

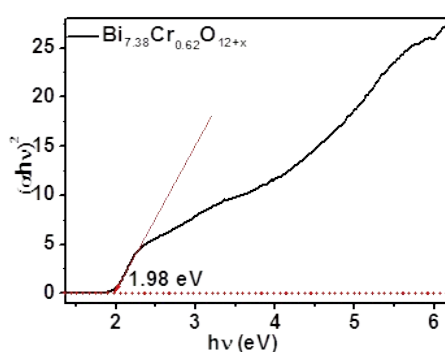
Supporting information for

## **Bi<sub>7.38</sub>Cr<sub>0.62</sub>O<sub>12+x</sub> crystal as a novel Visible-Light-Active Photocatalyst up to ~650 nm**

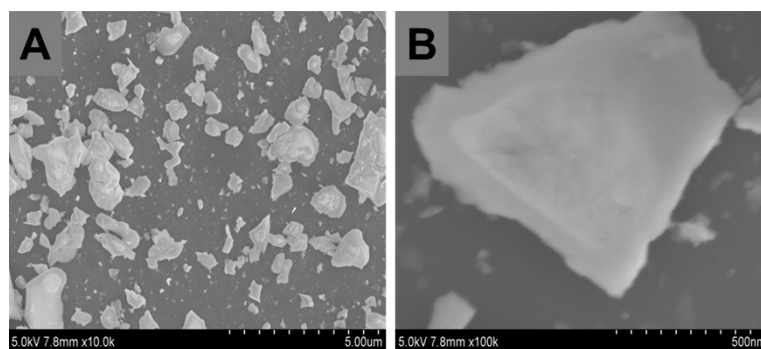
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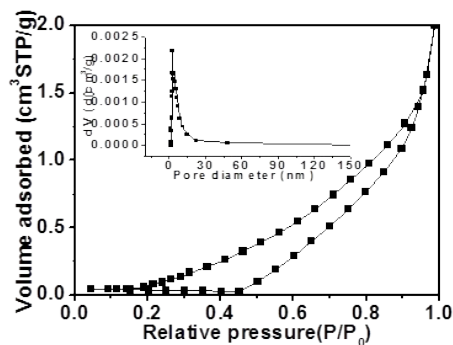
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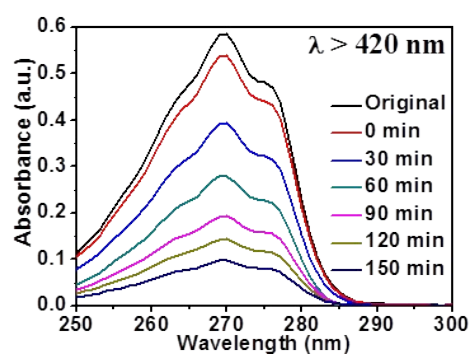
**Fig. S1.** The plot of transformed Kubelka-Munk function vs the energy of Bi<sub>7.38</sub>Cr<sub>0.62</sub>O<sub>12+x</sub> crystal.



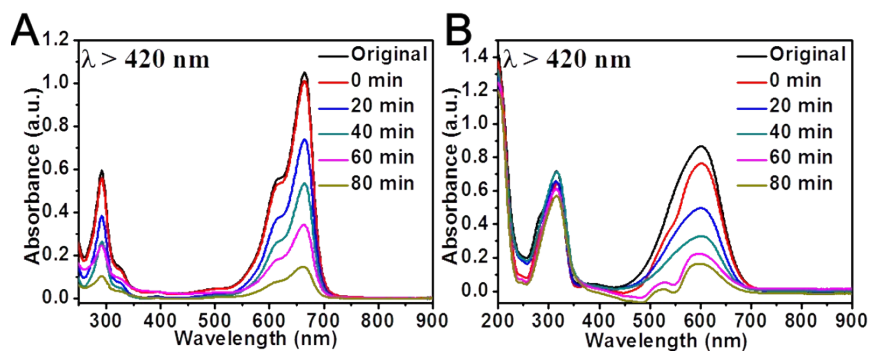
**Fig. S2.** The FE-SEM images of Bi<sub>7.38</sub>Cr<sub>0.62</sub>O<sub>12+x</sub> crystal.



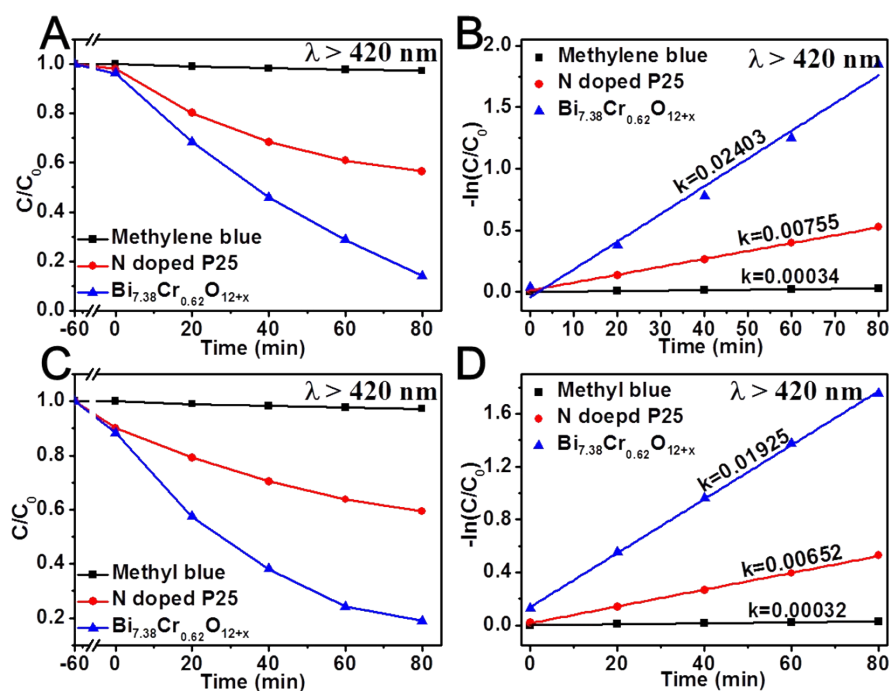
**Fig. S3.** The N<sub>2</sub> adsorption-desorption curve of Bi<sub>7.38</sub>Cr<sub>0.62</sub>O<sub>12+x</sub> crystal. Inset is the pore size distribution curve.



