Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

The Oxygen Evolution Reaction (OER) Activity Sites in $BiVO_4$ Studied by Density Functional Theory and experiment

Qingyan Zhang[1], Guowei Liu[1], Taifeng Liu*[1]

[1]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

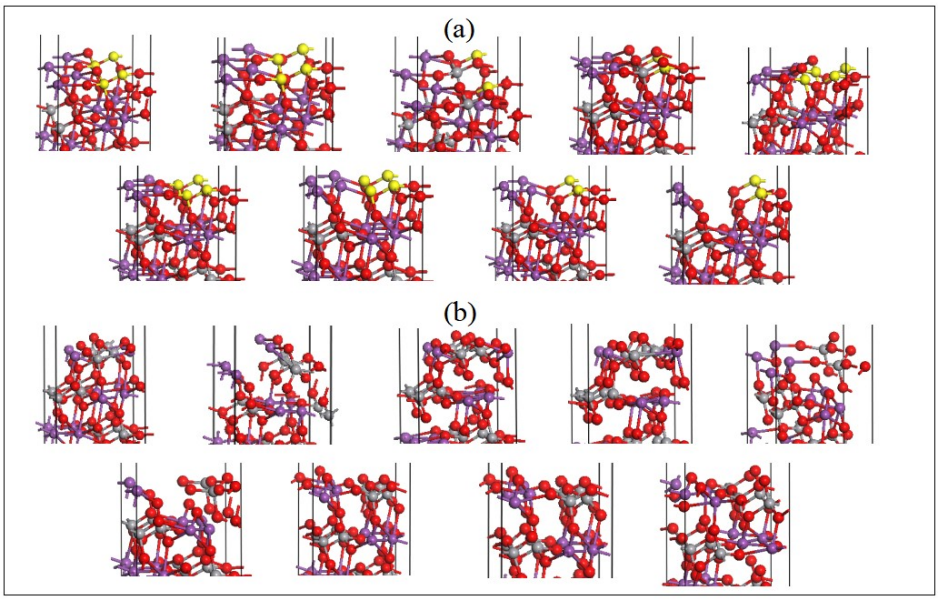

Figure S1. Different termination of (112) surface (a) before and (b) after optimization. In the optimization, strong surface reconstruction occur and the V site on the surface becomes four coordinated as in the bulk. The lattice parameters of this slab are a=7.250 Å，b=13.671 Å，c=33.922 Å，α=β=90.0°，γ=89.8°. The K-points in the calculation are 3×2×1.

