Supporting information

Hydrothermal route to metastable phase $FeVO_4$ ultrathin nanosheets with exposed {010} facets: synthesis, photocatalysis and gas-sensing

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Figure S1 displays the XRD pattern of the as-prepared $FeVO_4$-I. All the diffraction peaks may be readily indexed as a triclinic phase of $FeVO_4$-I (JCPDS 38-1372). No peaks from other phases have been detected. The sharp and narrow diffraction peaks reveal high crystallization of the as-prepared products.

Figure S2 is the thickness dispersion of the $FeVO_4$-II nanosheets.

Figure S3 is the XRD pattern of the sample with hexagonal nanosheet morphology obtained at pH of 12, which were identified as $Fe_{1.833}(OH)_{0.5}O_{0.5}$. All the diffraction peaks may be readily indexed as a hexagonal $Fe_{1.833}(OH)_{0.5}O_{0.5}$ (JCPDS 76-0182).

Figure S4 is the UV-Vis diffuse reflectance spectroscopy of $FeVO_4$-II and $FeVO_4$-I photocatalysts.

Figure S5 shows the plots of absorption squared (abs^2) versus energy and the square root of absorption ($abs^{1/2}$) versus energy for the $FeVO_4$-II absorption edge region. For semiconductors, the square of absorption coefficient is linear with respect to energy for direct optical transitions in the absorption edge region, whereas the

square root of absorption coefficient is linear with energy for indirect transition. The abs^2 versus energy plot in nearly linear, while the $abs^{1/2}$ versus energy deviates from the fitted straight line, which suggest that the absorption edge of $FeVO_4$-II is caused by direct transitions and its band gap can be determined as 2.0 eV.

The flat-band potential of $FeVO_4$-II was calculated employing an atom's Mulliken electronegativity theory [S1]: $E_{VB}=X_{FeVO4\text{-}II} - E^e + (1/2)E_g$, where E_{VB} is the potential of valance band top, $X_{FeVO4\text{-}II}$ is the electronegativity of the constituent atoms, E^e is the energy of free electrons on the hydrogen scale (ca. 4.5 eV) and Eg is the band gap energy of the $FeVO_4$-II (2.0 eV). Figure S6 shows a schematic band structure of $FeVO_4$-II semiconductor based on the earlier calculation. It is theoretically speculated that the band edge potentials of CB and VB of $FeVO_4$-II are 0.77 and 2.77 eV with respect to the vacuum level, respectively.

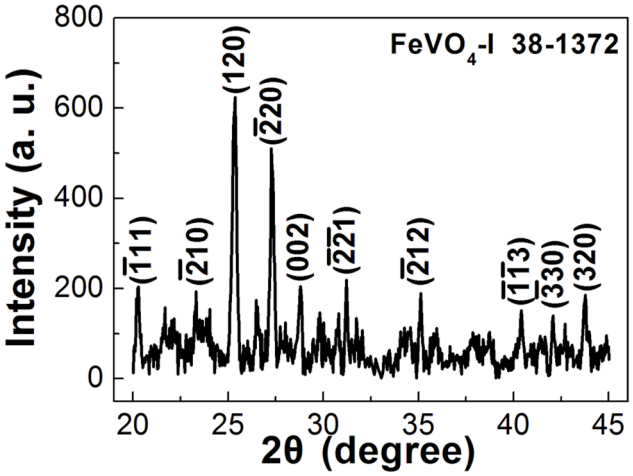

Fig. S1. (a) XRD pattern of the as-prepared products showing triclinic phase of $FeVO_4$-I.

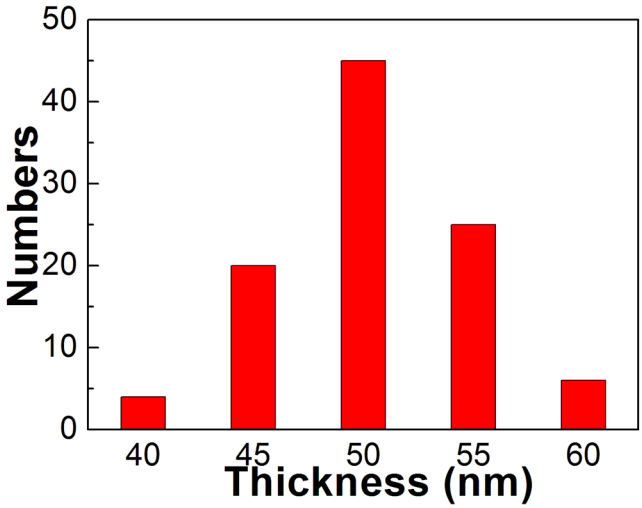

Fig. S2. The thickness dispersion of the $FeVO_4$-II nanosheets.

