Supplementary Materials

The Effects of Acid and Water in the Formation of Anodic Alumina: DFT and Experiment Study

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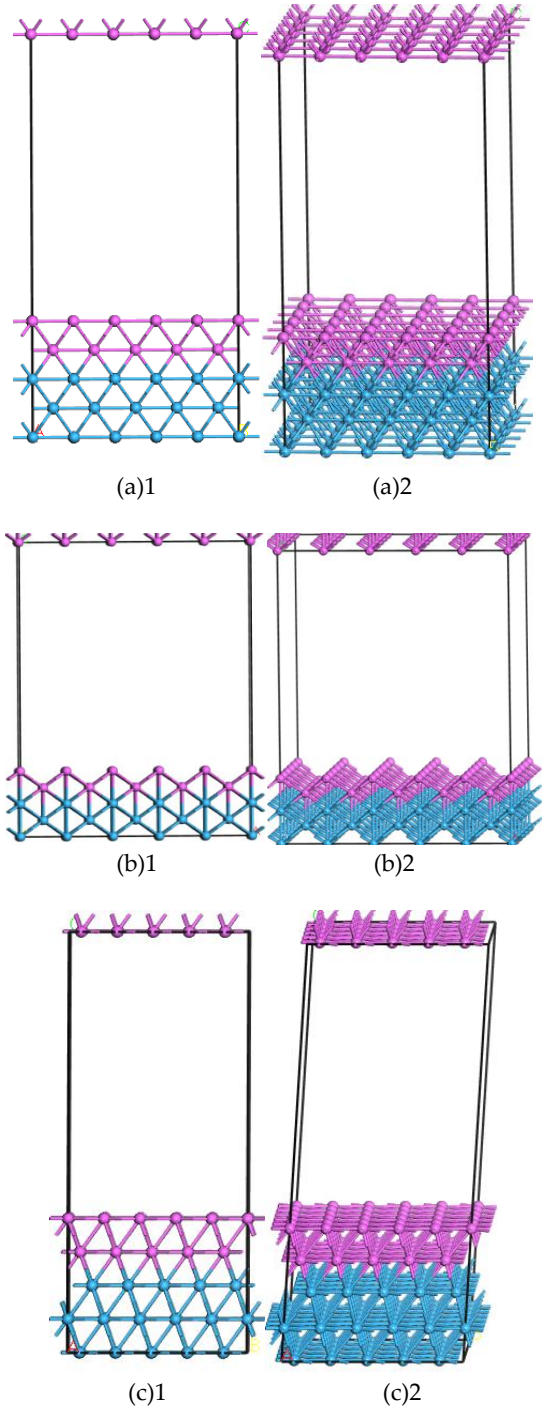
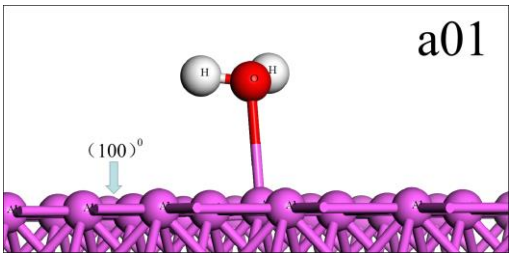


Figure S1. The aluminium slabs of three faces. The coordinates of the blue atoms are fixed, other atoms relax freely.
(a)1: the side view of (100) slab; (a)2: the oblique view of (100) slab;
(b)1: the side view of (110) slab; (b)2: the oblique view of (110) slab;
(c)1: the side view of (111) slab; (c)2: the oblique view of (111) slab.



