

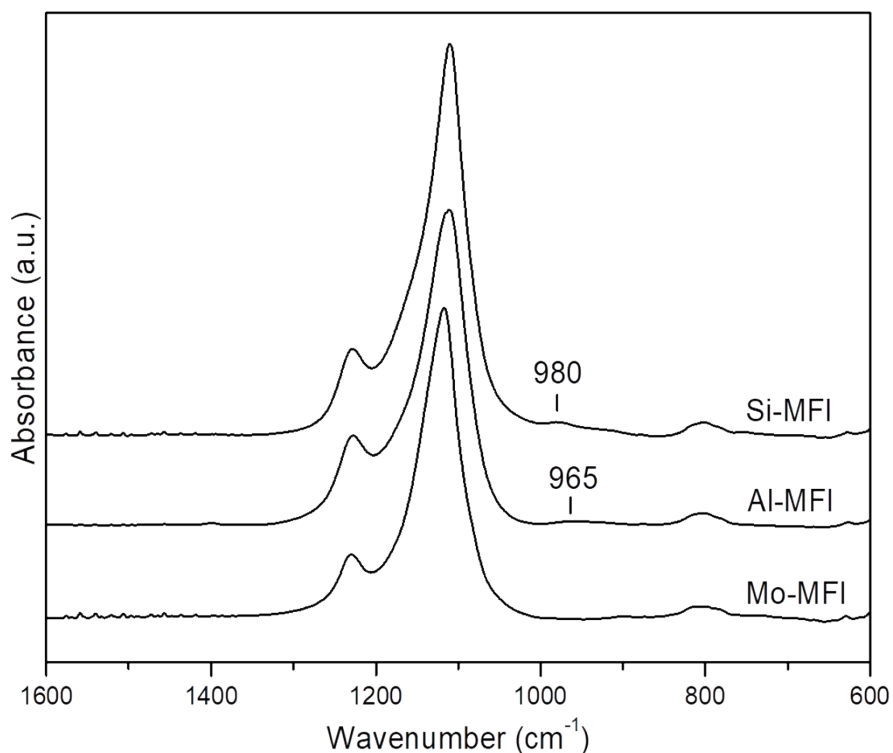
## Supporting Information

### The challenge of silanol species characterization in zeolites

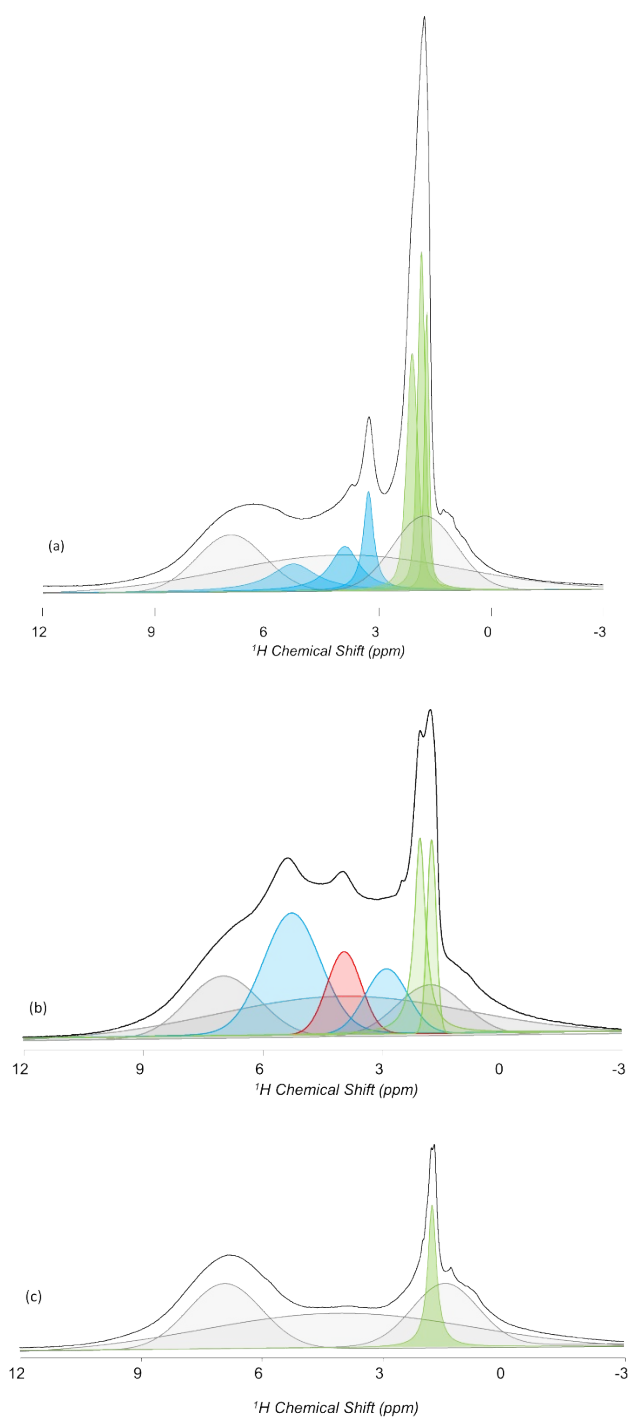
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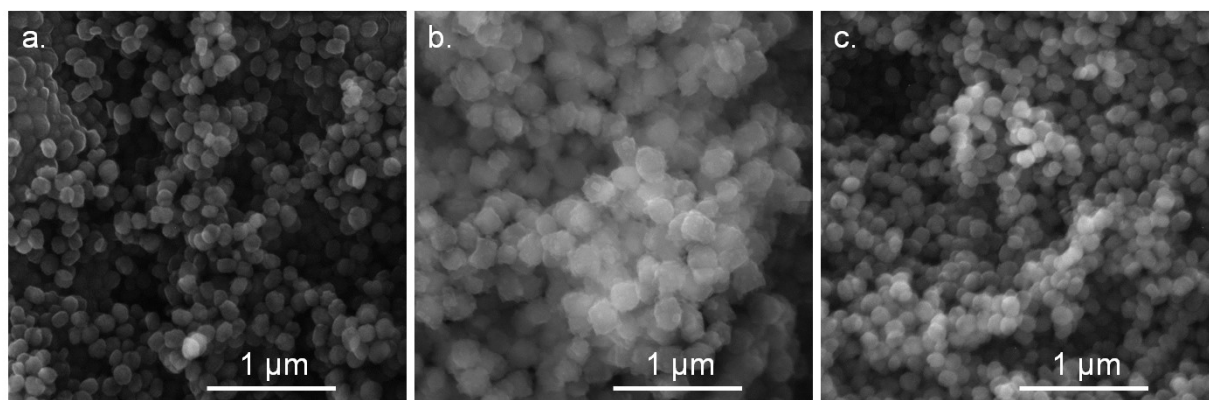


**Figure S1.** FTIR spectra of samples Si-MFI, Al-MFI, and Mo-MFI (spectra recorded under ambient conditions of zeolites dispersed in KBr).



**Figure S2.** Deconvolution of  $^1\text{H}$  MAS NMR spectra of samples (a) Si-MFI, (b) Al-MFI, and (c) Mo-MFI. The black line corresponds to the experimental  $^1\text{H}$  MAS NMR spectra, gray line corresponds to the rotor signal. The green lines correspond to isolated and weakly H-bonded

silanols, blue lines correspond to strongly H-bonded silanols, the red line correspond to Brønsted acid sites in the case of sample Al-MFI.



**Figure S3.** SEM images of samples (a) Si-MFI, (b) Al-MFI, and (c) Mo-MFI.

**Table S1.** Quantification of silanol species in samples Si-MFI, Al-MFI, and Mo-MFI based on integration and deconvolution of  $^1\text{H}$  MAS NMR spectra.

Silanols (mmol/g)	Si-MFI	Al-MFI	Mo-MFI
Isolated and weakly H bonded	3,2	4,9	0,2
Bronsted acid site	0	1,8	0
Strongly H bonded	1,7	4,6	0
<b>Total silanols (mmol/g)</b>	<b>4,9</b>	<b>11,3</b>	<b>0,2</b>

**Table S2.** Attribution of  $^{31}\text{P}$  MAS NMR chemical shifts observed for TMPO adsorbed in zeolite samples. [21]

Chemical shift [ppm]	Attribution
30	Physisorbed TMPO
45	TMPO interacting with framework Mo
50	TMPO interacting with silanols
64 and 75	TMPO interacting with bridging hydroxyl groups