Journal Name

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Supporting Information

1. Calculation methods

Before the single-point energy calculation, geometry optimization was done. The integration in reciprocal space was performed with a Monkhorst-Pack grid with a 7×2×5 *k*-point used for the bulk boehmite of size 2.90×12.34×3.74 $Å^3$. The self-consistent convergence accuracy was set at 1×10^{-5} eV/atom, the convergence criterion for the force between atoms was 3×10^{-2} eV/atom, and the maximum displacement was 1×10^{-3} Å.

Table S1. Optimized bulk lattice parameters of the γ-AlOOH crystal: our atomic orbital DFT calculations versus other DFT and experimental results.

Lattice parameter (Å)	GGA + PBE	GGA + PAW	Experimental result[1]	Experimental result[2]
a	2.90	2.90	2.87	2.85
b	12.18	11.97	12.23	12.24
c	3.73	3.71	3.69	3.69

Table S2. Parameters used for the calculation of the adsorption energy.

Crystal plane	100	010	001
Number of atoms	112 (+10)[a]	68 (+10)[a]	112 (+10)[a]
Slab thickness (Å)	15	15	15
Surface areas ($Å^2$)	92.4	43.6	71.8
Surface periodicity	$1b\times2c$	$2a\times2c$	$2a\times1b$
k-mesh	1×1×1	1×1×1	1×1×1

[a] Corresponding to three water molecules and one metal cation.

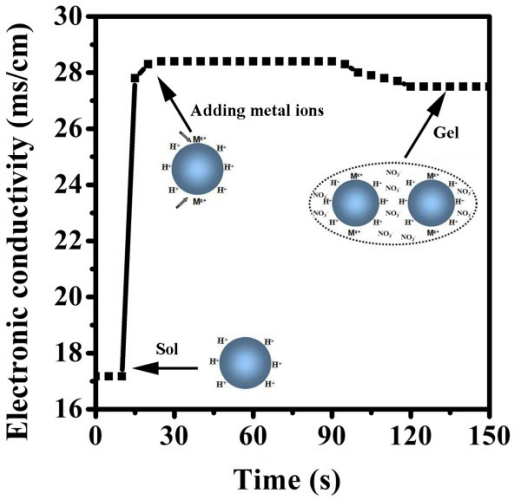

Fig. S1 The electrical conductivity change in γ-AlOOH sol-gel transformation.

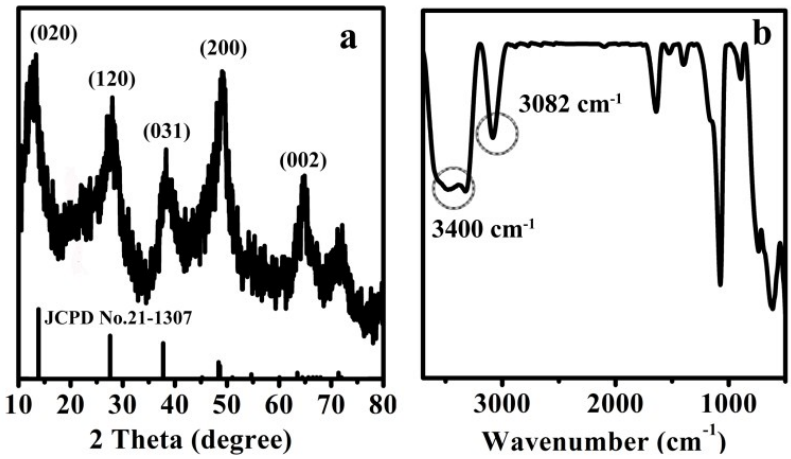

Fig. S2 The FTIR spectrum of as-prepared γ-AlOOH.

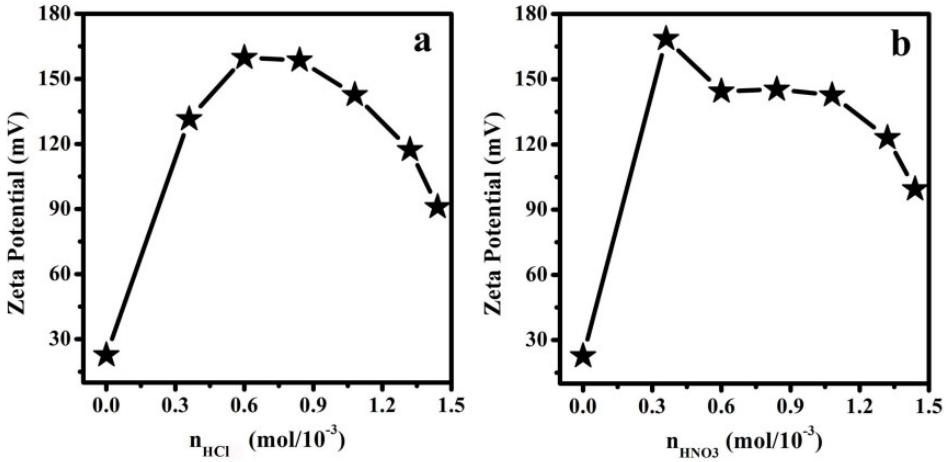

Fig. S3 Zeta potential of γ-AlOOH sol by adding (a) HCl and (b) HNO_3.

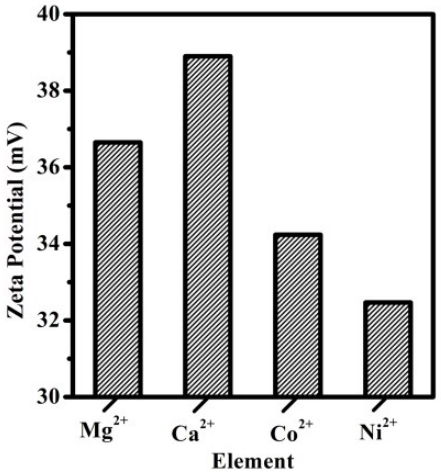

Fig. S4 Zeta potential of γ-AlOOH sol by adding different metal cations.