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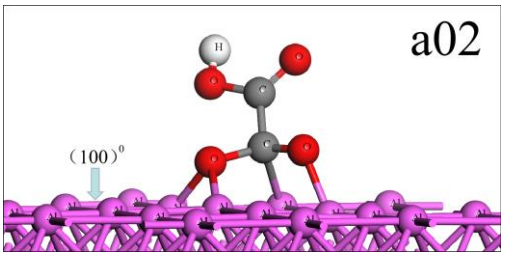

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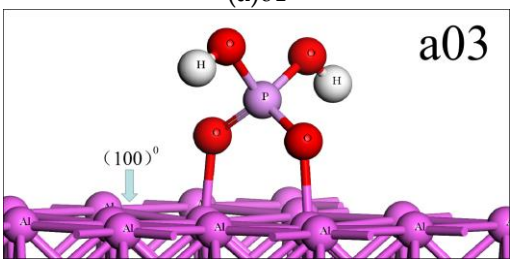

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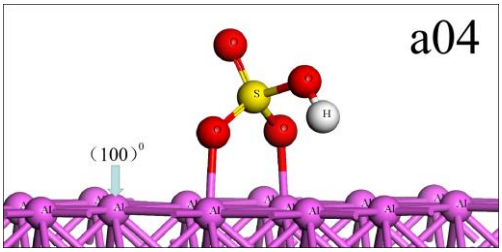

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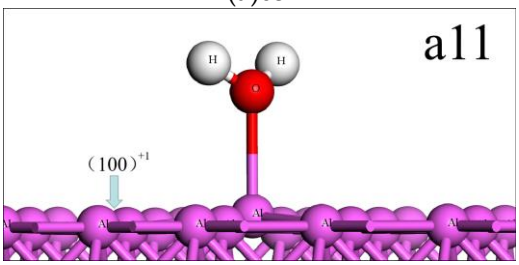

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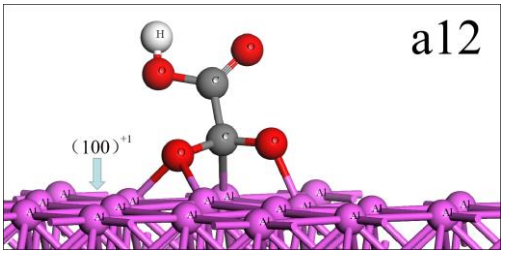

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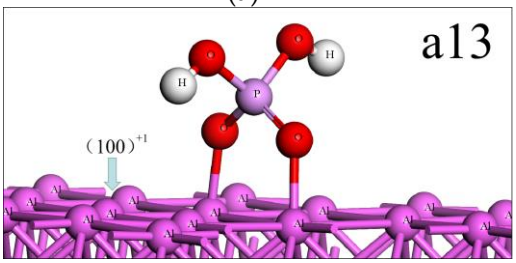

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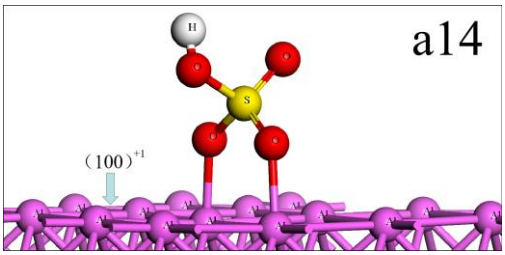

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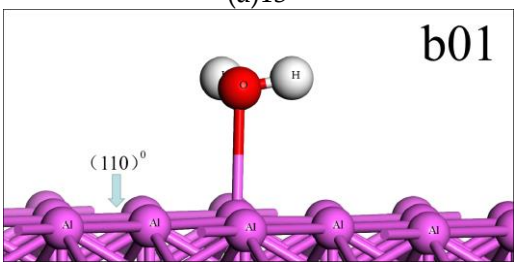

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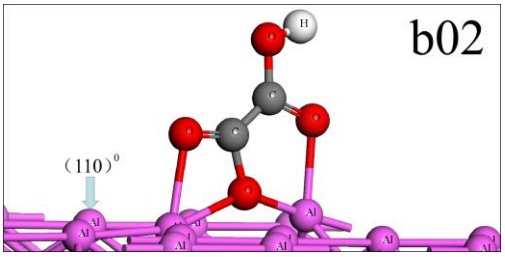