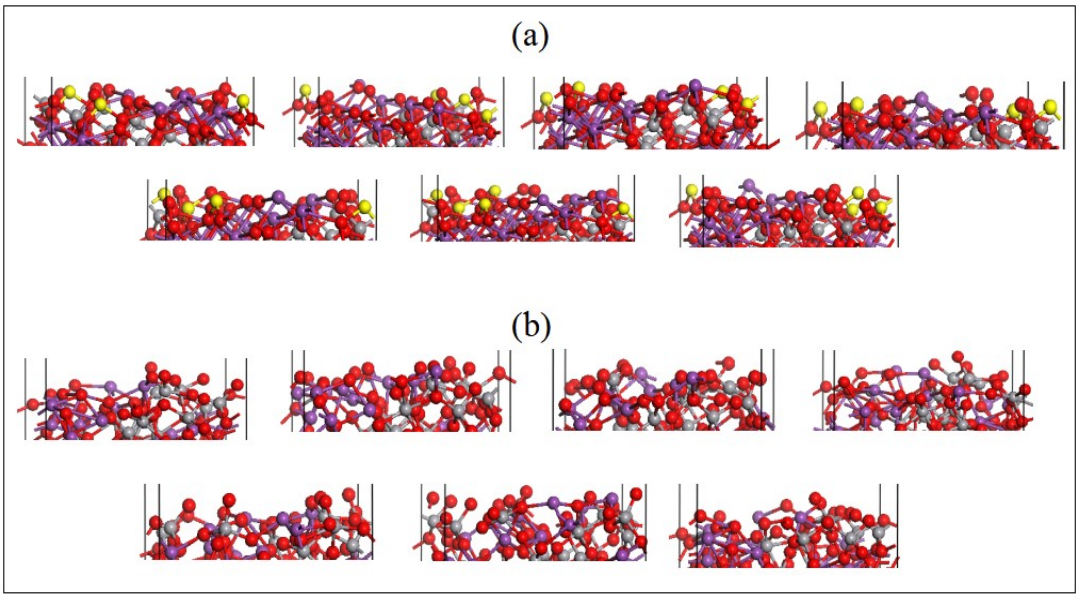

Figure S2. Different termination of (511) surface (a) before and (b) after optimization. In the optimization, strong surface reconstruction occur and the V site on the surface becomes four coordinated as in the bulk. The lattice parameters of this slab are a=5.138 Å，b=23.763 Å，c=27.471 Å，α=β=90.0°，γ=90.4°. The K-points in the calculation are 4×1×1.

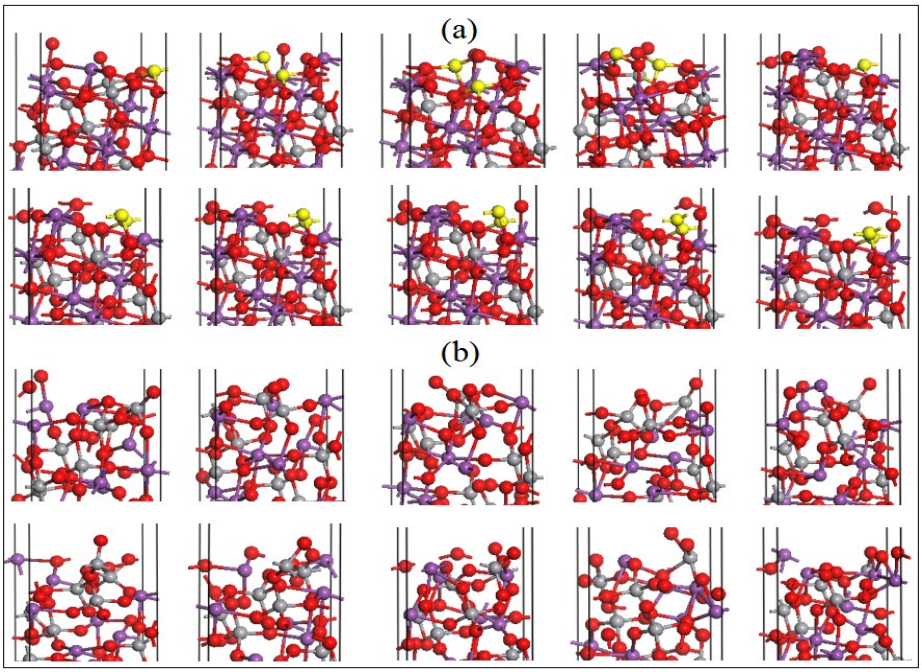

Figure S3. Different termination of (111) surface (a) before and (b) after optimization. In the optimization, strong surface reconstruction occur and the V site on the surface becomes four coordinated as in the bulk. The lattice parameters of this slab are a=7.250 Å，b=12.676 Å，c=30.241 Å，α=β=90.0°，γ=106.5°. The K-points in the calculation are 3×2×1.

