Supporting Information (SI)

Predicting Points of Zero Net Charge of Layered Double Hydroxides

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The SI contains 7 pages with 1 figure and 4 tables.

Physical constants, PZNCs or IEPs, and σ_{st} of (hydr)oxides including LDHs and the model plot for LDHs.

Table S1. Physical constants involved for LDH samples

(The O−H distance, *r*, is taken as 0.101 nm)

M−O bond	$\overline{L}$ (nm)	*v*	*v* / *L* (nm^{-1})
Mg–O	0.206	1/3	1.086
Al–O	0.189	1/2	1.724
Fe–O	0.200	1/2	1.661
Zn–O	0.195	1/3	1.689
Cr–O	0.269	1/2	1.351

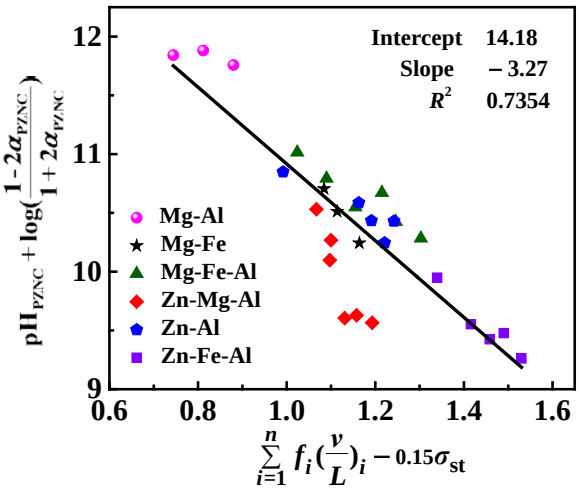

Figure S1. Linear regression plot of Eq. (10) for PZNC data of LDHs.

The units of *L* and σ_{st} are nm and mmol/g, respectively.

Table S2. Compositions, PZNCs, σ_{st}, and physical parameters of LDHs

Composition	pH_{PZNC}	$\sigma_{st,\ exp}$		$N_s \times 10^5$	$\log(\frac{1-2\alpha_{PZNC}}{1+2\alpha_{PZNC}})$	$\sum_{i=1}^{n} f_i(\frac{\nu}{L})_i$	Ref.
		mmol/g	C/m^2	($mmol/m^2$)			
$[Mg_{0.48}Al_{0.52}(OH)_2](NO_3)_{0.45}(OH)_{0.07}$	12.21	4.04	0.360	2.07	–0.329	1.4178	[S1]
$[Mg_{0.68}Al_{0.32}(OH)_2](NO_3)_{0.27}(OH)_{0.05}$	12.09	3.64	0.280	2.09	–0.248	1.2902	[S1]
$[Mg_{0.74}Al_{0.26}(OH)_2](NO_3)_{0.23}(OH)_{0.03}$	11.92	2.48	0.180	2.03	–0.162	1.2519	[S1]
$[Mg_{0.70}Fe_{0.30}(OH)_2]Cl_{0.06}(OH)_{0.24}$	10.78	1.16	0.081	1.95	–0.075	1.2585	[S2]
$[Mg_{0.68}Fe_{0.32}(OH)_2]Cl_{0.05}(OH)_{0.27}$	10.58	1.04	0.073	1.94	–0.068	1.2700	[S2]
$[Mg_{0.64}Fe_{0.36}(OH)_2]Cl_{0.03}(OH)_{0.33}$	10.30	0.86	0.060	1.93	–0.056	1.2930	[S2]
$[Mg_{0.72}Fe_{0.13}Al_{0.15}(OH)_2]Cl_{0.21}(OH)_{0.07}$	11.11	1.55	0.106	2.01	–0.095	1.2565	[S3]
$[Mg_{0.65}Fe_{0.03}Al_{0.32}(OH)_2]Cl_{0.14}(OH)_{0.21}$	10.88	1.45	0.100	2.07	–0.087	1.3074	[S3]
$[Mg_{0.52}Fe_{0.24}Al_{0.24}(OH)_2]Cl_{0.12}(OH)_{0.36}$	10.65	1.48	0.117	2.08	–0.102	1.3771	[S3]
$[Mg_{0.50}Fe_{0.16}Al_{0.34}(OH)_2]Cl_{0.12}(OH)_{0.38}$	10.75	1.20	0.090	2.08	–0.079	1.3949	[S3]
$[Mg_{0.46}Fe_{0.21}Al_{0.33}(OH)_2]Cl_{0.11}(OH)_{0.43}$	10.50	1.14	0.087	2.08	–0.076	1.4173	[S3]
$[Mg_{0.42}Fe_{0.29}Al_{0.29}(OH)_2]Cl_{0.10}(OH)_{0.48}$	10.35	0.90	0.074	2.01	–0.067	1.4378	[S3]
$[Zn_{0.19}Mg_{0.60}Al_{0.21}(OH)_2]Cl_{0.15}(OH)_{0.06}$	10.60	1.07	0.080	2.09	–0.069	1.3346	[S4]
$[Zn_{0.16}Mg_{0.60}Al_{0.24}(OH)_2]Cl_{0.16}(OH)_{0.08}$	10.33	0.97	0.072	2.09	–0.062	1.3356	[S4]
$[Zn_{0.08}Mg_{0.67}Al_{0.25}(OH)_2]Cl_{0.17}(OH)_{0.08}$	10.16	1.01	0.067	1.95	–0.062	1.2937	[S4]

