

## Supporting Information

### **Tailoring morphology of hierarchical catalysts for tuning pore diffusion behaviour: A rational guideline exploiting bench-top Pulsed-Field Gradient (PFG) Nuclear Magnetic Resonance (NMR)**

Luke Forster<sup>1</sup>, Michal Lutecki<sup>2</sup>, Henrik Fordsmand<sup>2</sup>, Le Yu<sup>1</sup>, Carmine D'Agostino\*<sup>1</sup>

<sup>1</sup> School of Chemical Engineering and Analytical Science, The University of Manchester, Oxford Road, Manchester, M13 9PL, United Kingdom

<sup>2</sup> Haldor Topsøe A/S, Haldor Topsøes Allé 1, DK-2800, Kongens Lyngby, Denmark

\*Corresponding author

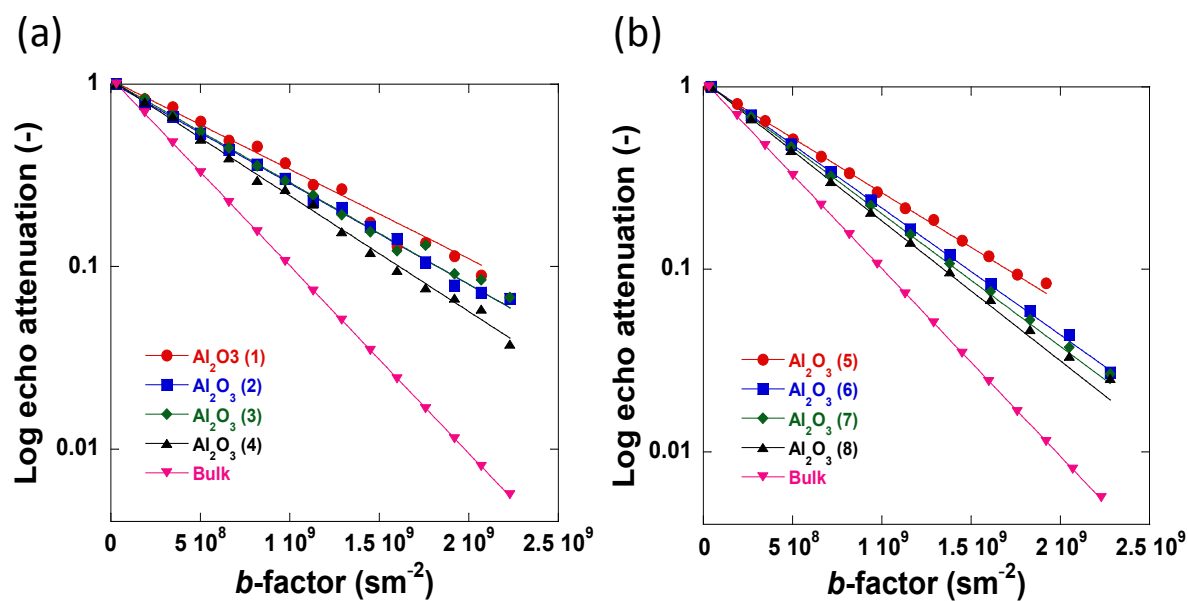
Carmine D'Agostino

Email: [carmine.dagostino@manchester.ac.uk](mailto:carmine.dagostino@manchester.ac.uk)

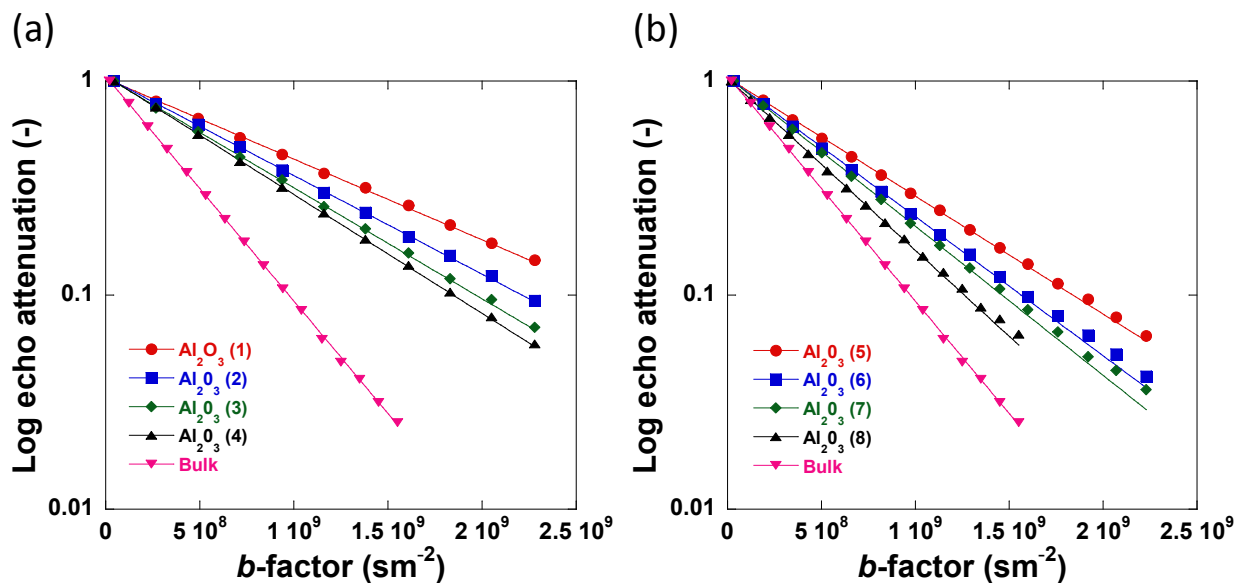
**Table S1.** Root mean squared displacements (*RMSD*) used to investigate the self-diffusivity of the guest molecules; *n*-octane, water, methanol and ethanol within the alumina carriers Al<sub>2</sub>O<sub>3</sub> (1) - Al<sub>2</sub>O<sub>3</sub> (8) during PFG

