

Supporting Information

Thermodynamic Evidence of Flexibility in H₂O and CO₂ Absorption of Transition Metal Ion Exchanged Zeolite LTA

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1. XRD patterns of transition metal ion exchanged zeolite LTA

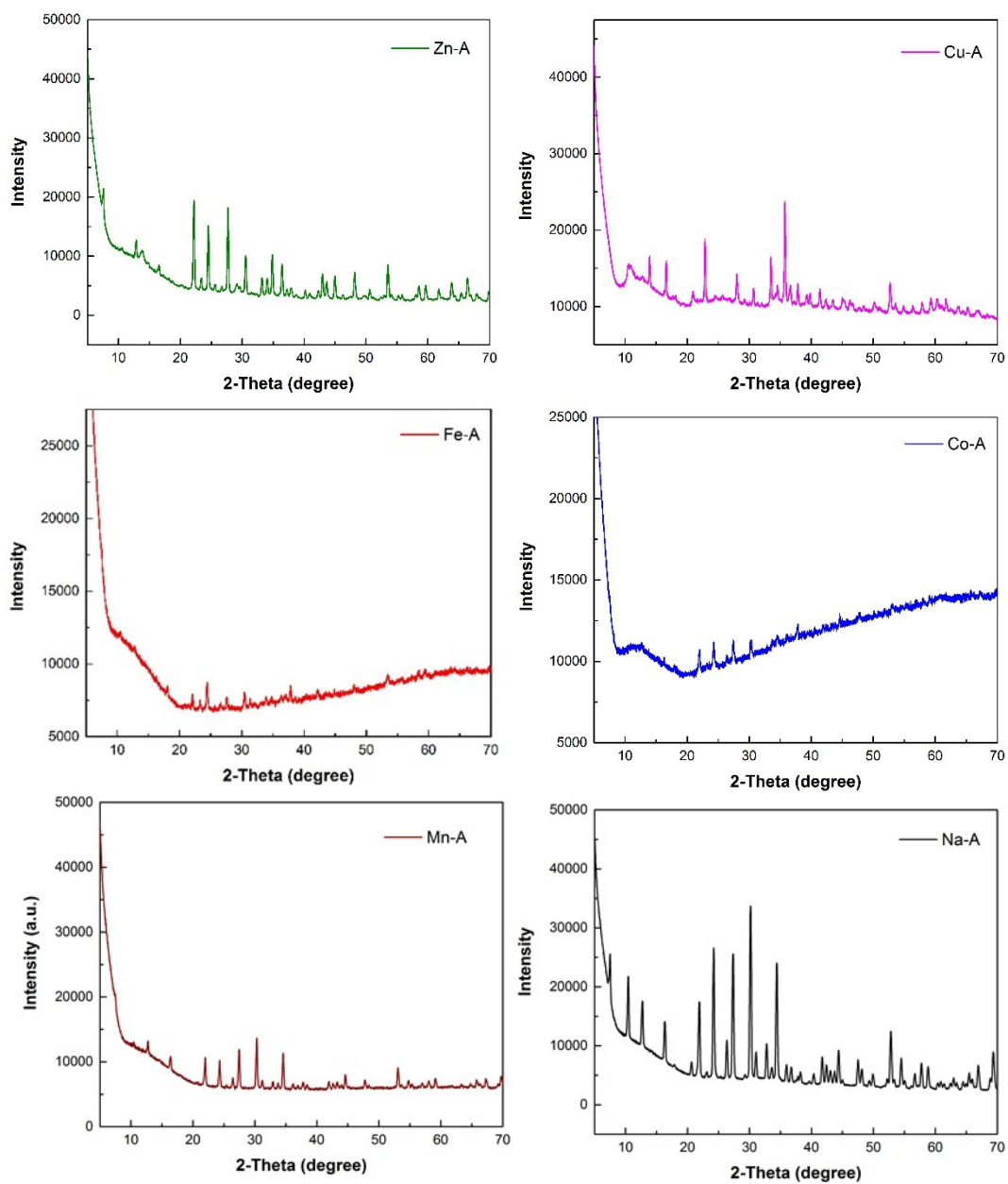


Figure S1. XRD patterns of transition metal ion exchanged zeolite A at room temperature.

