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Rapid Room Temperature Conversion of Hydroxy Double Salt to MOF-505 for CO_2 Capture

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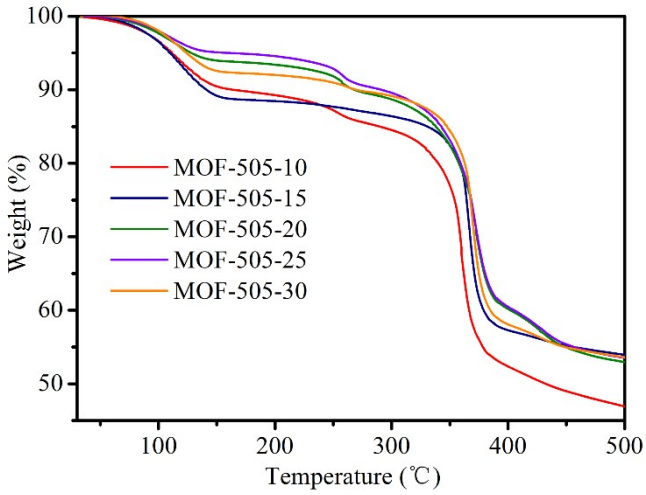

Figure S1. Thermogravimetric analysis (TGA) curves of MOF-505 products.

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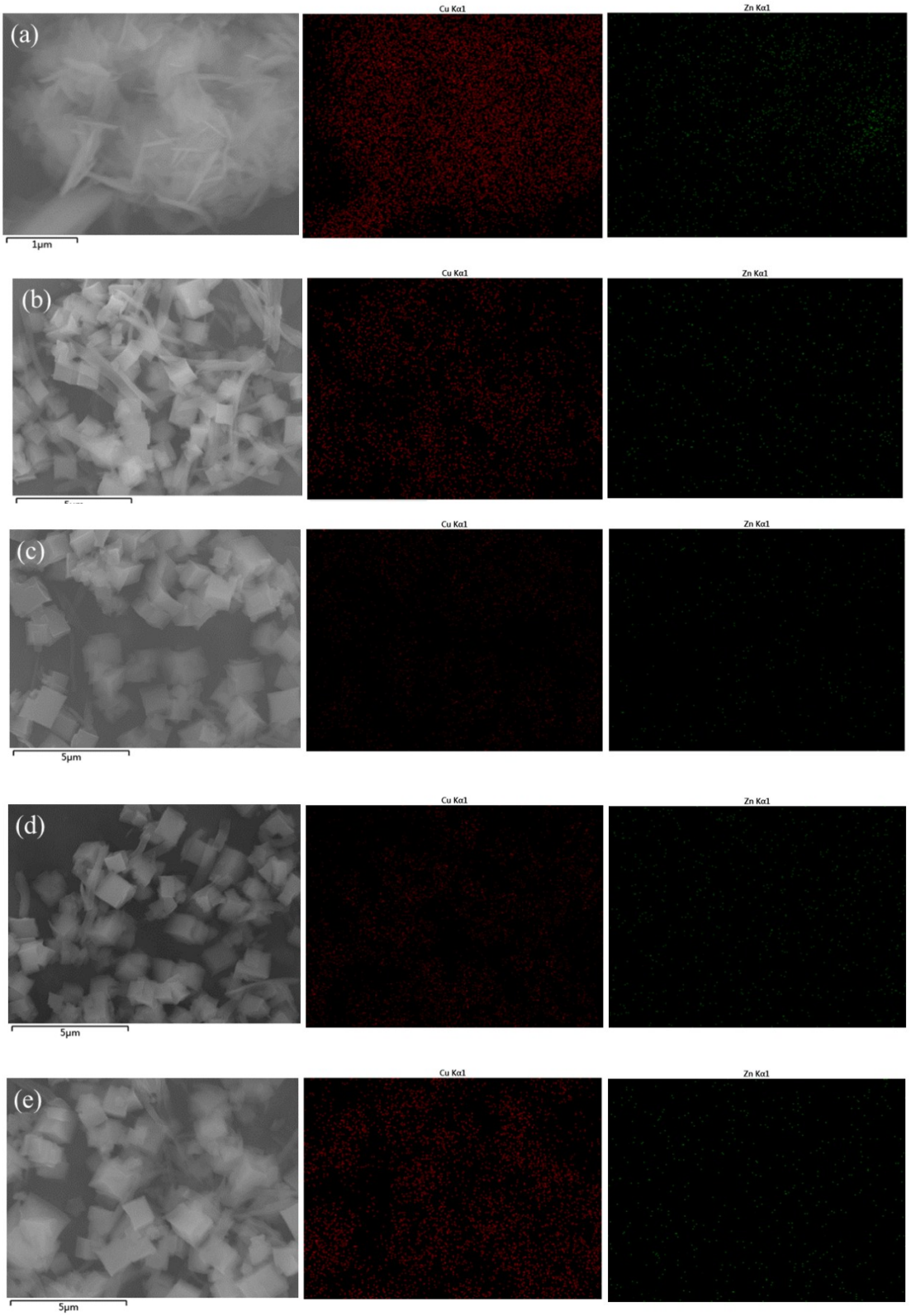
(a)
Cu Kα1
Zn Kα1
1μm
(b)
Cu Kα1
Zn Kα1
(c)
Cu Kα1
Zn Kα1
5μm
(d)
Cu Kα1
Zn Kα1
5μm
(e)
Cu Kα1
Zn Kα1
5μm