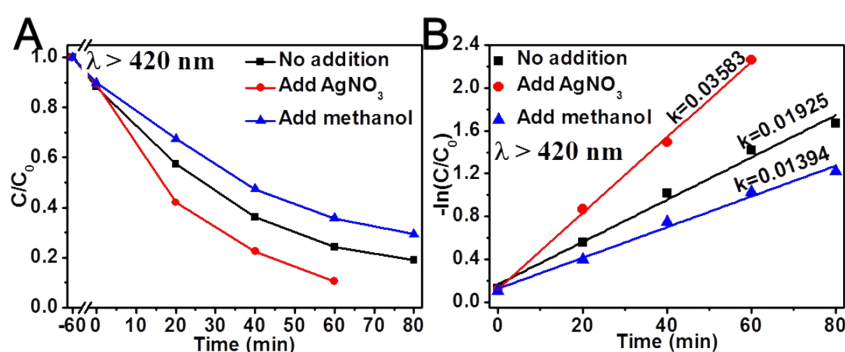
**Fig. S4.** The photocatalytic degradation ( $\lambda > 420$  nm) of phenol for Bi<sub>7.38</sub>Cr<sub>0.62</sub>O<sub>12+x</sub> crystal.



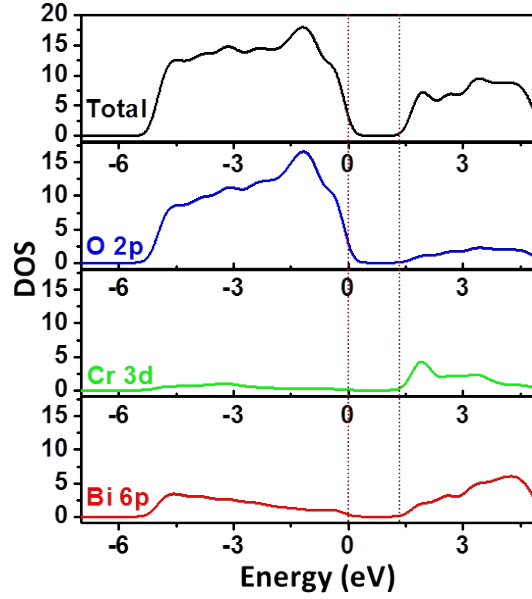
**Fig. S5.** The photocatalytic degradation ( $\lambda > 420$  nm) of methylene blue (A) and methyl blue (B) for Bi<sub>7.38</sub>Cr<sub>0.62</sub>O<sub>12+x</sub> crystal.



**Fig. S6.** The photocatalytic degradation ( $\lambda > 420$  nm) of methylene blue (A, B) and methyl blue (C, D) for N doped P25 and  $\text{Bi}_{7.38}\text{Cr}_{0.62}\text{O}_{12+x}$  crystal.



**Fig. S7.** The photocatalytic degradation ( $\lambda > 420$  nm) of methyl blue (A and B) by the addition of 100 mg of  $\text{AgNO}_3$  (electrons scavenger) and 5 mL of methanol (holes scavenger), respectively.



**Fig. S8.** The calculated density of state (DOS) of  $\text{Bi}_{7.38}\text{Cr}_{0.62}\text{O}_{12+x}$  was carried out by using the periodic density functional theory package of Cambridge Serial Total Energy Package (CASTEP) codes.

#### Calculation Method:

In this work, all of the calculations were carried out using the periodic density functional theory package of Cambridge Serial Total Energy Package (CASTEP) codes. CASTEP is a state-of-the-art quantum mechanics-based program designed specifically for solid-state materials science. The core electrons were treated with the ultrasoft pseudopotential. The exchange-correlation effects of valence electrons were described through the generalized gradient (GGA), within the Perdew-Burke-Ernzerhof (PBE) function. The  $\text{Bi}_{7.38}\text{Cr}_{0.62}\text{O}_{12}$  crystal structure was built based on the tetragonal  $\text{Bi}_2\text{O}_3$ , space group P-421 c(114), the  $2 \times 2 \times 2$  supercell of  $\text{Bi}_2\text{O}_3$  was built and one Bi atom was replaced by the Cr, which the formula approximate to  $\text{Bi}_{7.38}\text{Cr}_{0.62}\text{O}_{12}$ . The Monkhorst-Pack scheme  $k$ -points grid sampling was set as  $3 \times 3 \times 3$  for the irreducible Brillouin zone. An energy cutoff of 450 eV was used for expanding the Kohn-Sham wave functions. The convergence criteria were set as the force on the atoms less than  $0.01 \text{ eV } \text{\AA}^{-1}$ , the stress on the atoms less than 0.02 GPa, the atomic displacement less than  $5 \times 10^{-4} \text{ \AA}$ , and the energy change per atom less than  $5 \times 10^{-6} \text{ eV}$ .