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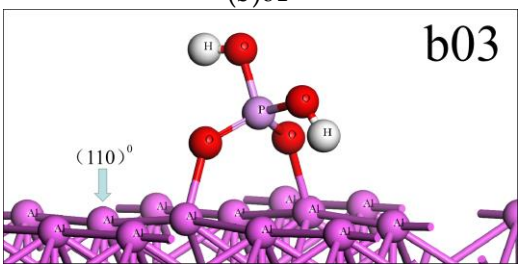

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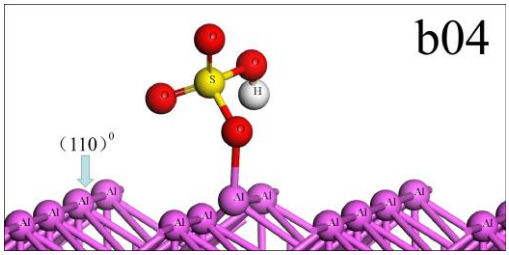

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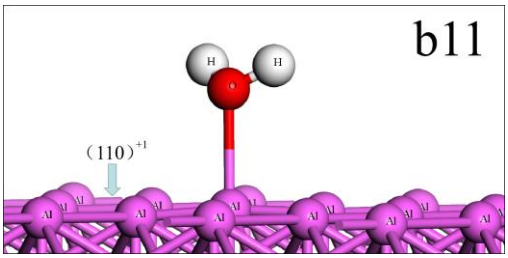

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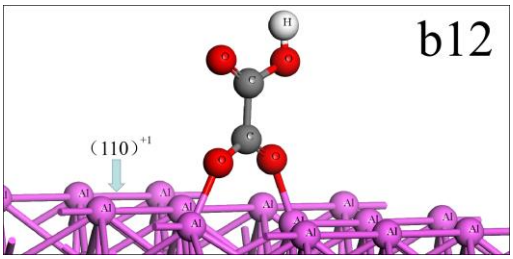

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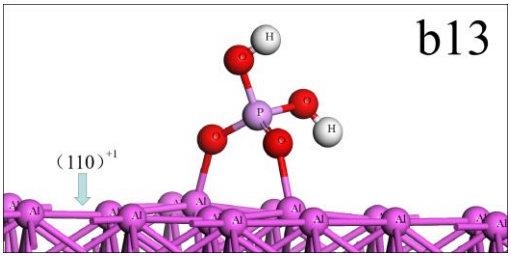

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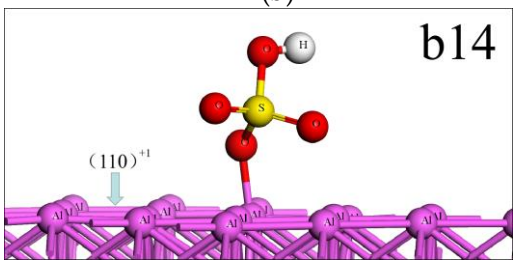

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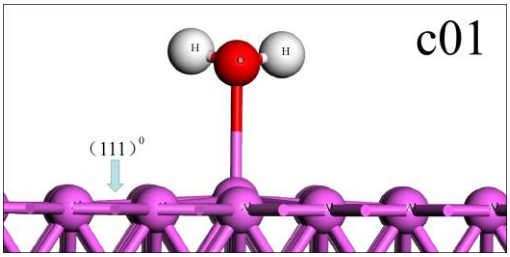

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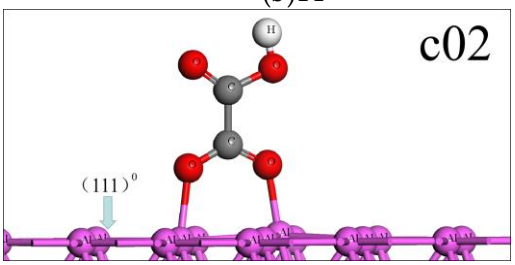

