

Description of Additional Supplementary Files

File Name: Supplementary Data 1

Description: Atomic coordinates for the optimized structures of $\text{Zn}_3(\text{PO}_4)_2$ before adsorption.

File Name: Supplementary Data 2

Description: Atomic coordinates for the optimized structures of Zn adsorption on $\text{Zn}_3(\text{PO}_4)_2$ at the site 1.

File Name: Supplementary Data 3

Description: Atomic coordinates for the optimized structures of Zn adsorption on $\text{Zn}_3(\text{PO}_4)_2$ at the site 2.

File Name: Supplementary Data 4

Description: Atomic coordinates for the optimized structures of SO_4^{2-} adsorption on $\text{Zn}_3(\text{PO}_4)_2$ at the site 1.

File Name: Supplementary Data 5

Description: Atomic coordinates for the optimized structures of SO_4^{2-} adsorption on $\text{Zn}_3(\text{PO}_4)_2$ at the site 2.

File Name: Supplementary Data 6

Description: Atomic coordinates for the optimized structures of SO_4^{2-} adsorption on $\text{Zn}_3(\text{PO}_4)_2$ at the site 3.