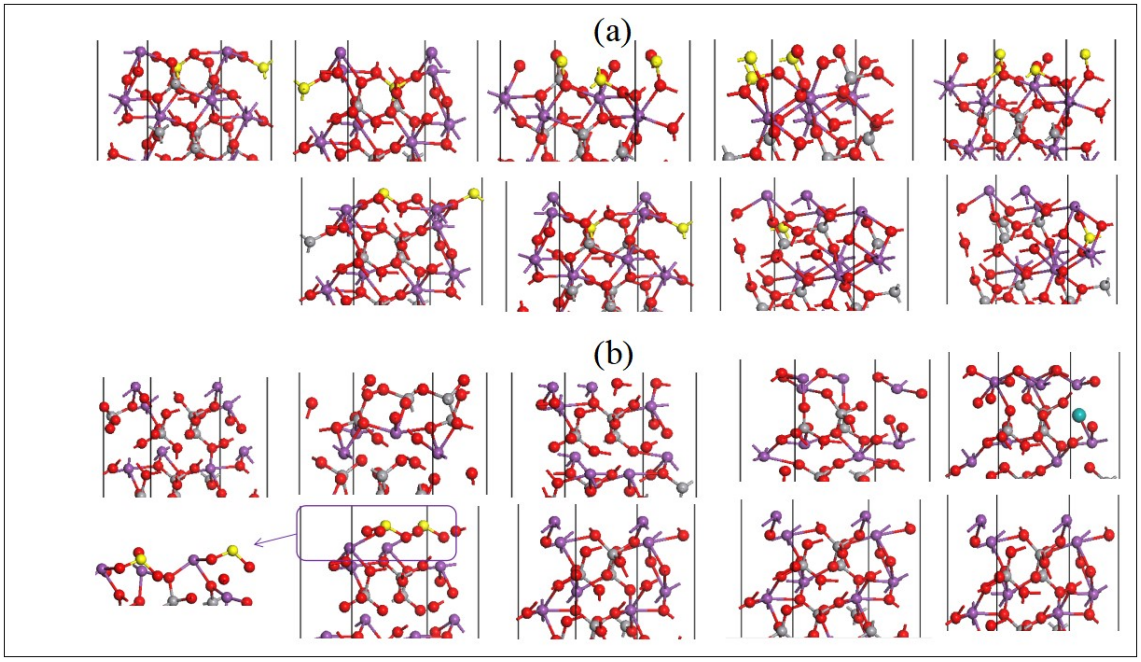

Figure S4. Different termination of (011) surface (a) before and (b) after optimization. In the optimization, strong surface reconstruction occur and the V site on most of the surface becomes four coordinated as in the bulk. However, we did find that there is one slab with unsaturated V site. The lattice parameters of this slab are a=5.138 Å，b=12.676 Å，c=33.720 Å，α=β=90.0°，γ=90.1°. The K-points in the calculation are 4×2×1.