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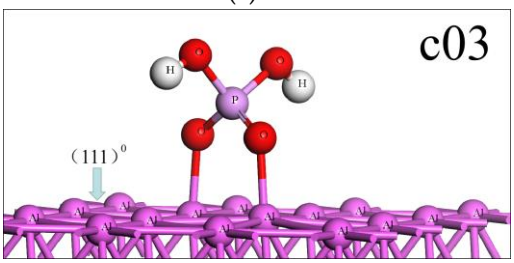

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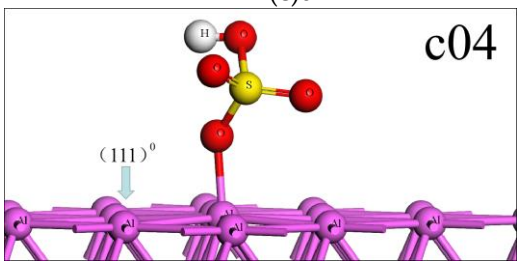

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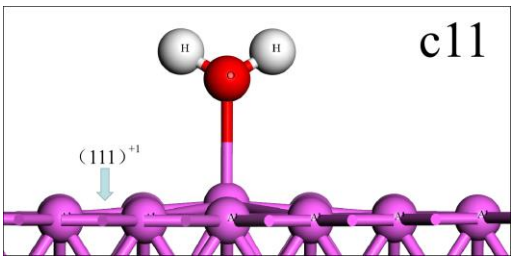

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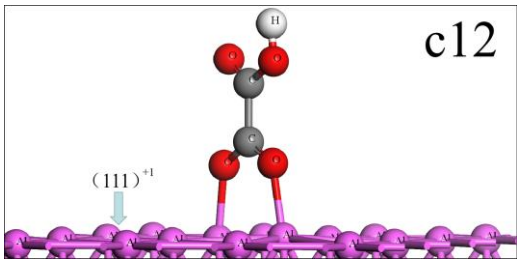

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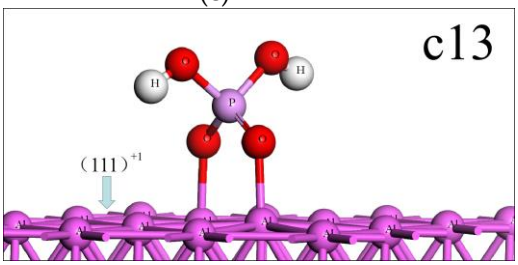

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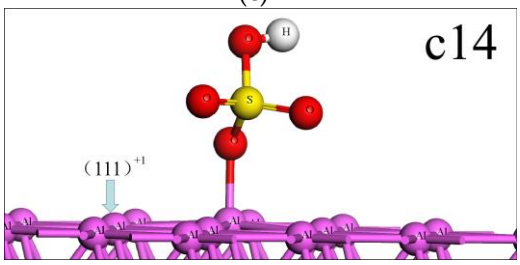


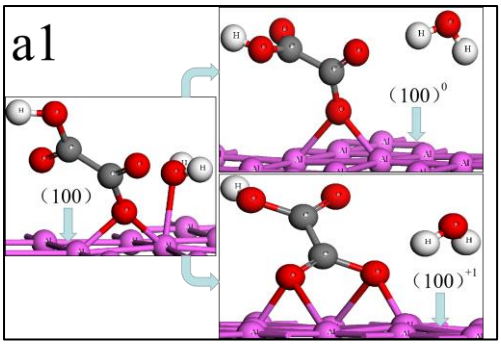
(c)14

Figure S2. The acid radicals and water adsorb on the natural and positively charged slabs. (a)01: the H_2O adsorbs on the natural (100) salb; (a)02: the $HC_2O_4^-$ adsorbs on the natural (100)

