

Supporting Information Available

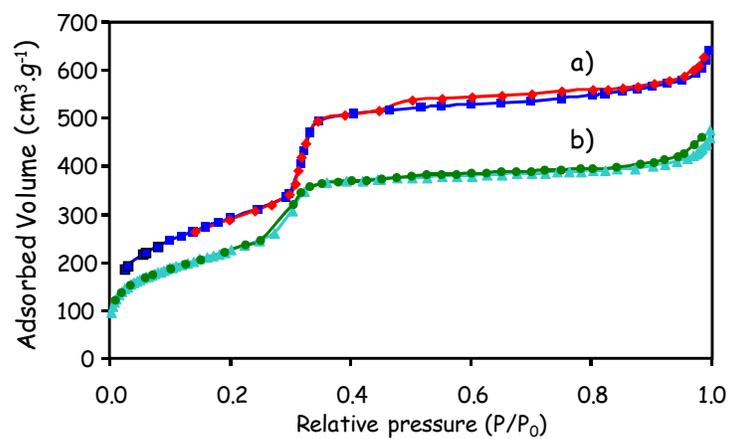
## A Molecular Picture of the Adsorption of Glycine in Mesoporous Silica through NMR Experiments Combined with DFT-D Calculations

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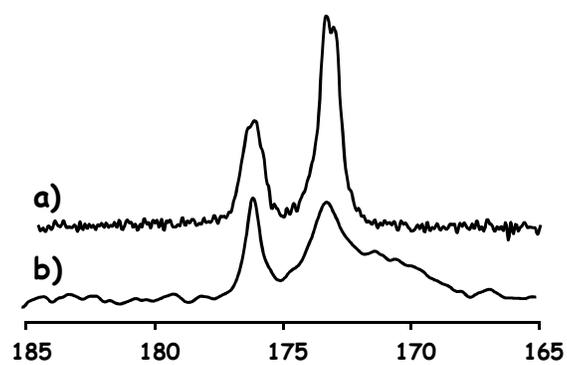
**Table S1:** Porosity Characteristics (BET Surface:  $S_{\text{BET}}$ , Porous volume:  $V_{\text{p}}$ , and average pore diameter) for unloaded and loaded MCM-41.

Sample	$S_{\text{BET}}$ ( $\pm 10 \text{ m}^2 \cdot \text{g}^{-1}$ )	Average pore diameter ( $\pm 2 \text{ \AA}$ )	$V_{\text{p}}$ ( $\pm 0.05 \text{ cm}^3 \cdot \text{g}^{-1}$ )
MCM-41	1060	33	1.1
Gly-MCM-41	830	29	0.7

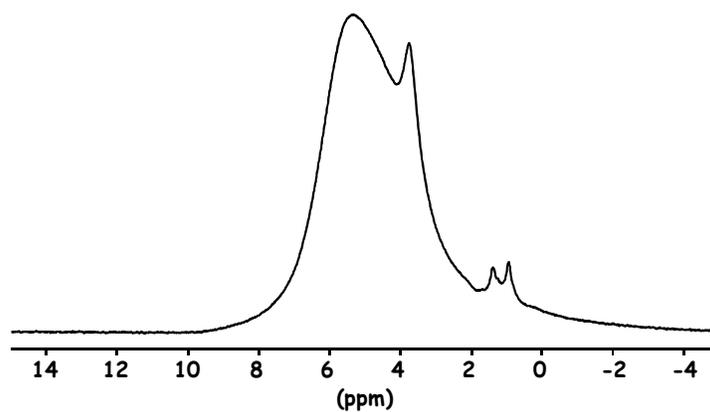
**Figure S1:** Nitrogen adsorption-desorption isotherms for both a) calcined MCM-41 and b) sample loaded with glycine.



**Figure S2:** Experimental <sup>13</sup>C a) MAS and b) CP MAS NMR spectra of glycine in MCM-41 sample.



**Figure S3:** Experimental  $^1\text{H}$  MAS NMR spectrum of glycine in MCM-41 sample.



**Figure S4:** Experimental and deconvoluted  $^{29}\text{Si}$  MAS NMR spectrum of calcined MCM-41 sample.

