

Supplementary Information

The first synthesis of organosilyl-substituted aluminophosphate molecular sieves

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Table S1 Compositions of as-synthesized Me-Si- $\text{AlPO}_4\text{-5}$ and organosilyl VPI-5 samples calculated from ICP-AES analysis.

OAS	Al_2O_3	P_2O_5	(R)SiO _{1.5}
MeSi-$\text{AlPO}_4\text{-5}$			
0.6	1	1.02	0.08
0.8	1	0.97	0.13
1.0	1	0.98	0.18
MeSi-VPI-5			
0.1	1	0.99	0.021
0.2	1	1.05	0.038
bisSi-VPI-5			
0.05	1	0.99	0.037
0.10	1	1.01	0.084
0.15	1	0.99	0.096

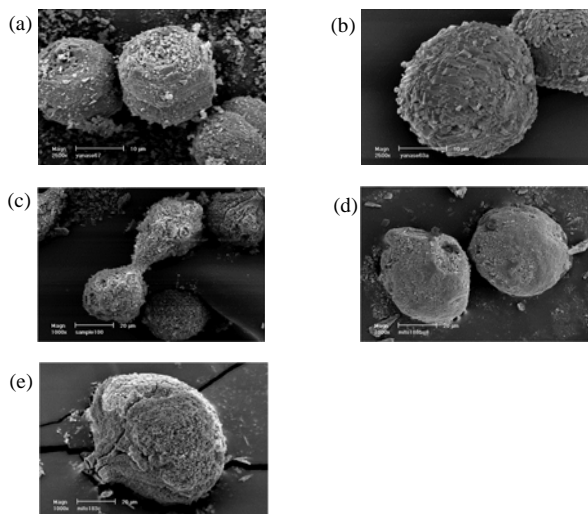


Fig. S1 SEM images of: (a) SAPO-5 (0.6TEOS), (b) MeSi- $\text{AlPO}_4\text{-5}$ (0.6MTES), (c) VPI-5, (d) bisSi-VPI-5 (0.15BTESM), (e) MeSi-VPI-5 (0.15MTES).

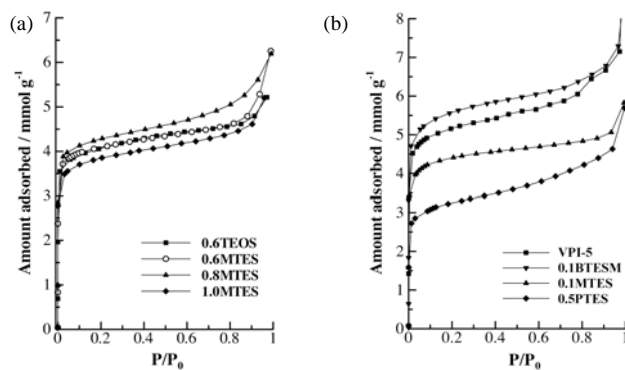


Fig. S2 Nitrogen adsorption isotherms at 77 K of: organosilyl-substituted (a) $\text{AlPO}_4\text{-5}$ and (b) VPI-5.

Preparation procedures of the organosilyl-substituted $\text{AlPO}_4\text{-5}$ and VPI-5

Organosilyl-substituted $\text{AlPO}_4\text{-5}$

The composition of the starting gel for AFI synthesis was $x\text{OAS}\cdot 1\text{Al}_2\text{O}_3\cdot (1.3-x/2)\text{P}_2\text{O}_5\cdot 1\text{Et}_3\text{N}\cdot 40\text{H}_2\text{O}$ ($x=0.6\text{--}2.0$). The gel was typically prepared as follows: A mixture of pseudo-boehmite and water were stirred for 5 min. After phosphoric acid was added, the mixture was stirred for 60 min. After Et_3N was added, the mixture was stirred for 90 min. After an organoalkoxysilane was added, the mixture was stirred for 10 min. The gel was hydrothermally reacted at 200°C for 18 h in a Teflon-lined autoclave. The template occluded in the product was removed with HCl/MeOH at 100°C for 20 h in a Teflon-lined autoclave.

Organosilyl-substituted VPI-5

The composition of the starting gel for VFI synthesis was $x\text{OAS}\cdot 1\text{Al}_2\text{O}_3\cdot 1\text{P}_2\text{O}_5\cdot 1\text{Pr}_2\text{NH}\cdot 40\text{H}_2\text{O}$ ($x=0.1\text{--}0.5$). The gel was typically prepared as follows: A mixture of pseudo-boehmite and water were stirred for 30 min. After phosphoric acid was added, the mixture was stirred for another 30 min. After the gel was aged for 24 h at an ambient temperature, Pr_2NH was added and stirred for 1 h. After an organoalkoxysilane was added, the mixture was stirred for 2 h. The gel was hydrothermally reacted at 140°C for 24 h in a Teflon-lined autoclave. The template occluded in the product was removed with HCl/MeOH at 100°C for 16 h in a Teflon-lined autoclave.