Supporting Information

to

Restricted Dynamics of a deuterated linker grafted on SBA-15 revealed by Deuterium MAS NMR

S. Jayanthi[1†], M. Werner[2†], Y. Xu[2], G. Buntkowsky[2*] and S. Vega[1*]

[1]Department of Chemical Physics, Weizmann Institute of Science, Rehovot, Israel – 76100.
[2] Eduard-Zintl-Institut für Anorganische und Physikalische Chemie, Technische Universität Darmstadt, Petersenstr. 20, D-64287 Darmstadt, Germany

[*]*Author for correspondence:* *Gerd.Buntkowsky@chemie.tu-darmstadt.de*, Fax no. +49 6151 16-4347
Shimon.Vega@Weizmann.ac.il, Fax no. +972-8-934-4123

Contents

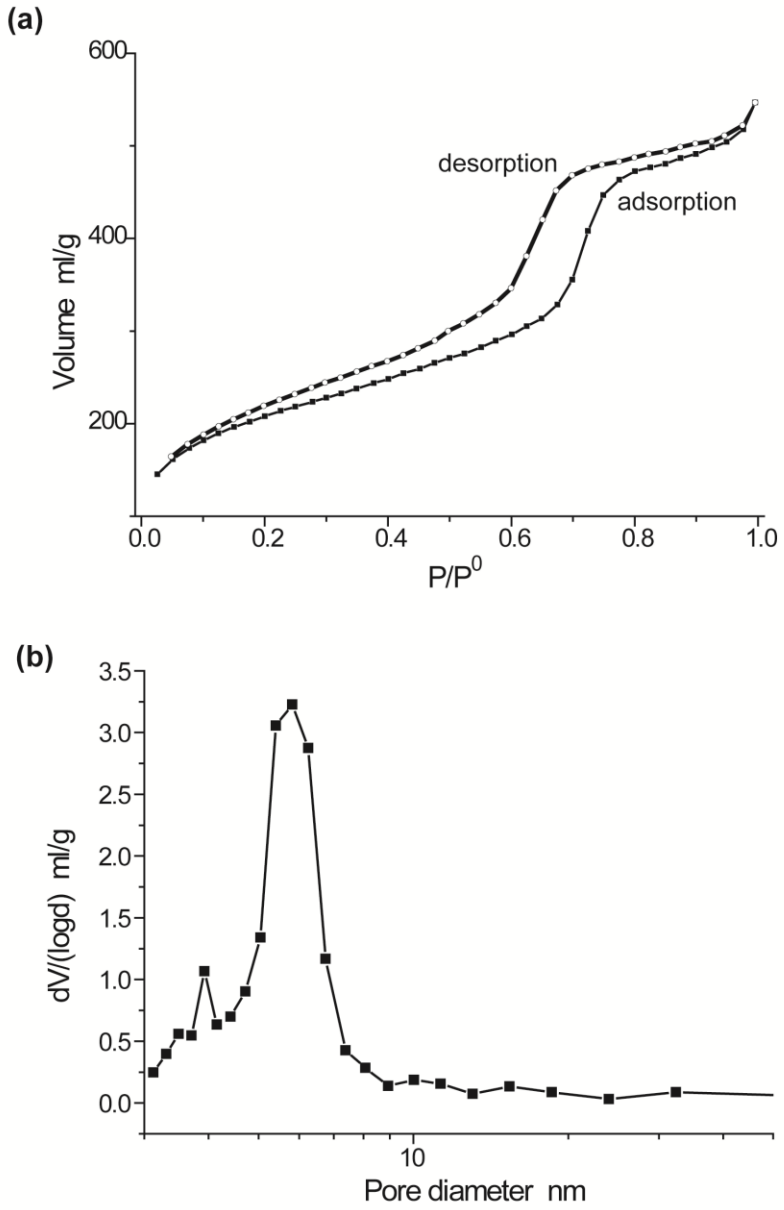

Figure S1: (a) BET adsorption – desorption curve of the synthesized SBA-15. Specific surface area observed is 737 m^2/g. (b) shows the BJH curve for the same sample. Average pore diameter and pore volume observed are 5.8 nm and 0.81 ml/g.