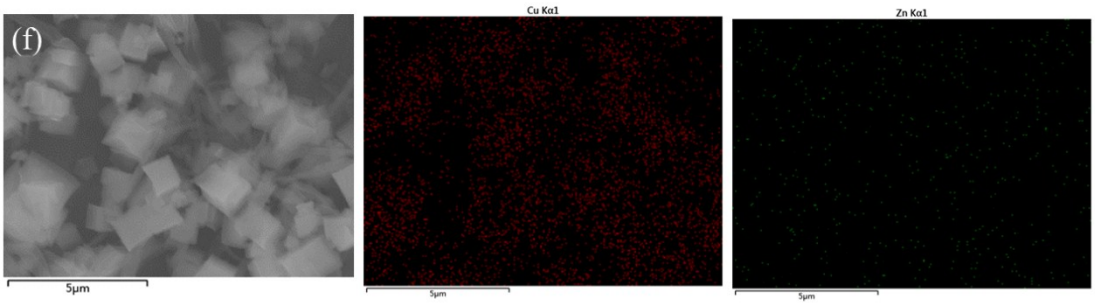

Figure S2. Elemental mapping images of (a) [(Zn,Cu)(OH)NO_3] intermediate and MOF-505 products synthesized by rapid room temperature method for (b) 10 min, (c) 15 min, (d) 20min, (e) 25 min, and (f) 30 min.

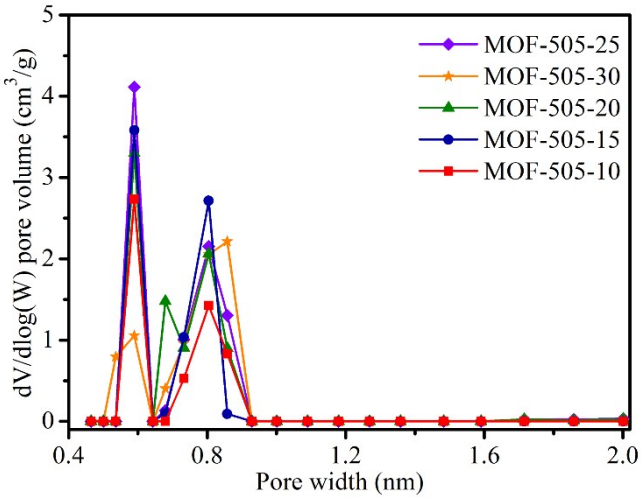

Figure S3. Density functional theory (DFT) pore size distribution of MOF-505 products.

Caculation of Adsorption Selectivity. The adsorption selectivities of CO_2/CH_4 and CO_2/N_2 for MOF-505-25 are calculated on the basis of ideal adsorbed solution theory (IAST), serving as a widely employed method to evaluate the separation performance of porous materials. Firstly, the measured single-component isotherms of CO_2, CH_4 and N_2 at 298 K are fitted to the Langmuir-Freundlich (L-F) model:

$$q = q_m \frac{b\,p^m}{1 + b\,p^m} \qquad (1)$$

where q (mmol/g) is the adsorbed amount; q_m (mmol/g) is the saturation capacity; p (kPa) is the pressure of the bulk gas at equilibrium with the adsorbed phase; b (1/kPa) is the affinity coefficient of the sites; m refers to the deviation from an ideal homogeneous surface. Here, all isotherms are well described by using the L-F model, giving the correlation coefficients (R^2) values high up to 0.9998, listed in Table S1. Then the adsorption selectivities of CO_2/CH_4 and CO_2/N_2 mixtures can be obtained according to the following equation:

$$S = \frac{q_1/q_2}{p_1/p_2} \qquad (2)$$

where q_1 and q_2 are the adsorbed amounts of the adsorbed phase in the mixture; p_1 and p_2 are the pressures in the gas phase.

Table S1

Fitting parameters of the Langmuir-Freundlich model

Parameters	q_m	b	m	R^2
CO_2	9.13764	0.01147	0.86757	0.99988
CH_4	6.39268	0.00174	1.01547	0.99999
N_2	4.92541	5.05542E-4	1.03874	0.99992