Electronic Supplementary Information

Study of structural, electronic and optical properties of tungsten doped bismuth oxychloride by DFT calculations†

Wenjuan Yanga, Yanwei Wena, Rong Chenb, Dawen Zenga,*, Bin Shanac,*

a State Key Laboratory of Material Processing and Die and Mould Technology and School of Materials Science and Technology, Huazhong University of Science and Technology, Wuhan (430074), China

b State Key Laboratory of Digital Manufacturing Equipment and Technology, Huazhong University of Science and Technology, Wuhan (430074), Hubei, China

c Department of Materials Science and Engineering, The University of Texas at Dallas, Richardson, Texas (75080), USA

Corresponding author:

bshan@mail.hust.edu.cn (B. Shan); dwzeng@mail.hust.edu.cn (D. W. Zeng)
Fig. S1. The EDX of experimentally synthesized tungsten doped BiOX sample.
Fig. S2. The XPS of W element in experimentally synthesized tungsten doped BiOCl sample
Fig. S3. Band structure (spin up (left) and spin down (middle)) and PDOS (right) for the pure BiOCl using DFT-D2 correction. The fermi energy is set at the energy of zero.