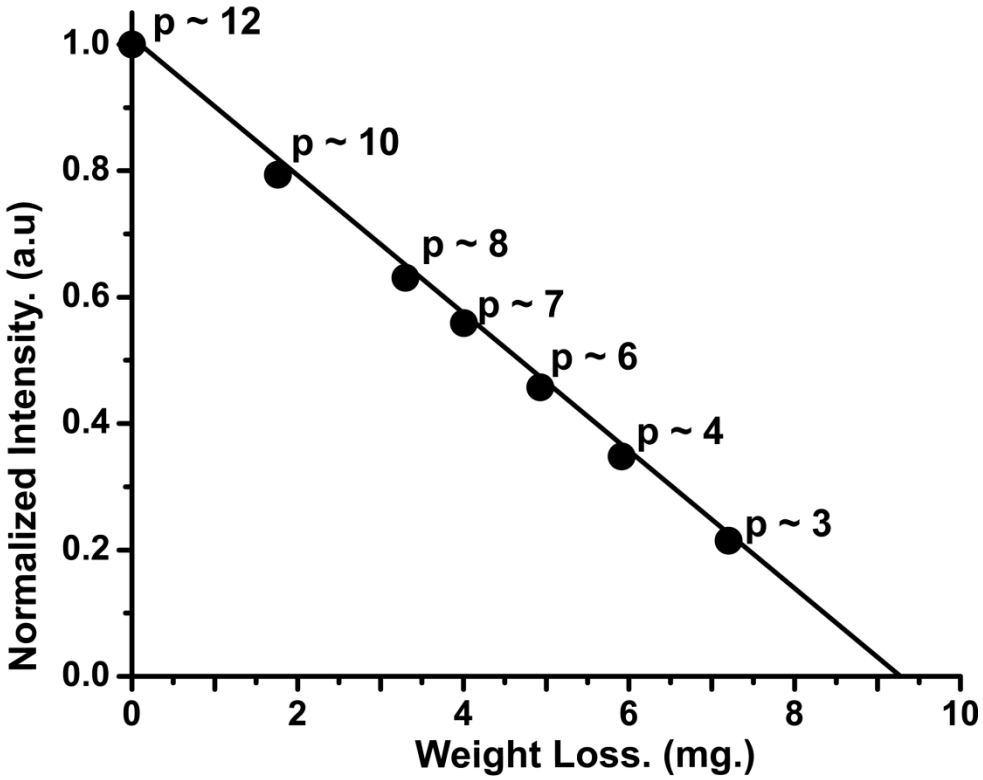

Figure S2: Plot shows the linear variation of integrated intensity of the proton spectra with weight loss of the post grafted sample at various levels of pumping. *p* values are calculated at each stage and shown therein.