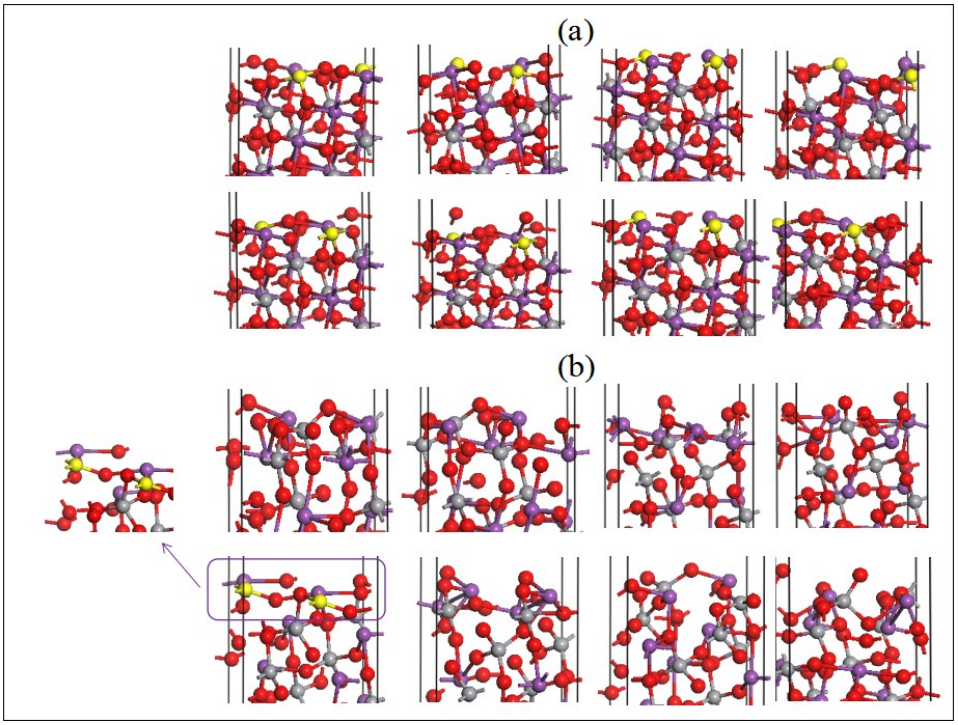

Figure S5. Different termination of (110) surface (a) before and (b) after optimization. In the optimization, strong surface reconstruction occur and the V site on most of the surface becomes four coordinated as in the bulk. However, we did find that there is one slab with unsaturated V site. The lattice parameters of this slab are a=11.604 Å， b=7.250 Å， c=30.451 Å， α=β=γ=90.0°. The K-points in the calculation are 2×4×1.

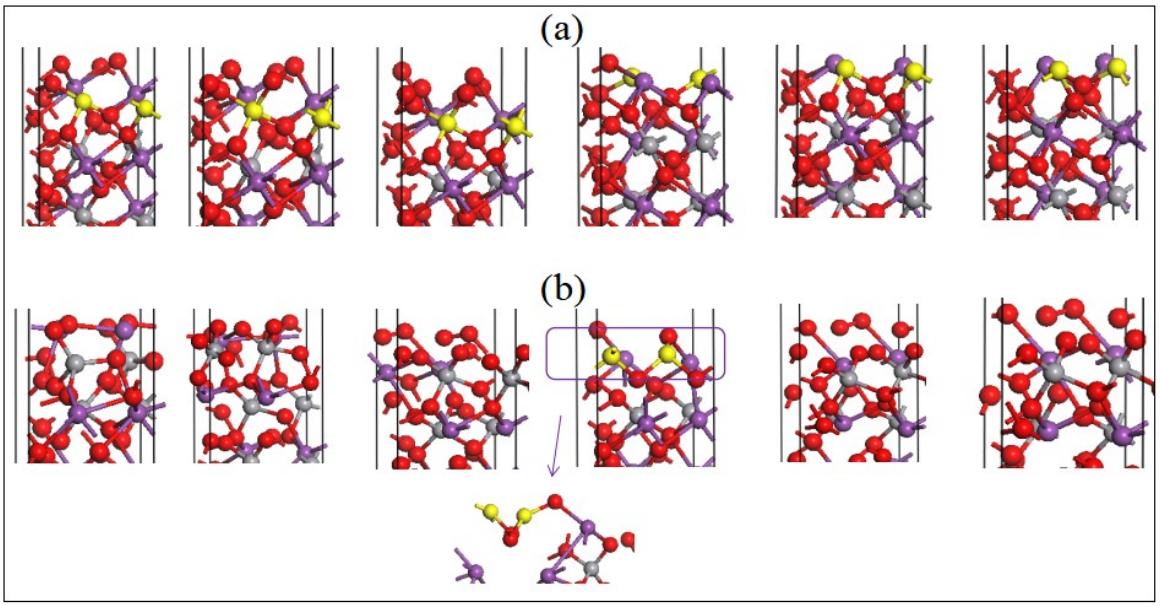

Figure S6. Different termination of (010) surface (a) before and (b) after optimization. In the optimization, strong surface reconstruction occur and the V site on most of the surface becomes four coordinated as in the bulk. However, we did find that there is one slab with unsaturated V site. The lattice parameters of this slab are a=11.605 Å， b=5.138 Å， c=34.582 Å， α=β=γ=90.0°. The K-points in the calculation are 2×4×1.