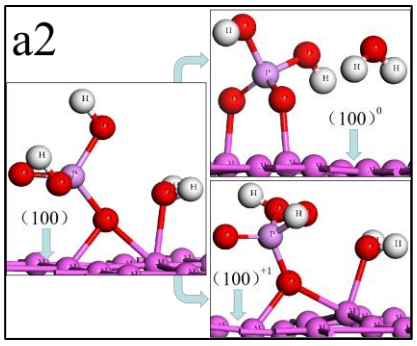
salb; (a)03: the $H_2PO_4^-$ adsorbs on the natural (100) salb; (a)04: the HSO_4^- adsorbs on the natural (100) salb; (a)11: the H_2O adsorbs on the positively charged (100) salb; (a)12: the $HC_2O_4^-$ adsorbs on the positively charged (100) salb; (a)13: the $H_2PO_4^-$ adsorbs on the positively charged (100) salb; (a)14: the HSO_4^- adsorbs on the positively charged (100) salb.

(b)01: the H_2O adsorbs on the natural (110) salb; (b)02: the $HC_2O_4^-$ adsorbs on the natural (110) salb; (b)03: the $H_2PO_4^-$ adsorbs on the natural (110) salb; (b)04: the HSO_4^- adsorbs on the natural (110) salb; (b)11: the H_2O adsorbs on the positively charged (110) salb; (b)12: the $HC_2O_4^-$ adsorbs on the positively charged (110) salb; (b)13: the $H_2PO_4^-$ adsorbs on the positively charged (110) salb; (b)14: the HSO_4^- adsorbs on the positively charged (110) salb.

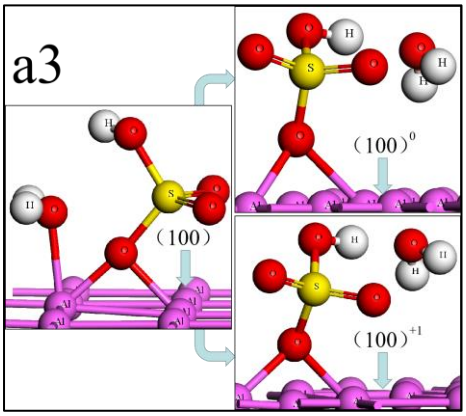
(c)01: the H_2O adsorbs on the natural (111) salb; (c)02: the $HC_2O_4^-$ adsorbs on the natural (111) salb; (c)03: the $H_2PO_4^-$ adsorbs on the natural (111) salb; (c)04: the HSO_4^- adsorbs on the natural (111) salb; (c)11: the H_2O adsorbs on the positively charged (111) salb; (c)12: the $HC_2O_4^-$ adsorbs on the positively charged (111) salb; (c)13: the $H_2PO_4^-$ adsorbs on the positively charged (111) salb; (c)14: the HSO_4^- adsorbs on the positively charged (111) salb.



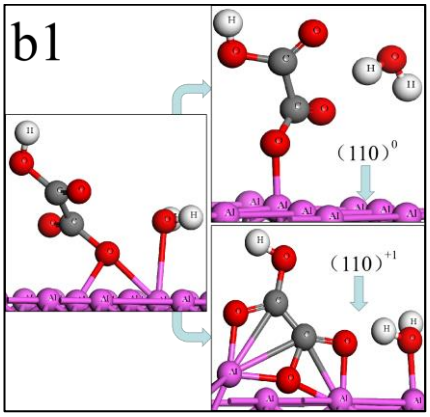
(a)1



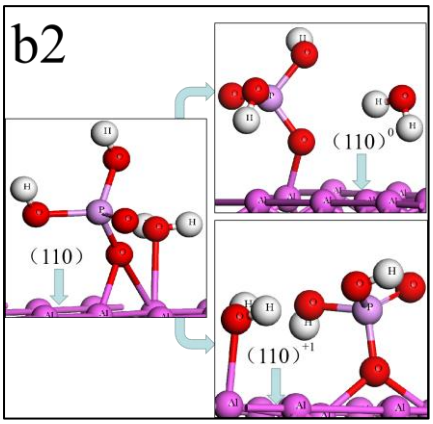
(a)2



(a)3



(b)1



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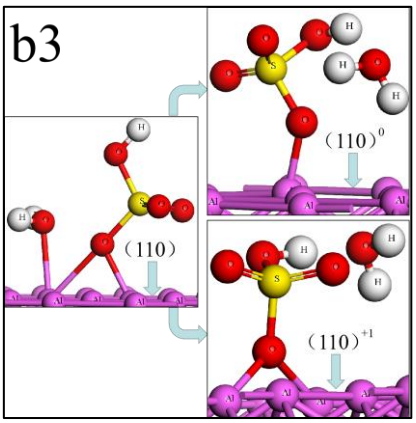