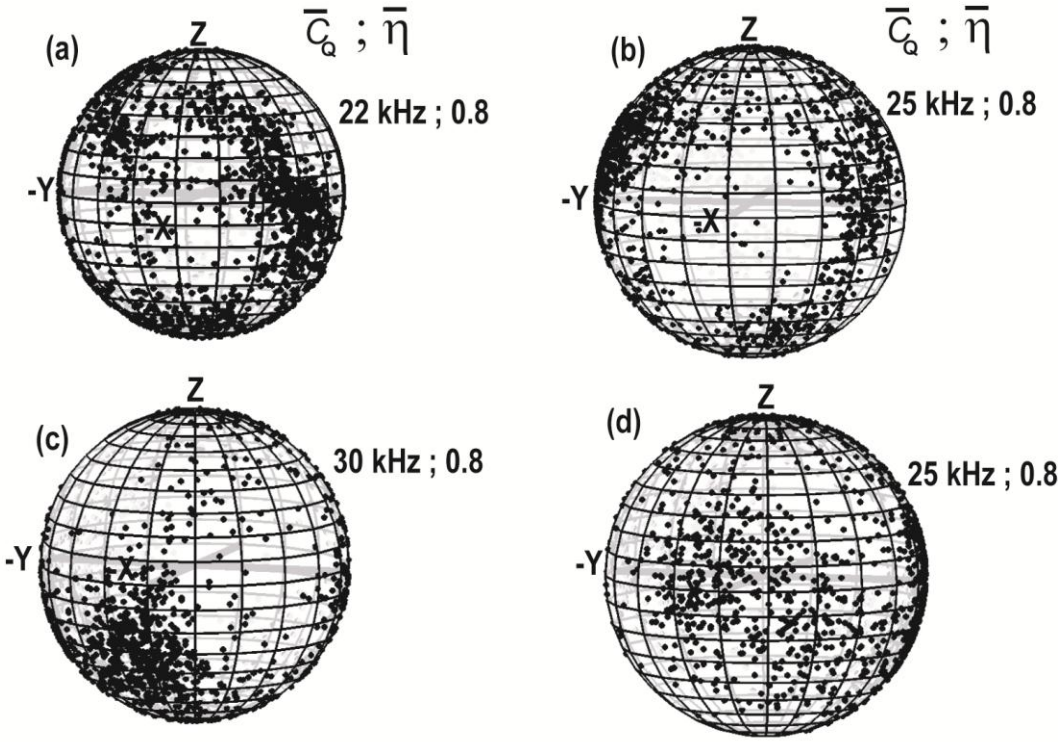

Figure S3: Distribution of the trajectory vectors derived from MD representing the spatial variation of C_1-$D_{1,2}$ and C_2-$D_{3,4}$ drawn on a unit sphere are shown in (a,b) and (c,d) respectively. Data points correspond to those behind the sphere shown in Figure 7.