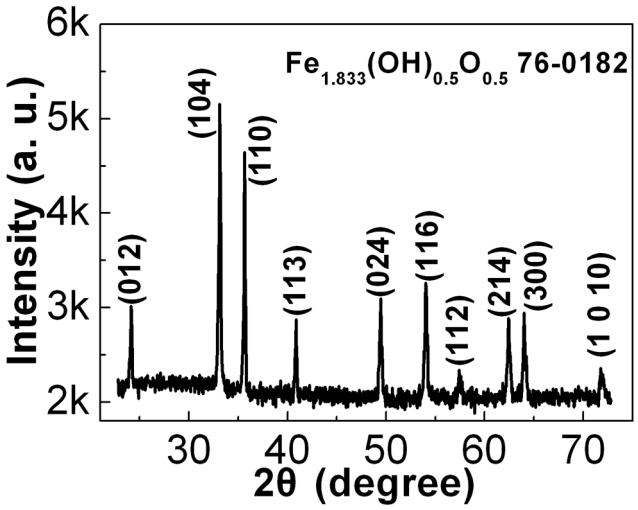

Fig. S3. XRD pattern of the products showing hexagonal $Fe_{1.833}(OH)_{0.5}O_{0.5}$ at pH 12.

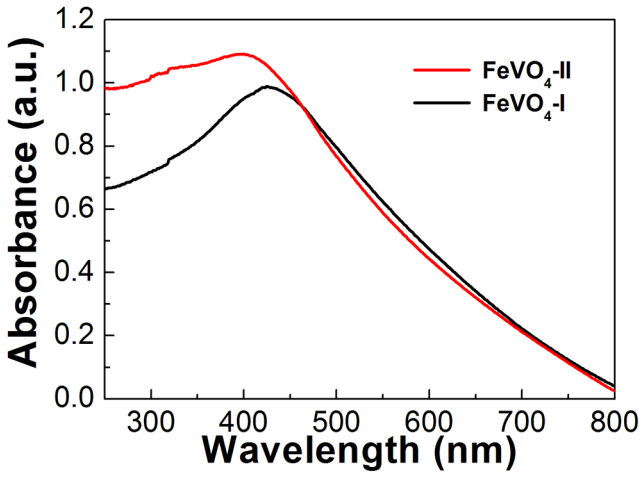

Fig. S4. UV-Vis diffuse reflectance spectroscopy of $FeVO_4$-II and $FeVO_4$-I photocatalysts.

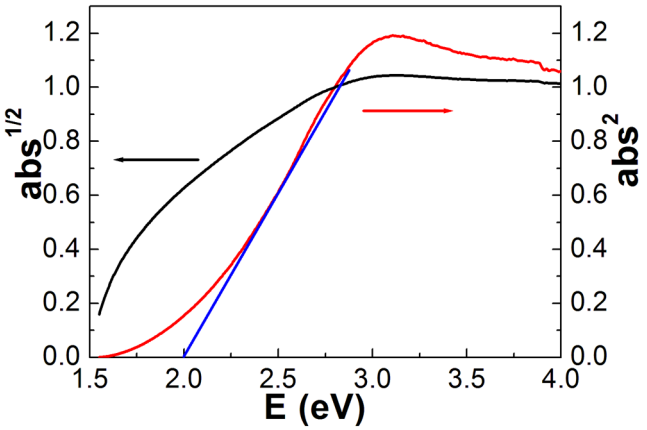

Fig. S5. The plots of absorption squared (abs^2) and the square root of absorption (abs1/2) versus energy for the $FeVO_4$-II absorption in the absorption edge region of $FeVO_4$-II sample.

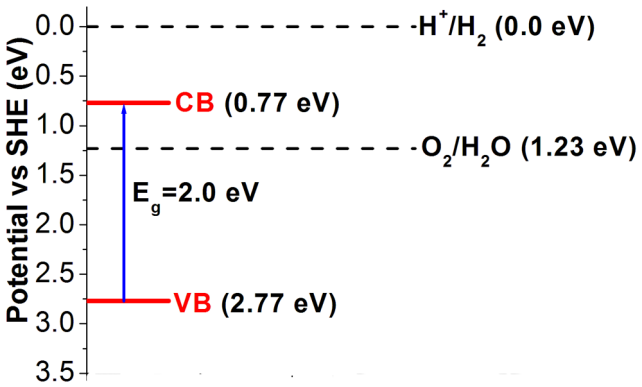

Fig. S6. Schematic band structure of $FeVO_4$-II.

[S1] Z. Jiang, F. Yang, G. D. Yang, L. Kong, M. O. Jones, T. C. Xiao, P. P. Edwards, Journal of Photochemistry and Photobiology A: Chemistry, 2010, 212, 8-13.