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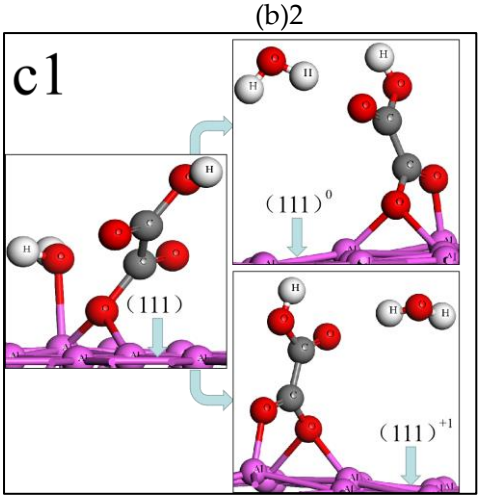

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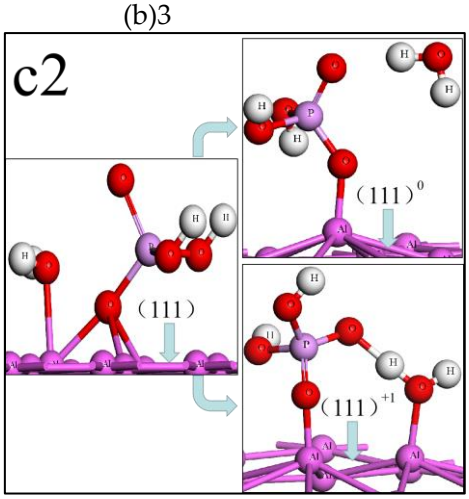

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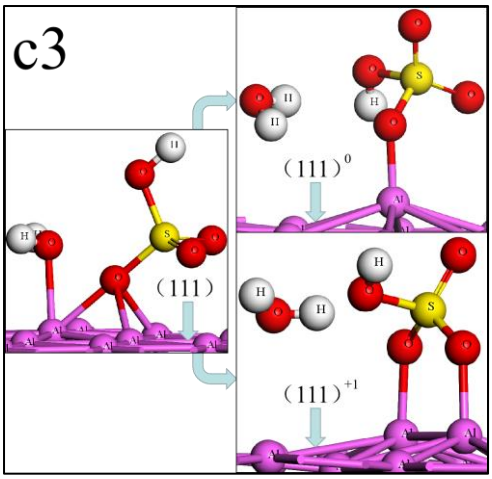

(c)3

Figure S3. The acid radicals substitute water on the natural and positively charged slabs.
(a)1: the $HC_2O_4^-$ substitute H_2O on the natural and positively charged slab of (100);
(a)2: the $H_2PO_4^-$ substitute H_2O on the natural and positively charged slab of (100);
(a)3: the HSO_4^- substitute H_2O on the natural and positively charged slab of (100);
(b)1: the $HC_2O_4^-$ substitute H_2O on the natural and positively charged slab of (110);
(b)2: the $H_2PO_4^-$ substitute H_2O on the natural and positively charged slab of (110);
(b)3: the HSO_4^- substitute H_2O on the natural and positively charged slab of (110);
(c)1: the $HC_2O_4^-$ substitute H_2O on the natural and positively charged slab of (111);
(c)2: the $H_2PO_4^-$ substitute H_2O on the natural and positively charged slab of (111);
(c)3: the HSO_4^- substitute H_2O on the natural and positively charged slab of (111);