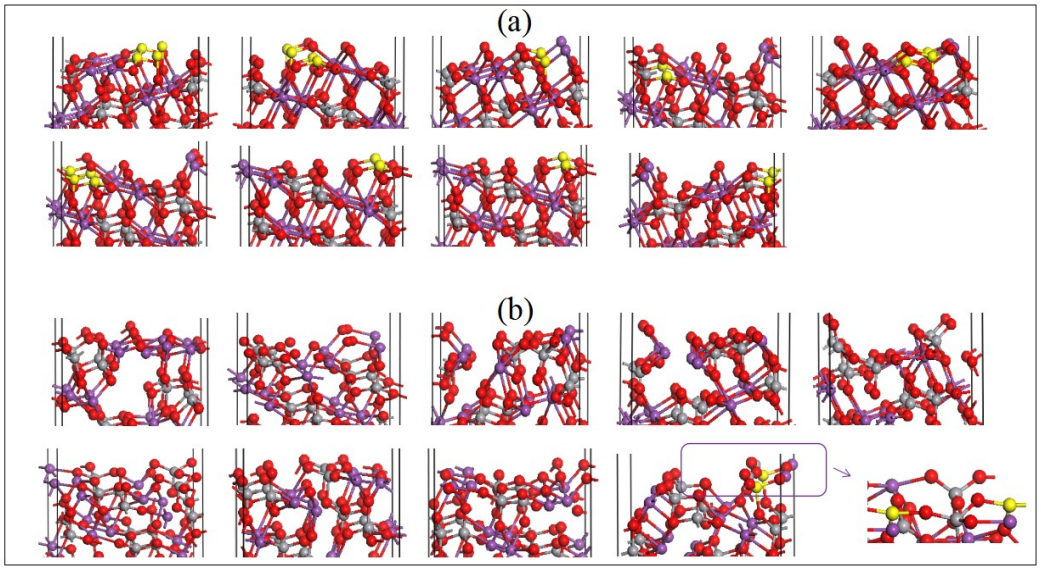

Figure S7. Different termination of (123) surface (a) before and (b) after optimization. In the optimization, strong surface reconstruction occur and the V site on most of the surface becomes four coordinated as in the bulk. However, we did find that there is one slab with unsaturated V site. The lattice parameters of this slab are a=11.486 Å，b=13.671 Å，c=29.673 Å，α=β=90.0°，γ=80.2°. The K-points in the calculation are 2×2×1.

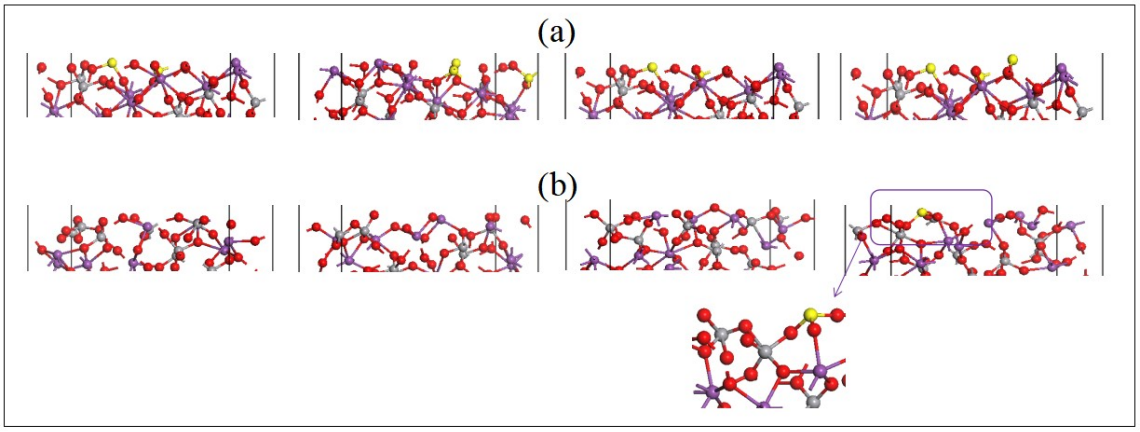

Figure S8. Different termination of (021) surface (a) before and (b) after optimization. In the optimization, strong surface reconstruction occur and the V site on most of the surface becomes four coordinated as in the bulk. However, we did find that there is one slab with unsaturated V site. The lattice parameters of this slab are a=5.138 Å，b=23.763 Å，c=27.471 Å，α=β=γ=90.0°，γ=80.2°. The K-points in the calculation are 4×2×1.

