The quantum size and spin-orbit coupling effect in BiVO$_4$ with several atomic layers studied by density functional theory

Taifeng Liu* and Yongqiang Zheng

National & Local Joint Engineering Research Center for Applied Technology of Hybrid Nanomaterials, Henan University, Kaifeng 475004, China

Corresponding author: Taifeng Liu: tfliu@vip.henu.edu.cn

Figure S1. (a) The geometry structure and (b) density of state (DOS) of the bulk BVO. In the DOS, the black line is the result without spin-orbit coupling (SOC), and the red line is the result with SOC. The red, purple, and grey spheres are O, Bi, and V atoms.
Figure S2. The geometry of (001) slabs. The red, purple, and grey spheres are O, Bi, and V atoms.

Figure S3. The geometry of (101) slabs. The red, purple, and grey spheres are O, Bi, and V atoms.
Figure S4. The DOS of all the (001)-slabs. From top to the bottom is the DOS of 1 to 8 Bi layers slab. The black line is the result without spin-orbit coupling (SOC), and the red line is the result with SOC.
Figure S5. The DOS of all the (101)-slabs. From the top to the bottom is the DOS of 2, 4, 6, 8 and 10 Bi layers slab. The black line is the result without spin-orbit coupling (SOC), and the red line is the result with SOC.

Figure S6. The structure of OER intermediates (a, d) OH*, (b, e) O*, and (c, f) OOH* on (001) and (101) slabs respectively. The red, purple, grey, and white spheres are O, Bi, V, and H atoms.
Figure S7. The structure of HER intermediates (a, d) H* on Bi site, (b, e) H* on O site, and (c, f) H* on V site on (001) and (101) slabs respectively. The red, purple, grey, and white spheres are O, Bi, V, and H atoms.