

Supporting Information

Metallic Tungsten Carbide Nanoparticles as Near-infrared Driven Photocatalyst

Weicheng Huang^{#a}, Hongxue Meng^{#c}, Yan Gao^b, Jinxin Wang^a, Chunyu Yang^b, Danqing Liu^{*d}, Jian Liu^a, Chongshen Guo^{*b}, Bin Yang^{*a}, Wenwu Cao^{a,e}

^a School of Instrumentation Science and Engineering, Harbin Institute of Technology, Harbin 150080, China. E-mail: binyang@hit.edu.cn

^b School of Chemistry and Chemical Engineering, Harbin Institute of Technology, Harbin 150080, China. E-mail: chongshenguo@hit.edu.cn

^c Department of Pathology, Harbin Medical University Cancer Hospital, Harbin, China.

^d School of Chemical and Environmental Engineering, Harbin University of Science and Technology, Harbin 150040, China. Email: danqingliu76@163.com

^e Department of Mathematics and Materials Research Institute, The Pennsylvania State University, Pennsylvania 16802, USA

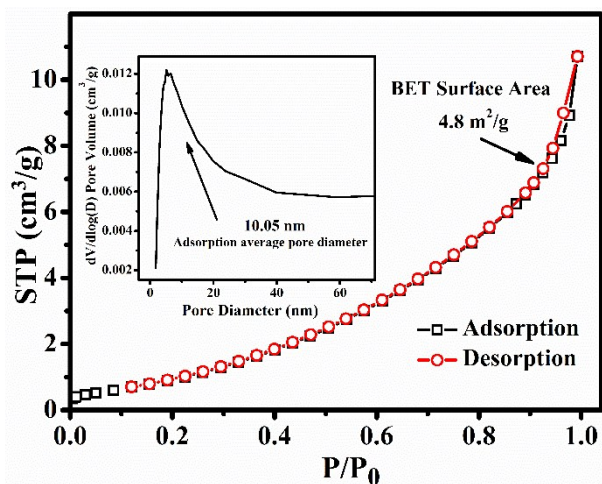


Figure S1 BET and corresponding pore size distribution curves.

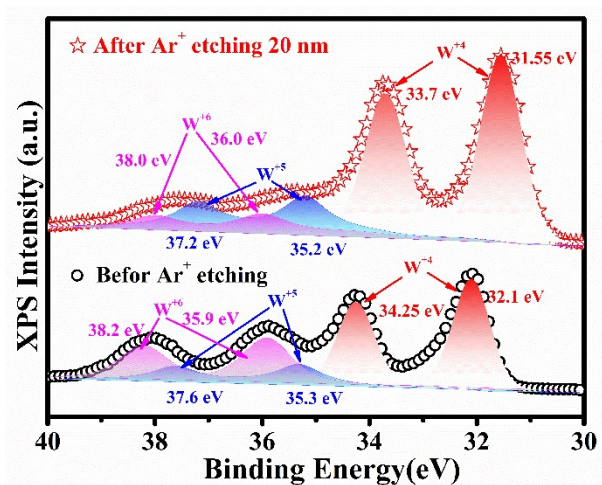


Figure S2 W 4f XPS spectra of WC nanoparticle before and after Ar⁺ etching 20 nm.

Table S1 Atomic analysis of W 4f before and after Ar⁺ etching

Chemical state	Atomic ratio	
	Before etching	After etching
W ⁴⁺ (W-C)	0.55	0.73
W ⁵⁺ (W-O)	0.15	0.19
W ⁶⁺ (W-O)	0.30	0.08

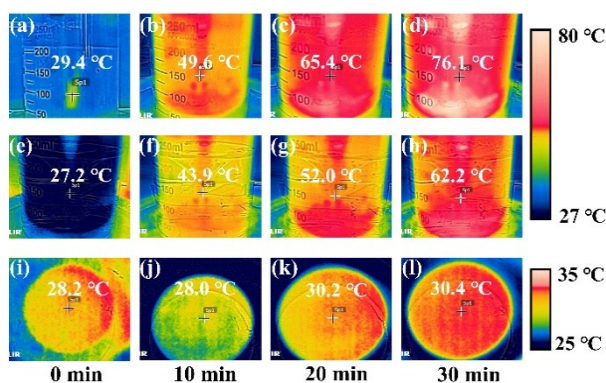


Figure S3 Temperature profiles of (a-d) the 1 mg/L WC aqueous dispersion without cooling water, (e-h) water without cooling water, (i-l) the 1 mg/L WC aqueous dispersion with cooling water under 30 min NIR irradiation.

