	70 ℃	15 min	30 mL	5.0 mL
F	0.15 mM	70 ℃	15 min	30 mL	10 mL
G	0.15 mM	70 ℃	15 min	30 mL	15 mL
J	0.15 mM	70 ℃	15 min	30 mL	20 mL

Table S2. The detailed experimental conditions of the products synthesized at 65 °C.

Sample	Concentration of $Zn(CH_3COO)_2$	Reaction temperature	Reaction time	The volume of ethanol	The volume of water
A	0.15 mM	65 ℃	15 min	30 mL	0.5 mL
B	0.15 mM	65 ℃	15 min	30 mL	1.0 mL
C	0.15 mM	65 ℃	15 min	30 mL	2.0 mL
D	0.15 mM	65 ℃	15 min	30 mL	3.0 mL
E	0.15 mM	65 ℃	15 min	30 mL	5.0 mL
F	0.15 mM	65 ℃	15 min	30 mL	10 mL
G	0.15 mM	65 ℃	15 min	30 mL	15 mL
J	0.15 mM	65 ℃	15 min	30 mL	20 mL

Table S3. The detailed experimental conditions of the products synthesized at 60 °C.

Sample	Concentration of $Zn(CH_3COO)_2$	Reaction temperature	Reaction time	The volume of ethanol	The volume of water
A	0.15 mM	60 ℃	15 min	30 mL	0.5 mL
B	0.15 mM	60 ℃	15 min	30 mL	1.0 mL
C	0.15 mM	60 ℃	15 min	30 mL	2.0 mL
D	0.15 mM	60 ℃	15 min	30 mL	3.0 mL
E	0.15 mM	60 ℃	15 min	30 mL	5.0 mL
F	0.15 mM	60 ℃	15 min	30 mL	10 mL
G	0.15 mM	60 ℃	15 min	30 mL	15 mL
J	0.15 mM	60 ℃	15 min	30 mL	20 mL

Table S4. The detailed experimental conditions of the products synthesized at 55 °C.

Sample	Concentration of $Zn(CH_3COO)_2$	Reaction temperature	Reaction time	The volume of ethanol	The volume of water
A	0.15 mM	55 ℃	15 min	30 mL	0.5 mL
B	0.15 mM	55 ℃	15 min	30 mL	1.0 mL
C	0.15 mM	55 ℃	15 min	30 mL	2.0 mL
D	0.15 mM	55 ℃	15 min	30 mL	3.0 mL
E	0.15 mM	55 ℃	15 min	30 mL	5.0 mL
F	0.15 mM	55 ℃	15 min	30 mL	10 mL
G	0.15 mM	55 ℃	15 min	30 mL	15 mL
J	0.15 mM	55 ℃	15 min	30 mL	20 mL

Table S5. The adsorption energy (E_a) for H_2O and C_2H_5OH molecules adsorbed on the different ZnO surfaces

Surface	Adsorption energy E_a (eV/molecule)	
	H_2O (water)	C_2H_5OH (ethanol)
$(000\bar{1})$	−0.32	−0.43
(0001)	−0.49	−0.12
$(10\bar{1}0)$	−1.03	−0.35
$(10\bar{1}1)$	−0.09	−1.13

Calculation method

Our first-principles calculations were based on DFT implemented in the Vienna ab initio simulation package (VASP) code.[1] The projected augmented wave (PAW) method[2] within the generalized gradient approximation of Perdew, Burke, and Ernzerhof (PBE)[3] was used. To separate the interactions between neighboring slabs, the periodic boundary conditions with a relatively large vacuum space of 20 Å were applied. The energy cutoff and convergence criteria for energy and force was set to be 450 eV, 10^{-4} eV, and 0.01 eV/Å, respectively. During the optimization, 3×3×1 K-point[4] was adopted, while 5×5×1 was used for total energy calculations.

[1] G. Kresse and J. Hafner, Phys. Rev. B 1993, 47, 558.
[2] P. E. Blöchl, Phys. Rev. B 1994, 50 17953.
[3] J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. 1996, 77, 3865.
[4] H. J. Monkhorst, J. D. Pack, Phys. Rev. B 1976, 13, 5188.