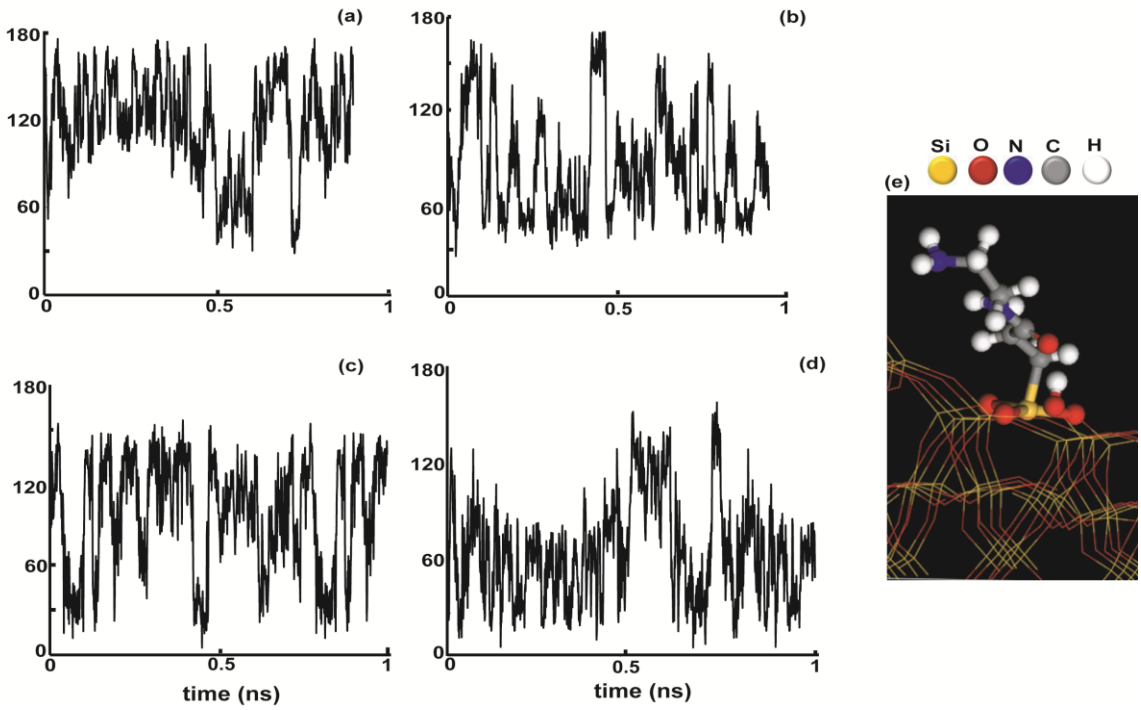

Figure S4: Variation of the time dependent polar angle θ for C_1-$D_{1,2}$ and C_2-$D_{3,4}$ are shown in (a,b) and (c,d) respectively for the model described in Figure 8. The molecular conformation where the mobility of the linker gets restricted through CO---HO hydrogen bonding derived from MD is shown in (e). MD calculation was performed at 295 K for a time period of ~ 1ns.