2. Calculated structural factor

The atomic form factor is the pre-exponential coefficient of structure factor F and can be well approximated by a sum of Gaussians of the form:

$$f(q) = \sum_{i=1}^4 a_i \exp\left(-b_i \left(\frac{q}{4\pi}\right)^2\right) + c$$

where $\mathbf{q}$ is the scattering vector, the coefficients of a_i , b_i and c for analytical approximation to the atomic form factors are obtained from International Tables for Crystallography [1] in **Table S1**.

Table S1. Coefficients for analytical approximation to the atomic form factors									
Element	a_1	b_1	a_2	b_2	a_3	b_3	a_4	b_4	c
Na ⁺	3.2565	2.6671	3.9362	6.1153	1.3998	0.2001	1.0032	14.039	0.404
Mn ²⁺	10.8061	5.2796	7.362	0.3435	3.5268	14.343	0.2184	41.3235	1.0874
Fe ³⁺	11.1764	4.6147	7.3863	0.3005	3.3948	11.6729	0.0724	38.5566	0.9707
Co ²⁺	11.2296	4.1231	7.3883	0.2726	4.7393	10.2443	0.7108	25.6466	0.9324
Cu ²⁺	11.8168	3.37484	7.11181	0.244078	5.78135	7.9876	1.14523	19.897	1.14431
Zn ²⁺	11.9719	2.9946	7.3862	0.2031	6.4668	7.0826	1.394	18.0995	0.7807

The calculated atomic form factors of Na⁺, Mn²⁺, Fe³⁺, Co²⁺, Cu²⁺, Zn²⁺ using above equation are 1.785, 6.364, 6.551, 6.740, 7.122, 7.414.

3. Time-resolved adsorption of Zeolite Na-A

The adsorption kinetics was investigated by using microbalance with a timer. Zeolite Na-A was first degassed at 300°C overnight under vacuum and then transferred to microbalance under the protection of nitrogen atmosphere in the tube. The weight increase is shown in Figure S2 and can be approximately fitted by an exponential function: $W = A \cdot \exp(x / \tau) + w_0$, in which A is the pre-exponential factor equal to -5.156, τ is time constant -30.604 and w_0 is the offset around 4.82.

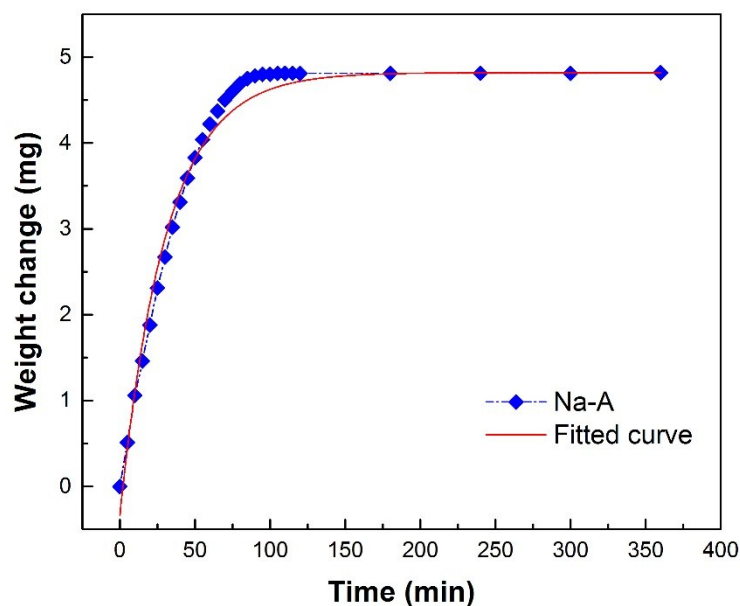


Figure S2. The time-resolved weight change of Zeolite Na-A, degassed at 300°C under vacuum. The dash line represents the experimental data and red line for fitting result.

The final weight increase in 24hrs is about 19.57% water content, comparable to the value 20.15% and 20.55% derived by isotherms and TG/DSC.

References

- (1) P. J. Brown, A. G. Fox, E. N. Maslen, M. A. O'Keefe and B. T. M. Willis, *International Tables for Crystallography*, 2006, **Vol. C**, **ch. 6.1**, pp. 554-595.