Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplemental Information

Spatial Distribution of Organic Functional Groups Supported on Mesoporous Silica Nanoparticles: A Study by DNP-Enhanced ^{29}Si-^{29}Si Solid-State NMR

Takeshi Kobayashi,[a] Dilini Singappuli-Arachchige,[a,b] Zhuoran Wang,[a,b] Igor I. Slowing,[a,b] and Marek Pruski[a,b,*]

[a]Ames Laboratory, U.S. Department of Energy, Ames, Iowa, 50011, U.S.A.
[b]Department of Chemistry, Iowa State University, Iowa 50011, U.S.A.

^{29}Si DPMAS NMR

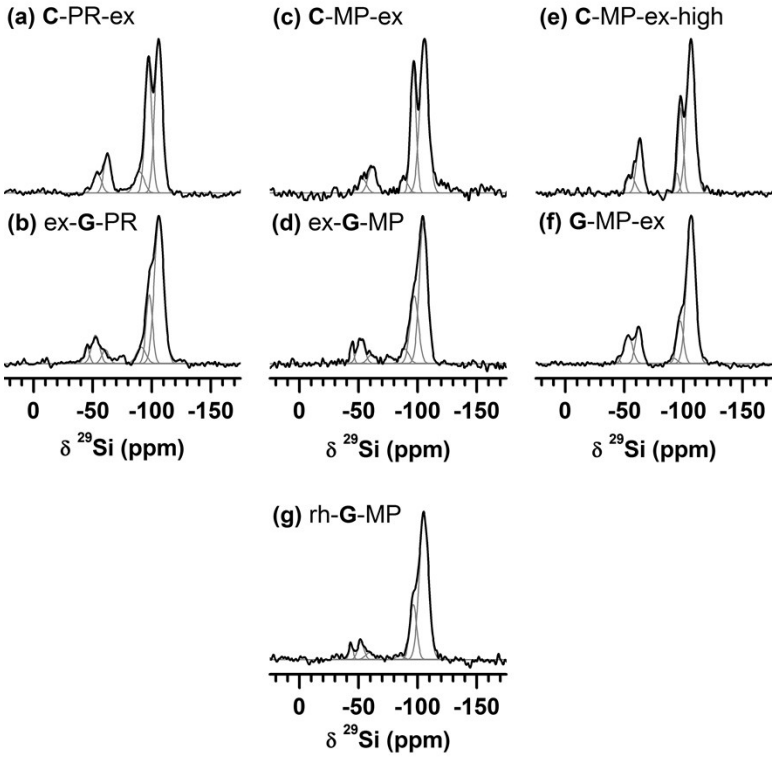

Fig. S1. Conventional ^{29}Si DPMAS spectra of functionalized MSNs obtained using ν_R = 10 kHz, SPINAL64 ^{1}H decoupling, τ_{RD} = 300 s and NS = 600. Note that the line widths corresponding to Q^3 sites are consistently smaller than those of Q^4, as the Si-O bonds associated with the latter are on average more strained.

DNP-enhanced $^{29}Si\{^{1}H\}$ CPMAS spectra of grafted MSNs as a function of MP loading.

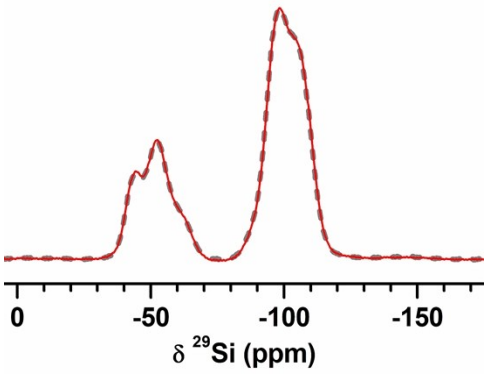

Fig. S2. DNP-enhanced $^{29}Si\{^{1}H\}$ CPMAS spectra of MP-grafted MSNs normalized to a constant height: dashed line represents ex-G-**MP**, which was synthesized as explained in the Experimental section using 4.57 mmol of alkoxysilane precursor per 250 mg of as-synthesized MSN; red line corresponds to a similar sample prepared with an increased precursor concentration of 5.38 mmol per 250 mg of as-synthesized MSN. The spectra were acquired using $\nu_R = 7.5$ kHz, $\tau_{CP} = 4$ ms, $\tau_{RD} = 13$ s and SPINAL64 ^{1}H decoupling.

DNP-enhanced $^{13}C\{^{1}H\}$ CPMAS NMR

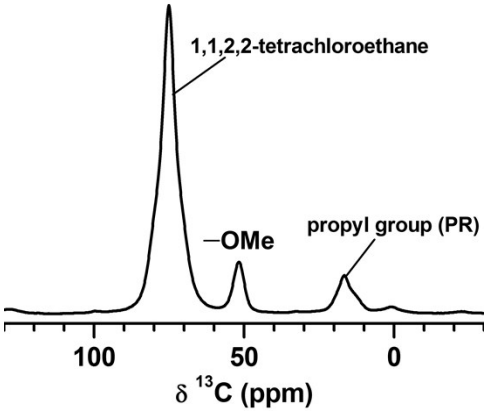

Fig. S3. DNP-enhanced $^{13}C\{^{1}H\}$ CPMAS spectrum of ex-**G**-PR. The spectrum was acquired using $\nu_R = 7.5$ kHz, $\tau_{CP} = 4$ ms, $\tau_{RD} = 13$ s and a SPINAL64 ^{1}H decoupling. The methoxy groups (at ~50 ppm), formed during the acid extraction of the surfactant, remained on the surface after the grafting process.

SIMPSON Simulation

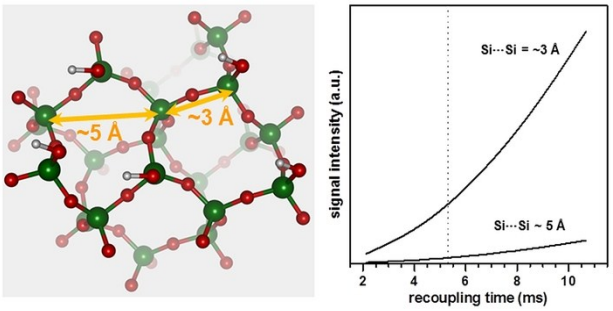

Fig. S4. [111] view of the cristobalite surface (left) and SIMPSON simulation of the polarization build-up using the SPC-5 homonuclear recoupling (right). The (111) surface was created based on the β-cristobalite crystal structure.[1] Si, O and H are represented in green, red, and gray, respectively. The average distance between nearest Si pair was presented. The dotted line drawn in the right panel indicates the total recoupling time, τ_{rec} = 5.3 ms, used in the present study.

References

1 D.R. Peacor, *Z. Kristallogr*. **1973**, *138*, 274-298.

2 M. Bak, J.T. Rasmussen, N.C. Nielsen, *J. Magn. Reson*. **2000**, *147*, 296-330.