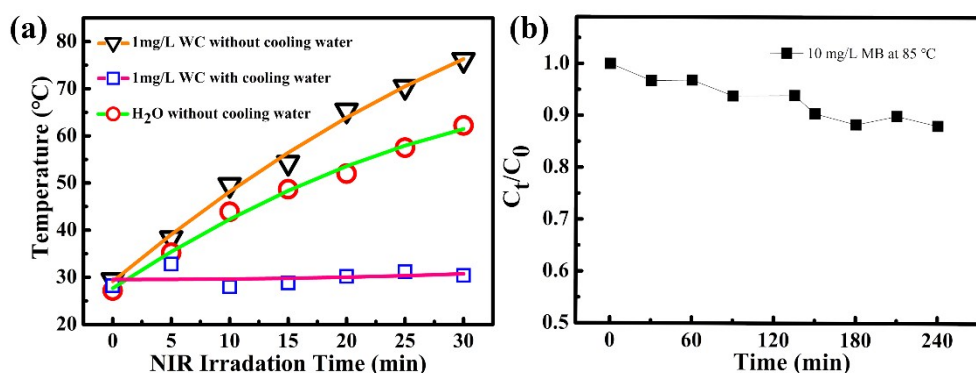


Figure S4 (a) Temperature-radiation time dependent of different solution. (b) C_t/C_0 of 10 mg/L MB in 85 °C water bath (under dark condition).

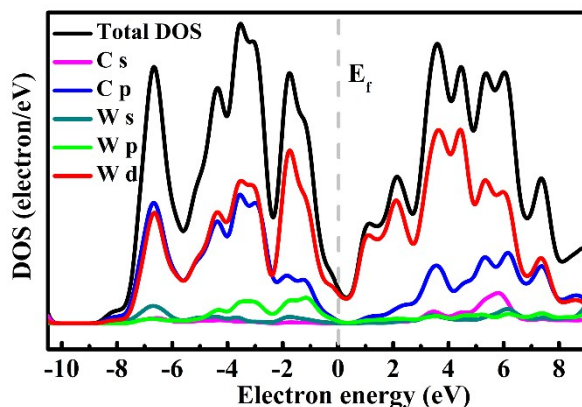


Figure S5 DFT calculated density of state (DOS) and the corresponding projected DOS of WC.

The DFT calculation of electronic structure of WC was performed on CATSEP, which is one of functional module in Material Studio package. The gradient corrected exchange-correlation with Perdew-Burke-Ernzerhof functional (GGA-PBE) and ultrasoft pseudopotential plane-wave methods were used for all the calculations. A hexagonal 4x4x2 supercell with 64 atoms was built for simulating WC. The cut-energy

of 340 eV and homogenate meshed 3x3x3 k-point were used throughout the calculation. The self-consistent geometry optimization was performed until it satisfies the convergence tolerances (0.01 GPa and 5×10^{-6} eV for maximum stress and energy change).

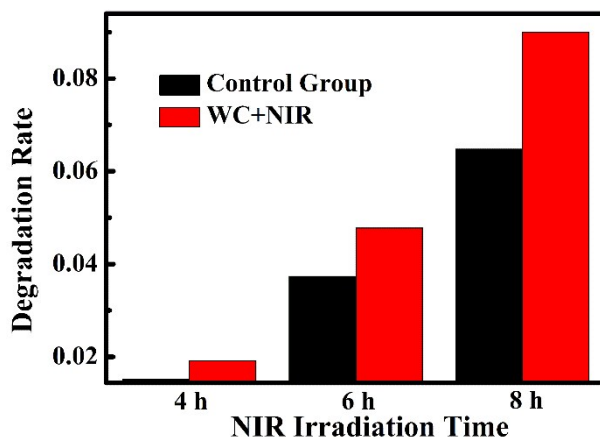


Figure S6 NIR photocatalytic degradation on Phenol of WC nanoparticles.

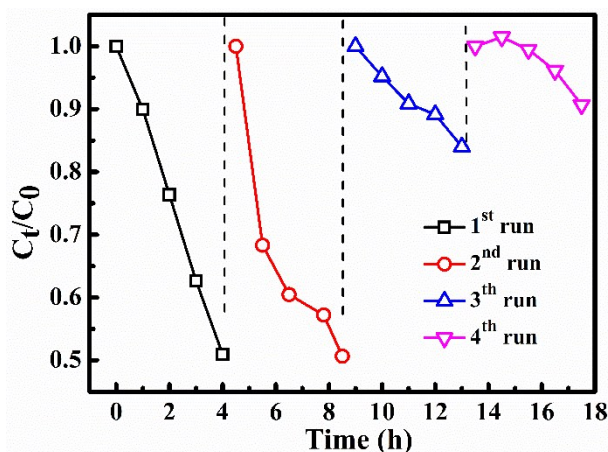


Figure S7 Recycle NIR photocatalytic degradation of MB for 4 runs.

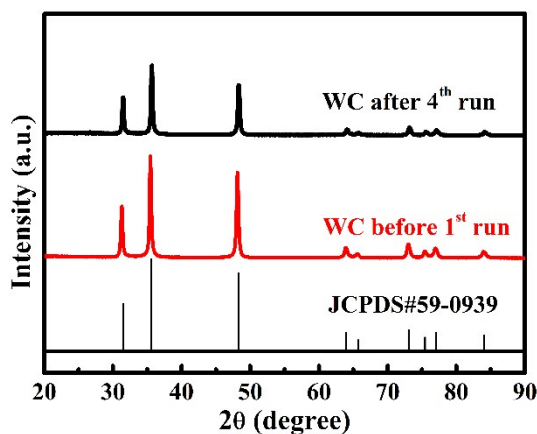


Figure S8 XRD spectra of WC nanoparticles before and after 4 run's photocatalyst.