Supporting Information for

Electron polarons in the subsurface layer of Mo/W-doped BiVO₄ surfaces

Jianhang Cen, Shunning Li*, Jiaxin Zheng, Feng Pan*

School of Advanced Materials, Peking University, Shenzhen Graduate School,

Shenzhen 518055, People's Republic of China

*Corresponding authors: S. Li (lisn@pkusz.edu.cn) and F. Pan

(panfeng@pkusz.edu.cn)

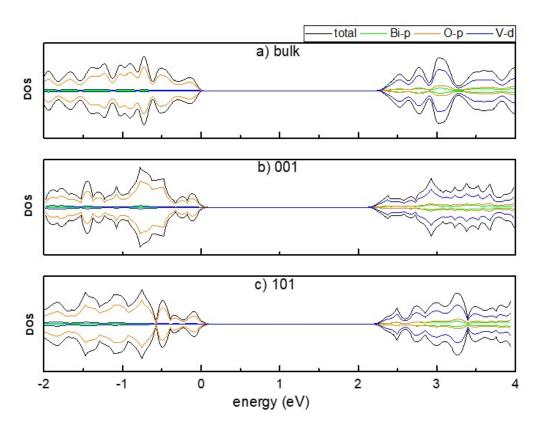


Fig. S1 DOS of (a) $BiVO_4\,bulk,$ (b) (001) surface, and (c) (101) surface.

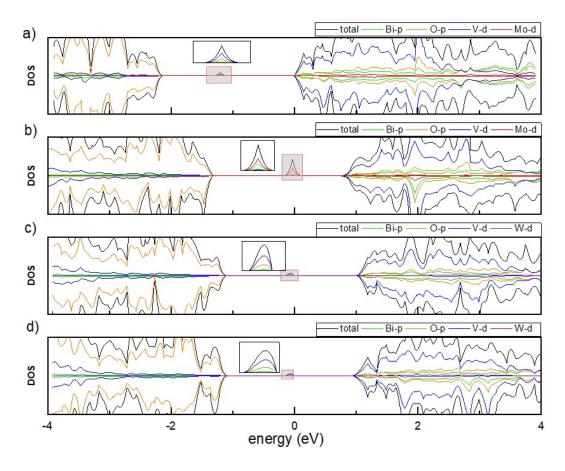


Fig S2 DOS for Mo/W-doped (001) surfaces. Mo doped in (a) the first and (b) second layers; W doped in (c) the first and (d) second layers.

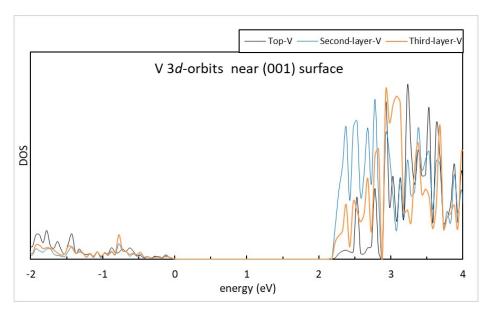


Fig. S3 Local DOS of V-3d orbitals near the (001) surface.

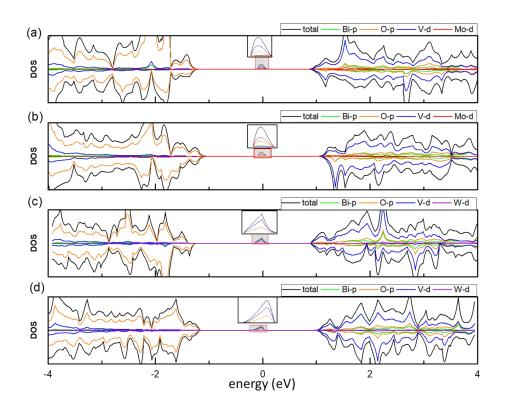


Fig S4 DOS for Mo/W-doped (101) surfaces. Mo doped in (a) the first and (b) second layers; W doped in (c) the first and (d) second layers.

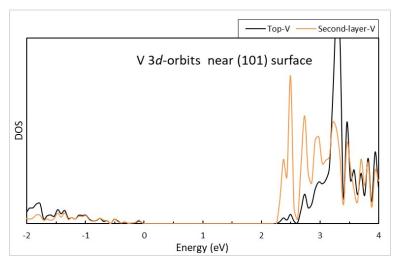


Fig. S5 Local DOS of V-3d orbitals near the (101) surface.