Analysis of Trivalent Cation Complexation to Functionalized Mesoporous Silica using Solid-State NMR Spectroscopy

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Supplemental Information

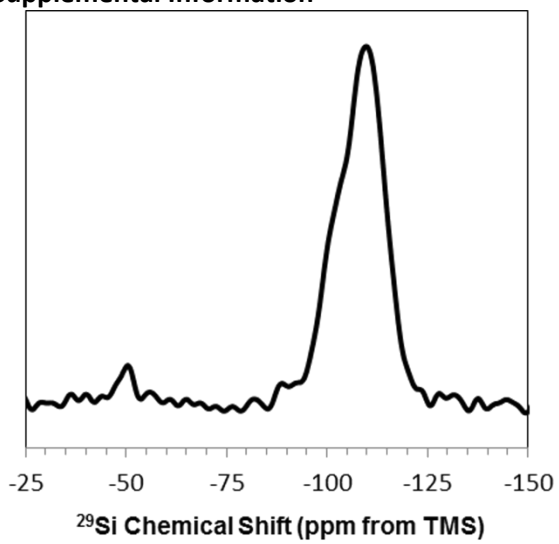

Figure S1. $^{29}Si\{^{1}H\}$ SP/MAS NMR spectra for pristine CA-SBA. The resonances for the bulk silicon atoms are the Q peaks (Q^2, Q^3, and Q^4 have shifts of δ_{Si} =-93, -97, and -107 ppm, respectively) and for the surface silicon atoms are the T peaks (T^1, T^2, and T^3 have shifts of δ_{Si} =-51, -58, and -66 ppm, respectively).

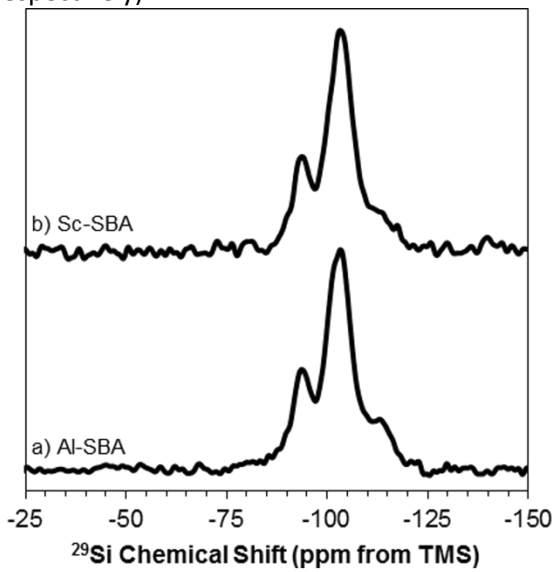

Figure S2. $^{29}Si\{^{1}H\}$ CP/MAS NMR spectra for solids from a) Al (Al-SBA and b) Sc (Sc- SBA) sorption to bare SBA-15. The resonances for the bulk silicon atoms are the Q peaks (Q^2, Q^3, and Q^4 have shifts of δ_{Si} =-93, -97, and -107 ppm, respectively).

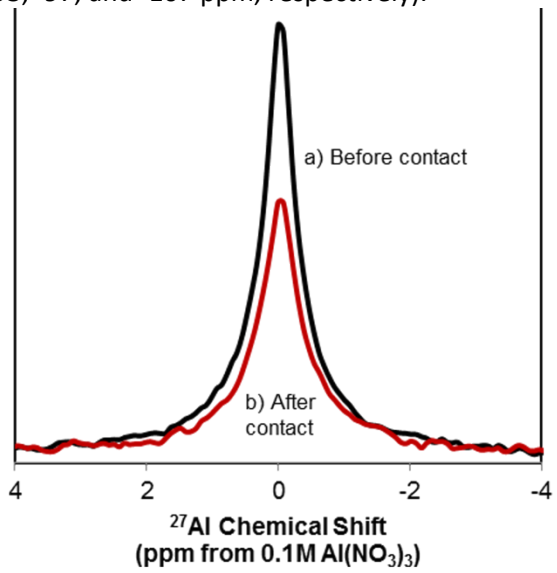

Figure S3. ^{27}Al SP/MAS NMR spectra of solution from Al sorption to CA functionalized SBA-15 a) before contact with CA-SBA and b) after contact with CA-SBA for 24 hours.