Sample	<i>RMSD</i> <sub>OCT</sub> (μm)	<i>RMSD</i> <sub>H<sub>2</sub>O</sub> (μm)	<i>RMSD</i> <sub>MeOH</sub> (μm)	<i>RMSD</i> <sub>EtOH</sub> (μm)
Al <sub>2</sub> O <sub>3</sub> (1)	9.70	10.63	9.31	6.39
Al <sub>2</sub> O <sub>3</sub> (2)	10.55	11.29	10.30	7.04
Al <sub>2</sub> O <sub>3</sub> (3)	11.14	11.34	10.93	7.35
Al <sub>2</sub> O <sub>3</sub> (4)	11.64	12.09	11.30	7.75
Al <sub>2</sub> O <sub>3</sub> (5)	11.58	11.74	11.26	7.52
Al <sub>2</sub> O <sub>3</sub> (6)	12.66	12.65	12.24	8.26
Al <sub>2</sub> O <sub>3</sub> (7)	12.70	12.94	12.66	8.69
Al <sub>2</sub> O <sub>3</sub> (8)	13.04	13.29	13.61	9.12

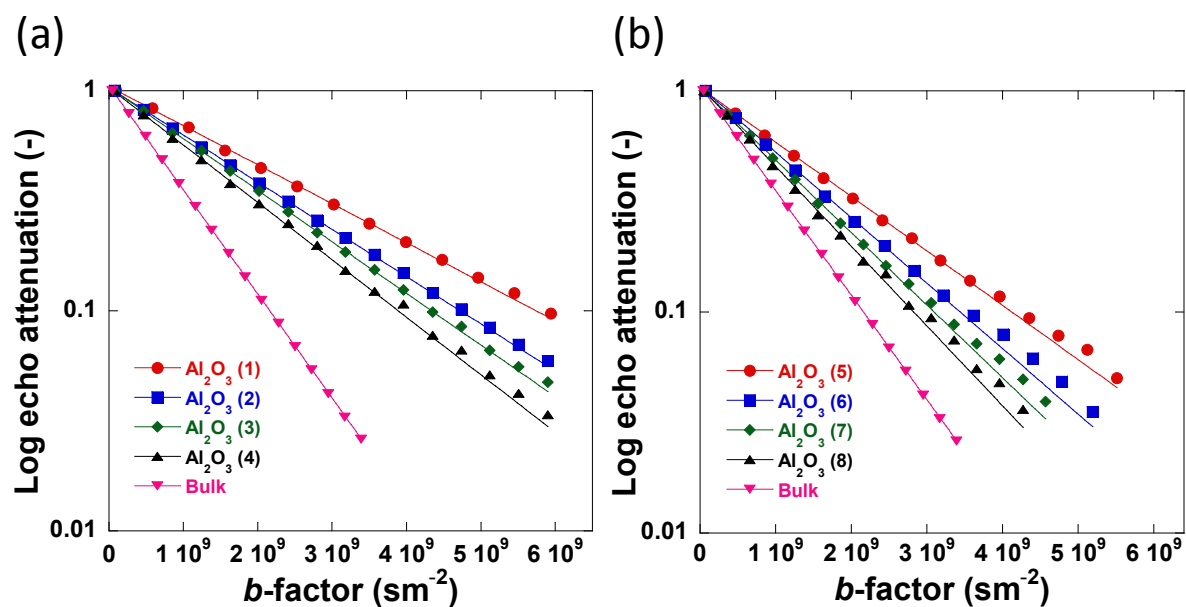
NMR diffusometry experiments.



**Figure S1.** Log attenuation plots of water imbibed within (a) Al<sub>2</sub>O<sub>3</sub> (1) – Al<sub>2</sub>O<sub>3</sub> (4) and (b) Al<sub>2</sub>O<sub>3</sub> (5) – Al<sub>2</sub>O<sub>3</sub> (8). Solid lines are fitting to Equation (1).



**Figure S2.** Log attenuation plots of methanol imbibed within (a)  $\text{Al}_2\text{O}_3$  (1) –  $\text{Al}_2\text{O}_3$  (4) and (b)  $\text{Al}_2\text{O}_3$  (5) –  $\text{Al}_2\text{O}_3$  (8). Solid lines are fitting to Equation (1).



**Figure S3.** Log attenuation plots of ethanol imbibed within (a)  $\text{Al}_2\text{O}_3$  (1) –  $\text{Al}_2\text{O}_3$  (4) and (b)  $\text{Al}_2\text{O}_3$  (5) –  $\text{Al}_2\text{O}_3$  (8). Solid lines are fitting to Equation (1).