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Supporting Information

Direct Synthesis of Shaped MgAPO-11 Molecular Sieve and the Catalytic Performance in *n*-Dodecane Hydroisomerization

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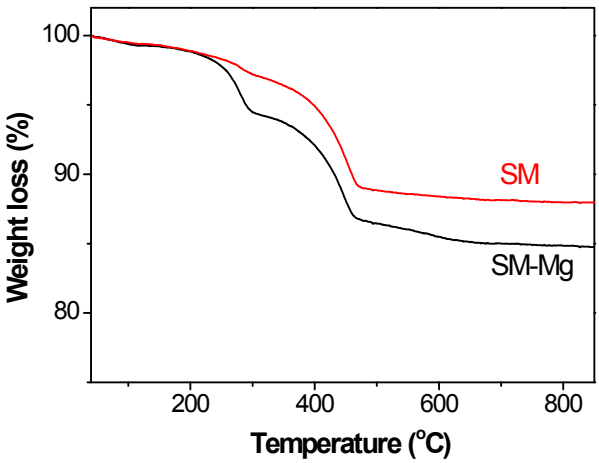

Fig. S1. TG curves of SM and SM-Mg.

As shown in Fig. S1, the TG curves of SM and SM-Mg consist of three major weight losses. The first loss below 110 °C is attributed to the removal of physisorbed water,[1] the second loss in the region of 100-300 °C is due to the decomposition of [EMIm]Br,[2] and the last weight loss in the region of 300-800 °C is corresponding to the decomposition of the organic molecules and the loss of -OH and -F groups in the

framework.[1]

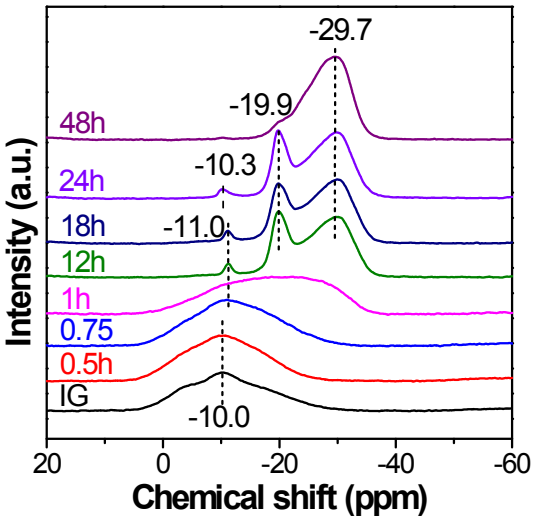

Fig. S2. ^{31}P NMR spectra of SM crystallized at 200 ^{o}C for (a) IDE, (b) 0.5 h, (c) 1 h, (d) 12 h, (e) 18 h, (f) 24 h, (g) 48 h and (h) 60 h.

The initial gel extrudate without Mg was denoted as IG. The experimental part was described in Ref 2. ^{31}P NMR spectrum (Fig. S2.) of the IG shows a very broad peak centered at around -10.0 ppm which can be attributed to the partially condensed phosphate species in amorphous $AlPO_x$ gel.[3] As the crystallization proceeds, peaks attributed to the partially condensed phosphate species become intense and shift to the high magnetic fields, indicating the depolymerization of the amorphous $AlPO_x$ gel. Three new peaks at -29.7 ppm, -19.9 ppm and -11.0 ppm show up in the ^{31}P NMR spectrum as increasing the crystallization time. The weak peak at -11.0 ppm is attributed to the structural P-OH groups in the framework, while the intense peak at -19.9 ppm is assigned to tetrahedral P. These two peaks also suggest the formation of -CLO intermediates.[4] (Because as shown in Fig. S3 in Ref 2, after crystallization for 1 h, an intermediate molecular sieve phase (-CLO) show up before the appearance of signals with pure AEL phase. When the crystallization time is between 1 h to 24 h, the product always contains -CLO type molecular sieve. After 48 h, AEL type molecular sieve was obtained.) Whereas, the -29.7 ppm peak is ascribed to the fully condensed coordination sphere around the P sites in the $AlPO_4$-11 framework.[5] Further increasing the crystallization time, the fully condensed P signals

become dominant, suggesting the formation of completely crystallized $AlPO_4$-11. These results illustrate the changing of coordination sphere of P species, from which the rearrangement partially condensed P into frame tetrahedral P sites can be demonstrated during the crystallization.

References

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