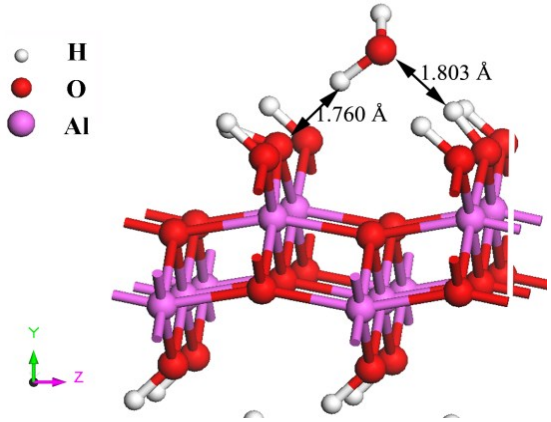

Fig.S5 Optimized structure of H2O on (010) crystal face.

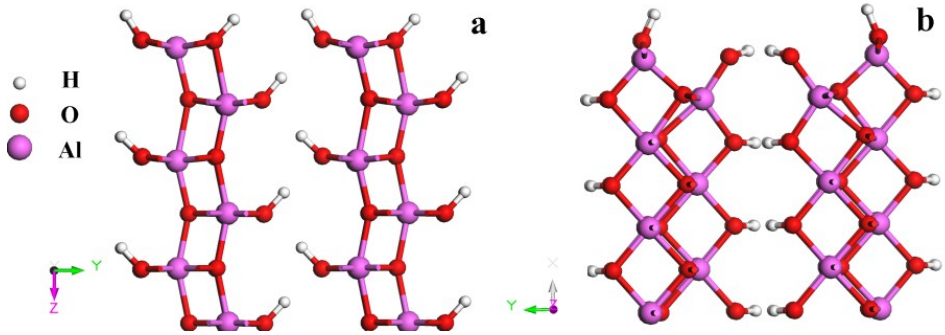

Fig. S6 Optimized structure of (a) hydroxylated (001) crystal face and (b) hydroxylated (100) crystal face.

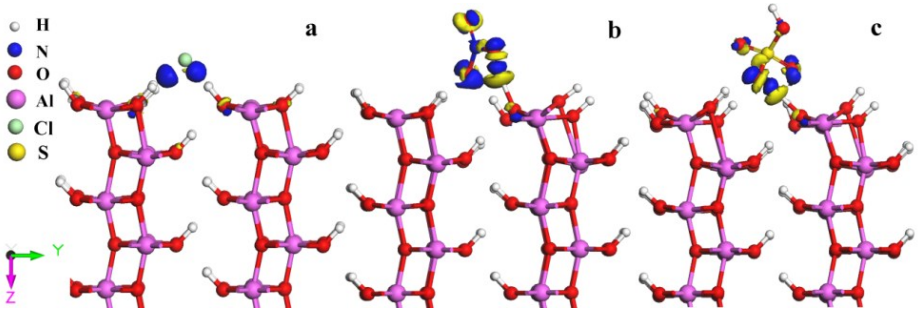

Fig. S7 Total charge density of (a) Cl^-, (b) NO_3^- and (c) HSO_4^- on hydroxylated (001) crystal face. The blue and yellow regions represent charge accumulation and depletion, respectively.

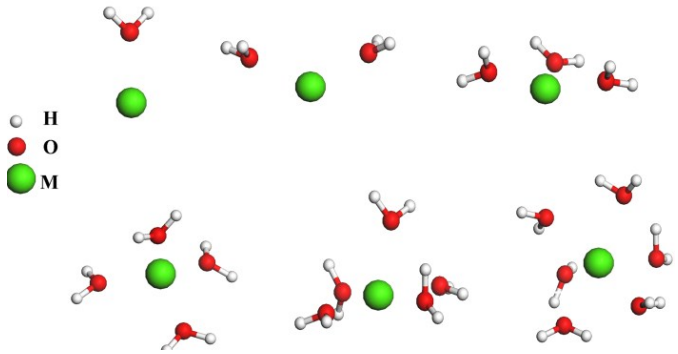

Fig. S8 The optimized geometry of $M^{2+}(H_2O)_6$ complex (M= Mg, Ca, Co, Ni).

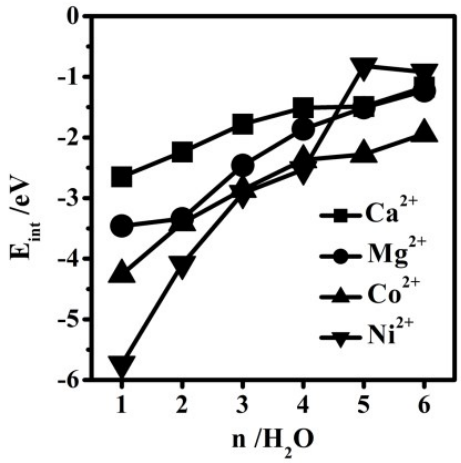

Fig. S9 Incremental binding energies for $M^{2+}(H_2O)_6$ complex, taking Ca^{2+}, Mg^{2+}, Co^{2+} and Ni^{2+} as representative.

References

1. C. E. Corbato, T. R. Tettenhorst and G. G. Christoph, *Clay.Clay. Miner.*, 1985**, 33**, 71-75.

2. P. P. Reichertz and W. J. Yost, *J. Chem. Phys.*, 1946, **14**, 495-501