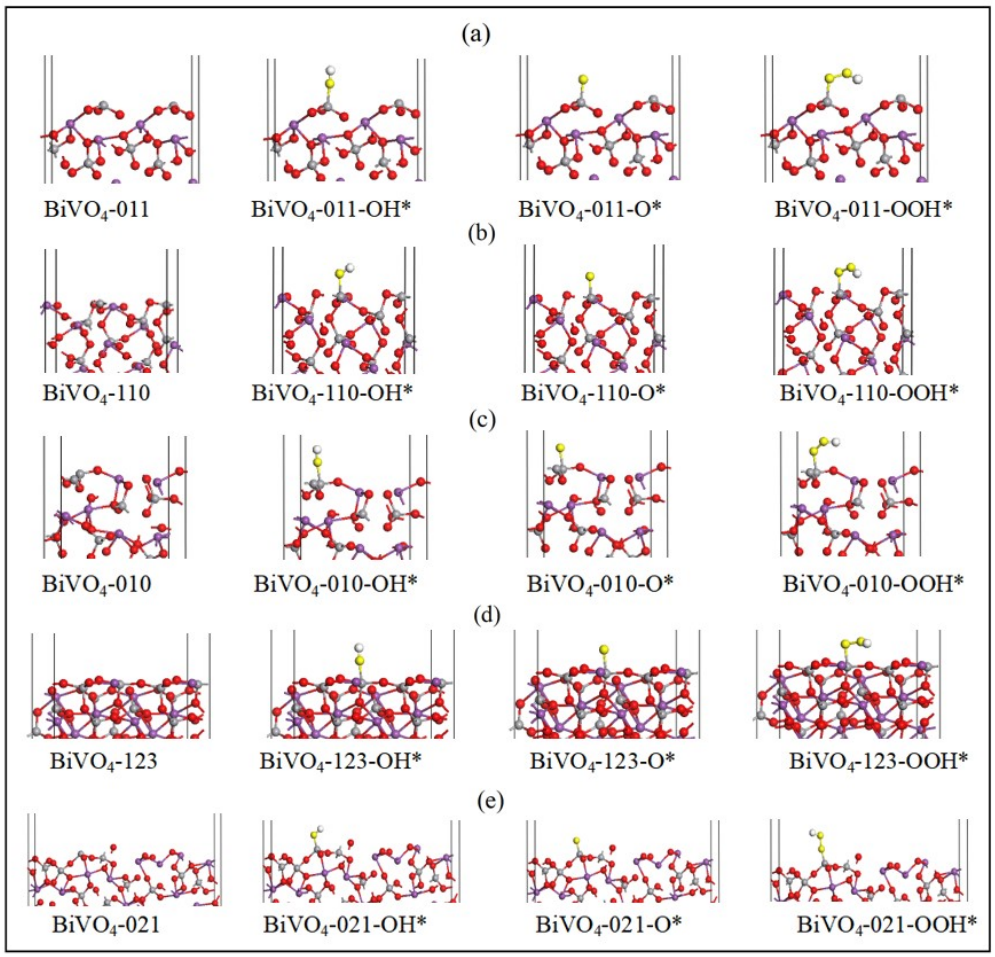

Figure S9. The intermediates of OER on V site of (011), (110), (010), (123), and (021) surfaces.

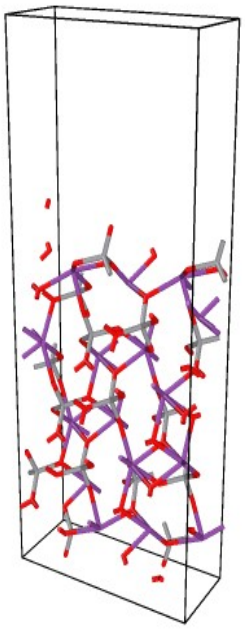

Figure S10. The geometry changes during the molecular dynamics simulation with 300 K.

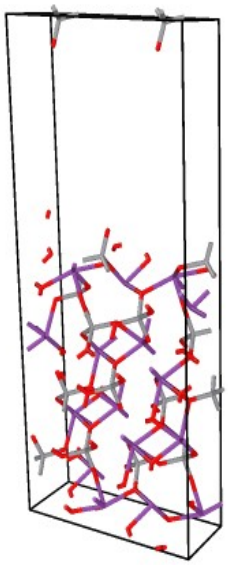

Figure S11. The geometry changes during the molecular dynamics simulation with 673 K.