Electronic Supplementary Material (ESI) for Journal of Materials Chemistry


# Electronic Supplementary Information

# Controlled synthesis of $Ag_2O$ microcrystals with facets-dependent photocatalytic activities

**Gang Wang[a], Baibiao Huang,*[a] Xiangchao Ma,[b] Hefeng Cheng,[a] Zeyan Wang,[a] Jie Zhan*[a] and Ying Dai[b]**

[a] State Key Laboratory of Crystal Materials, Shandong University, Jinan 250100 (P. R. China). E-mail: bbhuang@sdu.edu.cn, zhanjiesdu@yahoo.com.cn,

[b] School of Physics, Shandong University, Jinan 250100 (P. R. China)

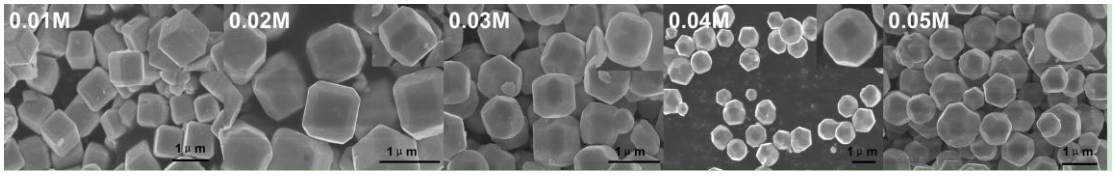


**Fig. S1** SEM images of $Ag_2O$ in different $CH_3COONH_4$ concentrations

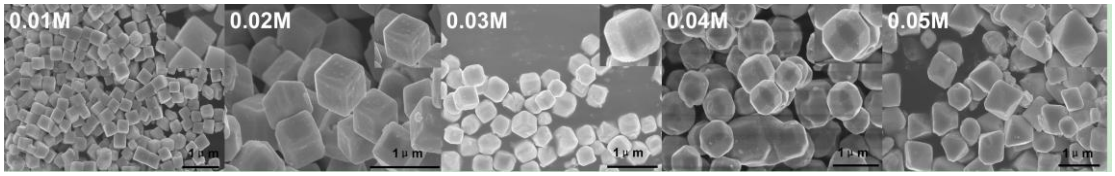


**Fig. S2** SEM images of $Ag_2O$ in different $NH_4NO_3$ concentrations

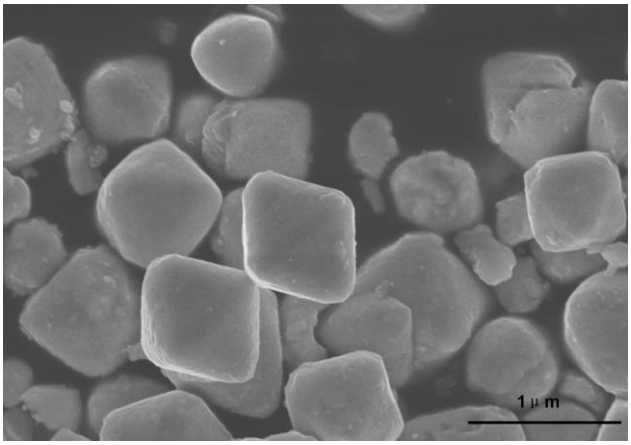


**Fig. S3** SEM image of $Ag_2O$ in 0.02M $(NH_4)_2HPO_4$ solution

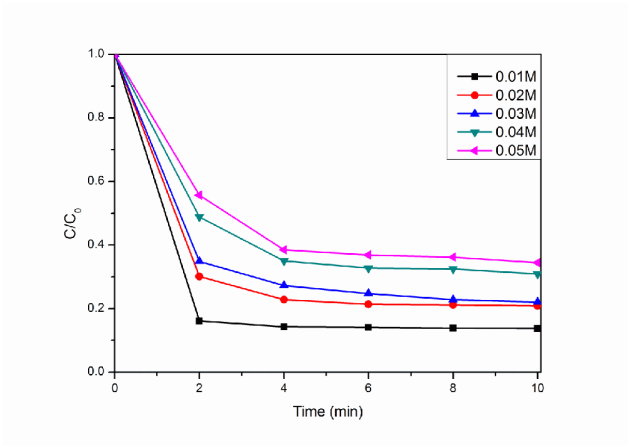


**Fig. S4** Different photocatalytic activities of two facets exposed $Ag@Ag_2O$ with the variation of $CH_3COONH_4$ concentrations