$[Zn_{0.17}Mg_{0.54}Al_{0.29}(OH)_2]Cl_{0.16}(OH)_{0.12}$	9.67	0.98	0.071	1.96	–0.065	1.3735	[S4]
$[Zn_{0.13}Mg_{0.58}Al_{0.29}(OH)_2]Cl_{0.12}(OH)_{0.17}$	9.68	0.79	0.061	2.15	–0.051	1.3494	[S4]
$[Zn_{0.27}Mg_{0.37}Al_{0.36}(OH)_2]Cl_{0.13}(OH)_{0.24}$	9.63	0.89	0.074	2.06	–0.065	1.4785	[S4]
$[Zn_{0.48}Al_{0.52}(OH)_2]Cl_{0.18}(OH)_{0.34}$	10.36	1.44	0.130	2.05	–0.115	1.7072	[S5]
$[Zn_{0.59}Al_{0.41}(OH)_2]Cl_{0.17}(OH)_{0.24}$	10.50	0.86	0.082	2.11	–0.070	1.7034	[S5]
$[Zn_{0.63}Al_{0.37}(OH)_2]Cl_{0.16}(OH)_{0.21}$	10.52	1.04	0.096	2.02	–0.086	1.7020	[S5]
$[Zn_{0.65}Al_{0.35}(OH)_2]Cl_{0.16}(OH)_{0.19}$	10.68	1.15	0.106	2.04	–0.094	1.7013	[S5]
$[Zn_{0.69}Al_{0.31}(OH)_2]Cl_{0.20}(OH)_{0.11}$	11.03	2.13	0.201	2.02	–0.181	1.6999	[S5]
$[Zn_{0.47}Fe_{0.26}Al_{0.27}(OH)_2]Cl_{0.32}(OH)_{0.21}$	10.00	0.58	0.060	2.10	–0.051	1.6912	[S5]
$[Zn_{0.35}Fe_{0.27}Al_{0.38}(OH)_2]Cl_{0.35}(OH)_{0.30}$	9.60	0.55	0.056	2.12	–0.048	1.6947	[S5]
$[Zn_{0.28}Fe_{0.42}Al_{0.30}(OH)_2]Cl_{0.06}(OH)_{0.66}$	9.50	0.27	0.027	2.12	–0.023	1.6877	[S5]
$[Zn_{0.26}Fe_{0.46}Al_{0.28}(OH)_2]Cl_{0.03}(OH)_{0.71}$	9.47	0.54	0.054	2.12	–0.046	1.6859	[S5]
$[Zn_{0.18}Fe_{0.59}Al_{0.23}(OH)_2]Cl_{0.06}(OH)_{0.76}$	9.29	0.33	0.033	2.10	–0.028	1.6805	[S5]
$[Zn_{0.67}Cr_{0.33}(OH)_2](CO_3)_{0.17}$	~10	0.08	0.010	2.17	–0.007	1.2003	[S6]

Table S3. PZNCs and IEPs of (nominal) hydroxides

Sample	$pH_{PZNC, exp}$ or IEP [S8-S9]	ν / L (nm^{-1})	$pH_{PZNC, cal}$
$Mg(OH)_2$	10.7 [S7], 11–12	1.086	10.61
$Al(OH)_3$	8.4–10.1	1.724	8.52
$Fe(OH)_3$	8.0–9.8	1.661	8.73
$Zn(OH)_2$	9.6–10	1.689	8.64
$Cr(OH)_3$	8.4–9.3	1.664	8.73

Table S4. PZNCs and physical parameters of (hydr)oxides

Sample	$pH_{PZNC, exp}$ or IEP [S8-S9]	ν / L	$pH_{PZNC, cal}$
HgO	5.8–7.3	0.931	11.12
MgO	9.8–12	1.070	10.66
$Co(OH)_2$	11–11.5	1.072	10.65
$Ni(OH)_2$	8.1–11.3	1.093	10.51
La_2O_3	6.7–9.6	1.449	9.42
ThO_2	9.0–9.8	1.456	9.40
PuO_2	9.0	1.492	9.28
Y_2O_3	7.9–9.0	1.520	9.18
ZrO_2	6.3–9.5	1.529	9.16
α-FeO(OH)	7.9–8.7	1.639	8.80
α-Fe_2O_3	8.3–9.5	1.654	8.75
γ-FeO(OH)	7.4–7.7	1.661	8.73
$Fe(OH)_2$	9.5–10	1.661	8.73
Cr_2O_3	6.6–9.8	1.664	8.73
ZnO	8.9–9.8	1.673	8.69
CuO	7.5–9.4	1.689	8.64
$Cu(OH)_2$	8.5–10.3	1.698	8.61
α-AlO(OH)	8.6–9.5	1.698	8.61
γ-AlO(OH)	7.50–9.5	1.711	8.57
Al_2O_3	7.2–9.6	1.712	8.56
BeO	7.1–10.2	1.880	8.01
SnO_2	3.8–6.60	2.177	7.04
TiO_2	5.2–6.8	2.245	6.82
WO_3	1.5–2	3.405	3.03
SiO_2	1.80, 1–3	3.817	1.68

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