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


# Bond lengths of pure and Mo-doped *m*$BiVO_4$ (010) surfaces.

# Geometric structures of adsorptive surfaces.

*Supporting information to accompany*

**"Why the photocatalytic activity of Mo-doped $BiVO_4$ is enhanced: a comprehensive density functional study"**

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Table S1. The bond lengths of the outmost layer of (010) surface.

| Bond | (010) surface |
|---|---|
| Bi-O/ Å | 2.530 ×2 |
| | 2.341 ×2 |
| | 2.355 ×2 |
| V-O/ Å | 1.683 ×2 |
| | 1.813 ×2 |

Table S2. The bond lengths of Mo-O bonds in Mo-doped (010) surfaces.

| The models of Mo-doped surfaces | | The bond lengths of Mo-O bond /Å |
|---|---|---|
| (010) | Mo@V_top | 1.774 ×2, 1.855 ×2 |
| | Mo@V_in | 1.861 ×2, 1.820 ×2 |
| | Mo@Bi_top | 1.906 ×2, 2.056 ×2, 2.129 ×2 |
| | Mo@Bi_in | 2.157 ×2, 2.136 ×2, 2.156 ×2, 2.476 ×2 |

Fig. S3. The spin electron denstiy of $Bi_{1-x}Mo_xVO_4$ predicted by the GGA level. (The issurface is at 0.03 $e$/Å$^3$)

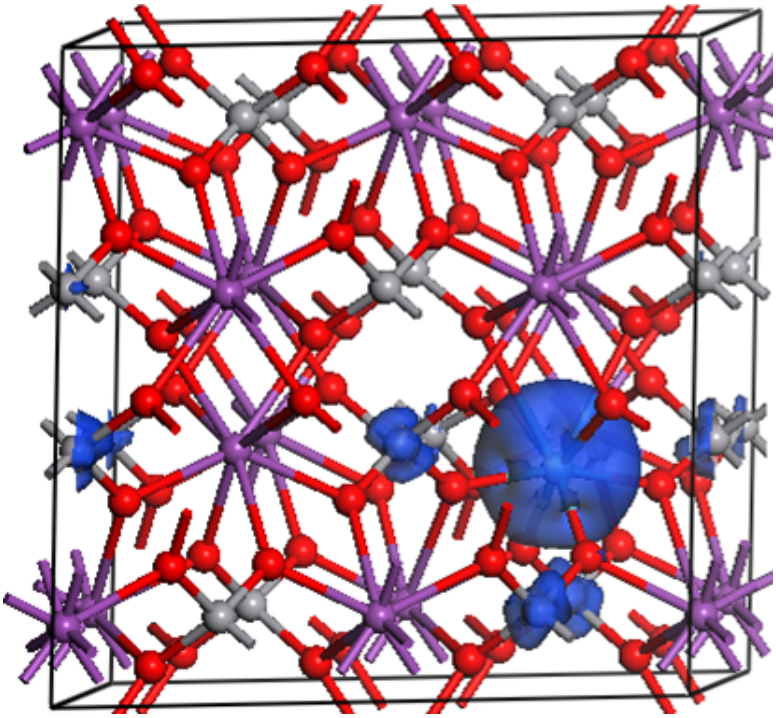

Fig. S4. The geometric structure of $H_2O$ adsorbed on Mo@V_top surface.

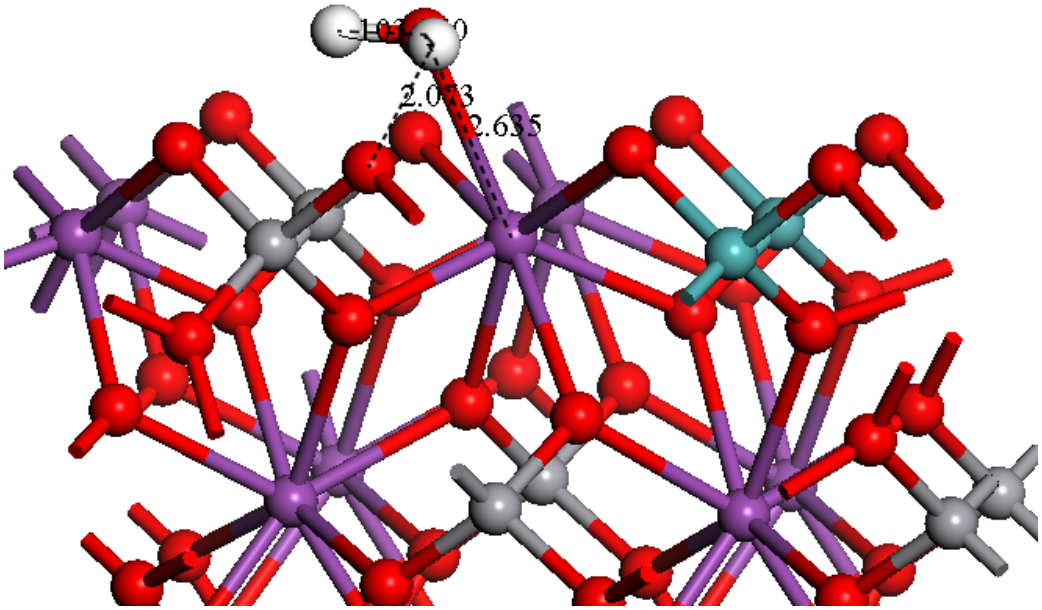

Fig. S5. The geometric structure of $H_2O$ adsorbed on Mo@V_in surface.

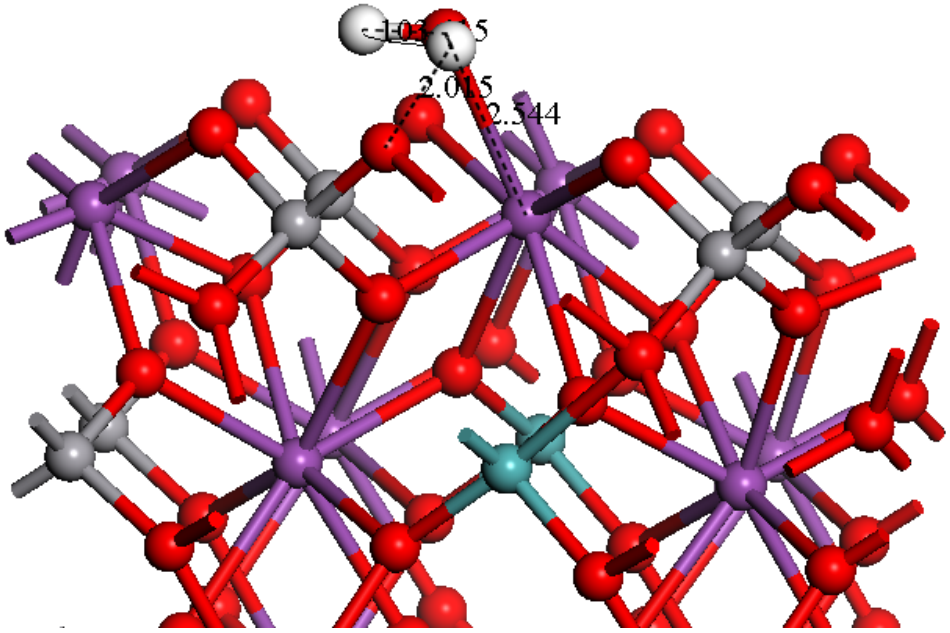

Fig. S6. The geometric structure of $H_2O$ adsorbed on Mo@Bi_in surface.