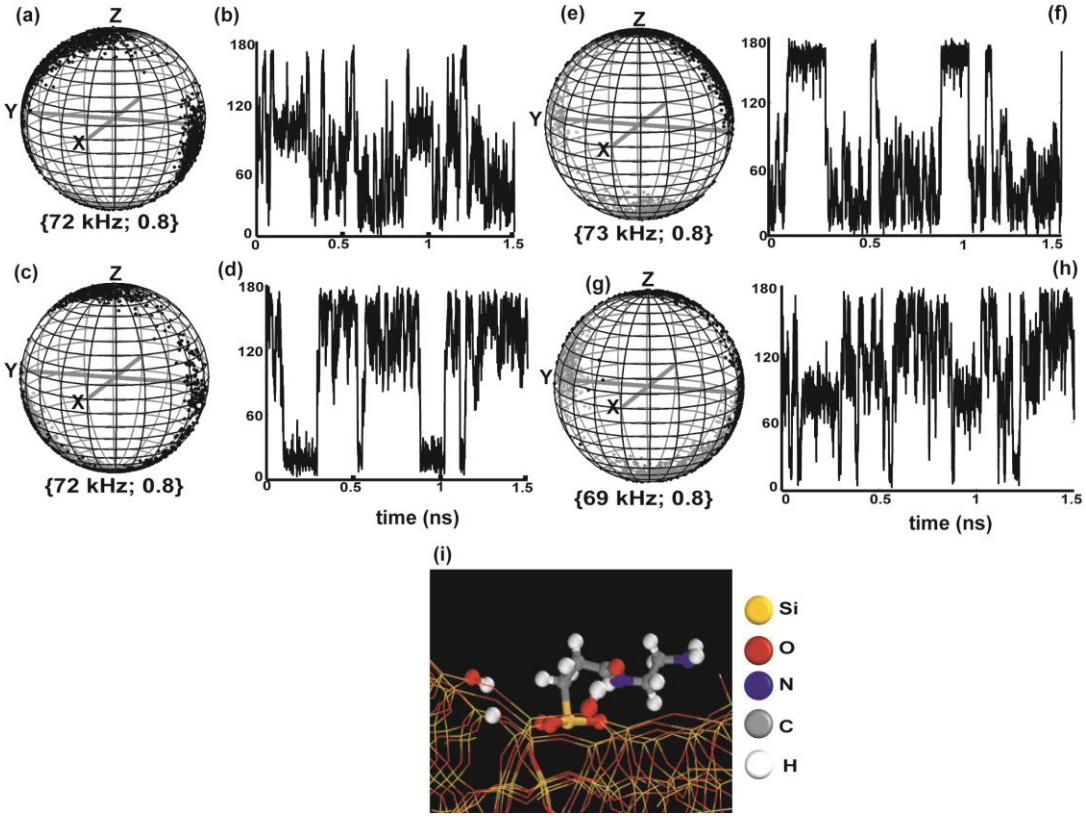

Figure S5: Distribution of the trajectory vectors drawn on a unit sphere along with the variation of the time dependent polar angle θ for C_1-$D_{1,2}$ and C_2-$D_{3,4}$ derived from MD calculation are shown in (a-d) and (e-h) for the model where more than one hydroxyl is introduced. The configuration shown in (i) corresponds to the restricted mobility of the linker through CO---HO hydrogen bonding. MD calculation was performed at 295 K for a time period of ~ 1.5 ns. Averaged quadrupolar parameters calculated are shown therein. Trajectories behind the sphere are drawn in grey.

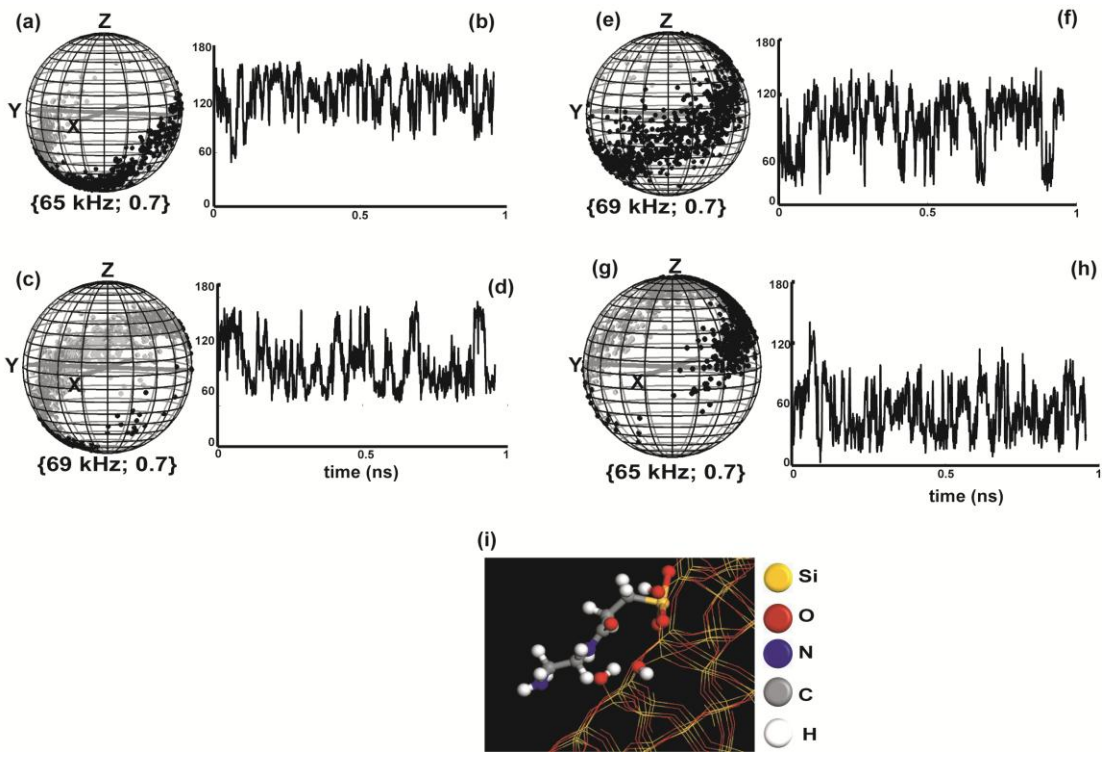

Figure S6: Distribution of the trajectory vectors drawn on a unit sphere along with the variation of the time dependent polar angle θ for C_1-$D_{1,2}$ and C_2-$D_{3,4}$ derived from the MD calculation are shown in (a-d) and (e-h) for the model with more than one hydroxyl on the surface. Molecular conformation where the linker gets bound to the surface hydroxyl through NH---OH hydrogen bonding is shown in (i). MD calculation was performed at 295 K for a time period of ~ 1 ns. Averaged quadrupolar parameters calculated are shown therein. Trajectories behind the sphere are drawn in grey.