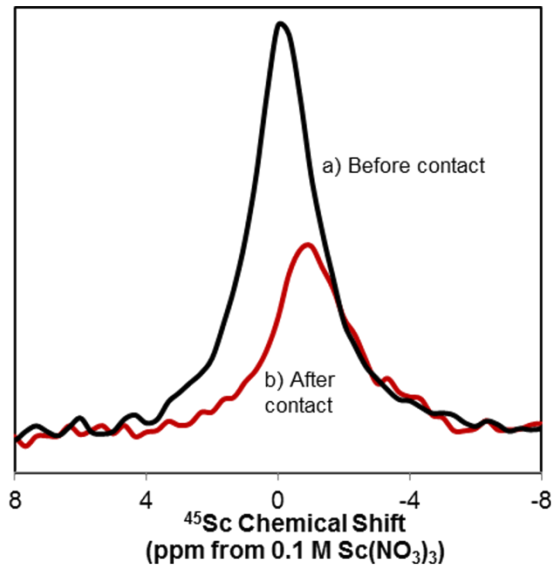

Figure S4. ^{45}Sc SP/MAS NMR spectra of solution from Sc sorption to CA functionalized SBA-15 a) before contact with CA-SBA and b) after contact with CA-SBA for 24 hours.

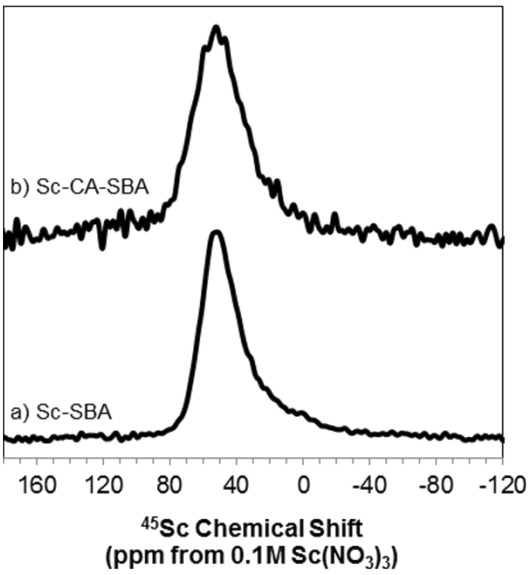

Figure S5. ^{45}Sc SP/MAS NMR spectra of solids from a) Sc sorption to bare SBA-15 (Sc-SBA) and b) CA functionalized SBA-15 (Sc-CA-SBA) collected on 500 MHz spectrometer. The chemical shifts for 6, 7, and 8-coordinated Sc occur in the ranges of δ_{Sc}=100 to 160 ppm, δ_{Sc} = 10 to 70 ppm, and δ_{Sc} =-10 to -50 ppm, respectively.[28]

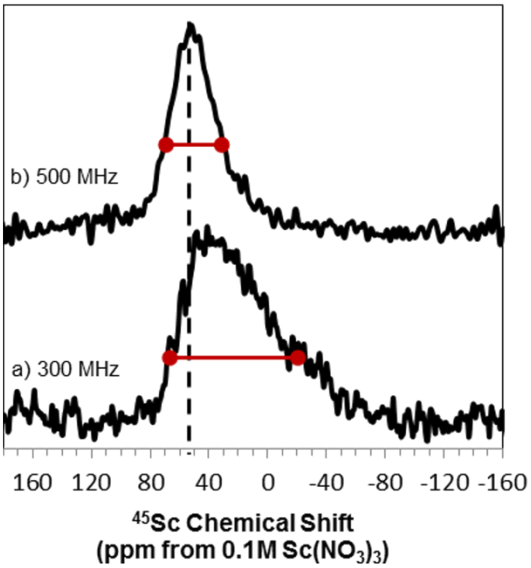

Figure S6. ^{45}Sc SP/MAS NMR spectra of solids from Sc sorption to CA functionalized SBA-15 (Sc-CA-SBA) on a) the 300 MHz spectrometer and b) the 500 MHz spectrometer. The chemical shifts for 6, 7, and 8-coordinated Sc occur in the ranges of δ_{Sc}=100 to 160 ppm, δ_{Sc} = 10 to 70 ppm, and δ_{Sc} =-10 to -50 ppm, respectively[28].