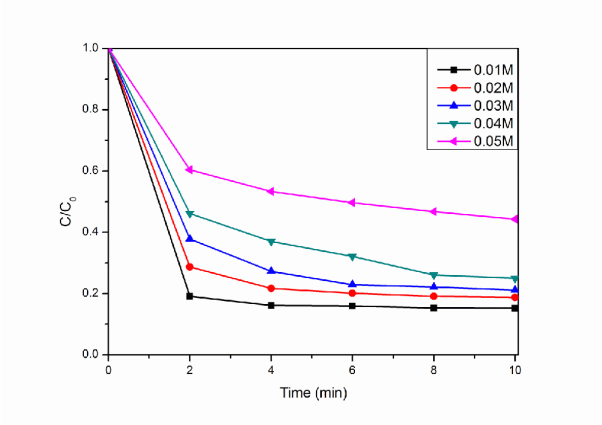


**Fig. S5** Different photocatalytic activities of all facets exposed Ag@$Ag_2O$ with the variation of $NH_4NO_3$ concentrations

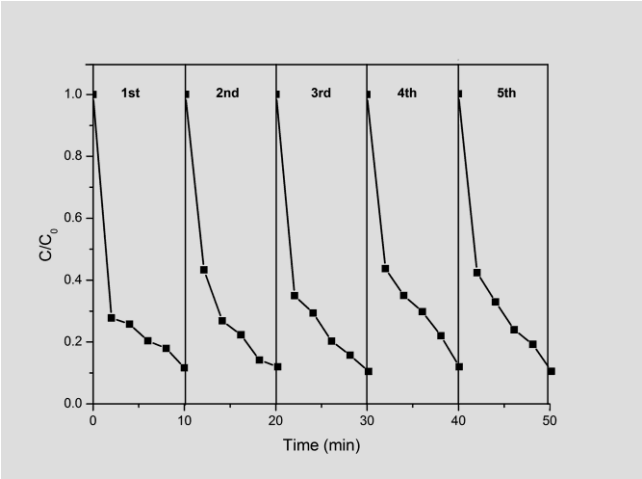


**Fig. S6** Repeating runs in the photocatalytic degradation of MO in the presence of cubic Ag@$Ag_2O$ photocatalyst under visible light irradiation

# The calculated method of estimation of the redox potentials of (100), (110), (111) surface

Our electronic structure calculations were based on the density functional theory within the local-density approximation (LDA). The calculations are performed using the projector augmented wave as implemented in the VASP code.[1, 2] The electronic wave functions are expanded in plane waves with an energy cutoff of 400 eV, which is found to be high enough for energy convergence. The 1×1 slab models using the experimental lattice parameters [4.73 Å] are used to construct the surface models. We have used a 10×10×1, 10×8×1, 8×8×1 Γ-centered k-points[3] sampling the Brillouin zones for the final calculations of energies for (100), (110) and (111) surfaces, respectively. The atomic positions are fully relaxed until the residual forces are below 0.03 eV/Å. In the case of slabs, a 20 Å thickness of vacuum layer are used. The total and projected densities of states (TDOS and PDOS) were calculated at the equilibrium volume using the tetrahedron method with BlcÖhl corrections for accuracy.[4]

1. G. Kresse and J. Hafner, *Physical Review B*, 1993, **47** (1), 558-561.

2. G. Kresse and J. Furthmüller, *Physical Review B*, 1996, **54** (16), 11169-11186.

3. H. J. Monkhorst and J. D. Pack, *Physical Review B*, 1976, **13** (12), 5188-5192.

4. P. E. BlcÖhl, O. Jepsen and O. K. Andersen, *Phys. Rev. B*, 1994, **49**, 16223 –16233.