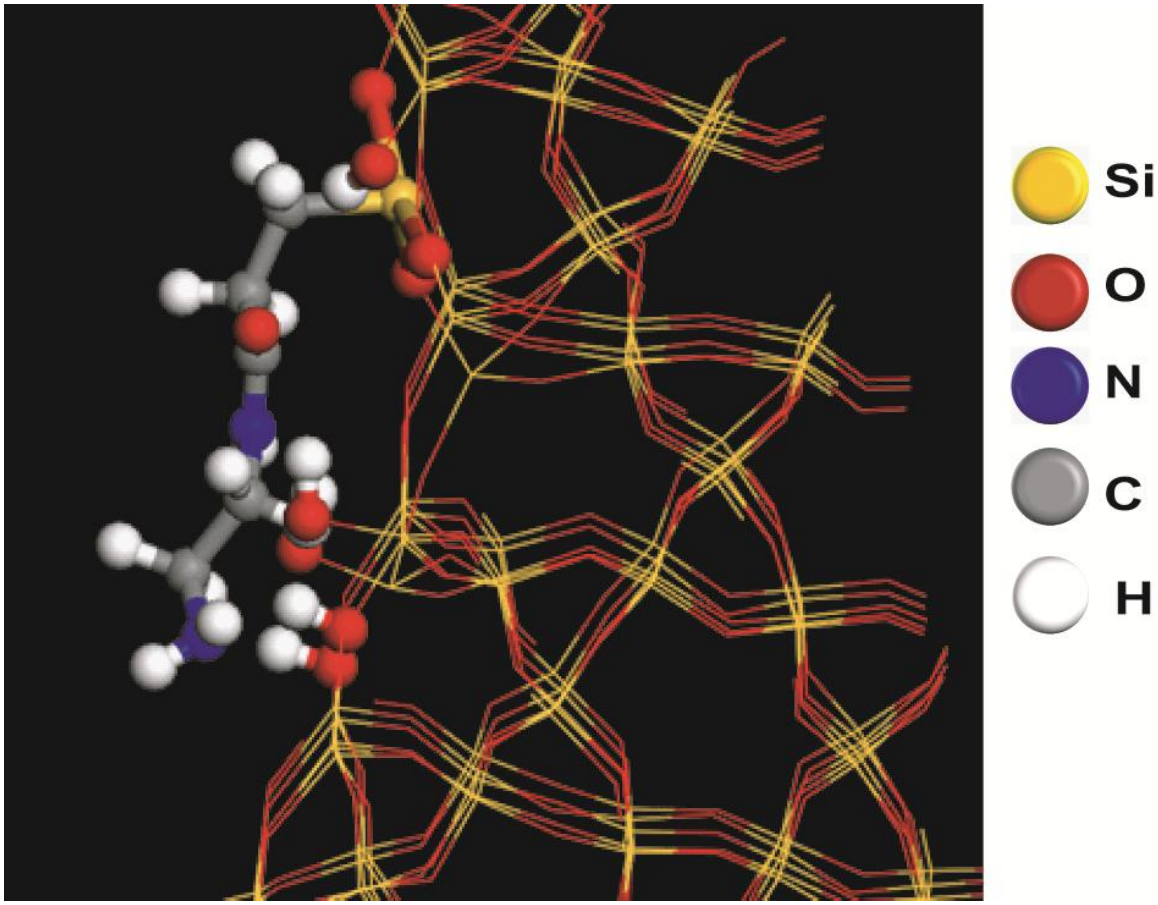

Figure S7: Molecular conformation where the linker gets bound to the surface through NH---OH and NH_2---OH hydrogen bonding thereby resulting in static quadrupolar interaction parameters is shown. MD calculation was performed at 295 K for a time period of ~ 2 ns.