

Supporting Information

Functionalized ordered mesoporous silica by vinyltriethoxysilane for the removal of VOCs through adsorption/desorption process

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Analysis of pore size distribution for the pure SiO₂ and vinyl-functionalized SiO₂

The pore size distribution of the pure and vinyl-functionalized SiO₂ were obtained by the DFT model, shown in the **Figure S1**. It can be seen that all the samples present a main mesoporous and different micropores. The main mesoporous were formed for the function of the template agent (P123). Meanwhile the micropores were formed due to the EO portion of the P123¹⁻². It also can be seen that there is a shoulder peak along the main mesoporous peak for the v-SiO₂(5%) and v-SiO₂(10%), which is attributed to the pore block caused by the vinyl functionalization. However, there are no shoulder peaks appearing in the v-SiO₂(15%) and v-SiO₂(20%), which indicates that structure transformation could weaken the pore block to some extent. Moreover, the mean pore size have decreased with more vinyl functionalized. This result suggests that the addition of the VTES could influence the size of the micelles formed by P123.

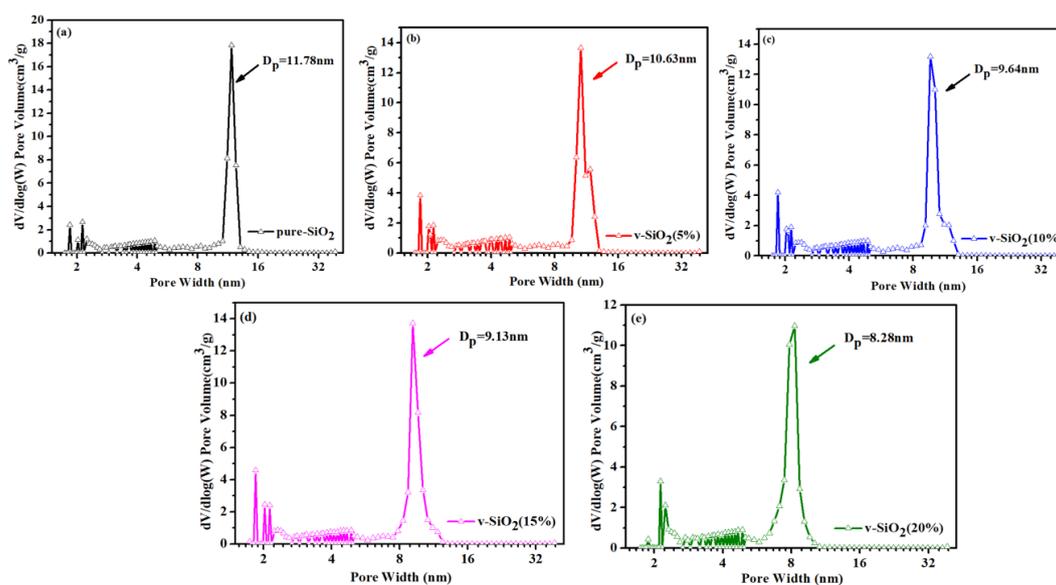


Figure S1. Pore size distribution for the (a) pure SiO₂ and (b-e) vinyl-functionalized SiO₂.

Table S1. Surface chemical composition of synthesized adsorbents from XPS

analysis.

Samples	C(1s)	Si(2p)	O(1s)
pure-SiO ₂	11.86	30.11	58.03
v-SiO ₂ (5%)	16.35	28.45	55.20
v-SiO ₂ (10%)	19.91	27.27	52.83
v-SiO ₂ (15%)	21.21	26.99	51.80
v-SiO ₂ (20%)	22.08	26.78	51.14

Table S2. Specific chemical composition of C1s in pure SiO₂ and v-SiO₂.

C(1s)	C-Si(-O)		C-O(-Si)		C-C(-H) / C=C(H)	
	Binding energy (eV)	Amount (%)	Binding energy (eV)	Amount (%)	Binding energy (eV)	Amount (%)
pure-SiO ₂	--	--	286.83	60.0	285.08	40.0
v-SiO ₂ (5%)	285.53	28.4	286.95	49.6	284.82	22.0
v-SiO ₂ (10%)	285.54	32.3	286.89	39.7	284.82	28.1
v-SiO ₂ (15%)	285.64	35.8	287.03	33.9	284.83	30.3
v-SiO ₂ (20%)	285.64	36.1	287.04	32.3	284.83	31.6

Table S3. Desorbed amount and ratio of *p*-xylene from different adsorbents under dry and wet condition.

Samples	Desorbed amount (mmol/g)		Desorption ratio	
	dry	wet	dry	wet
pure SiO ₂	0.73	0.32	92.1%	71.4%
v- SiO ₂ (5%)	0.81	0.53	91.3%	77.2%
v- SiO ₂ (10%)	0.86	0.62	90.6%	81.5%
v- SiO ₂ (15%)	0.82	0.65	89.2%	88.1%
v- SiO ₂ (20%)	0.71	0.60	88.5%	87.67%

Repeatability of adsorption process on different adsorbents under wet and dry conditions

The adsorption process of different adsorbents under different conditions were conducted on replicates to avoid the experimental error. The results are presented in the **Figure S2** and **Figure S3** in the form of error bars.

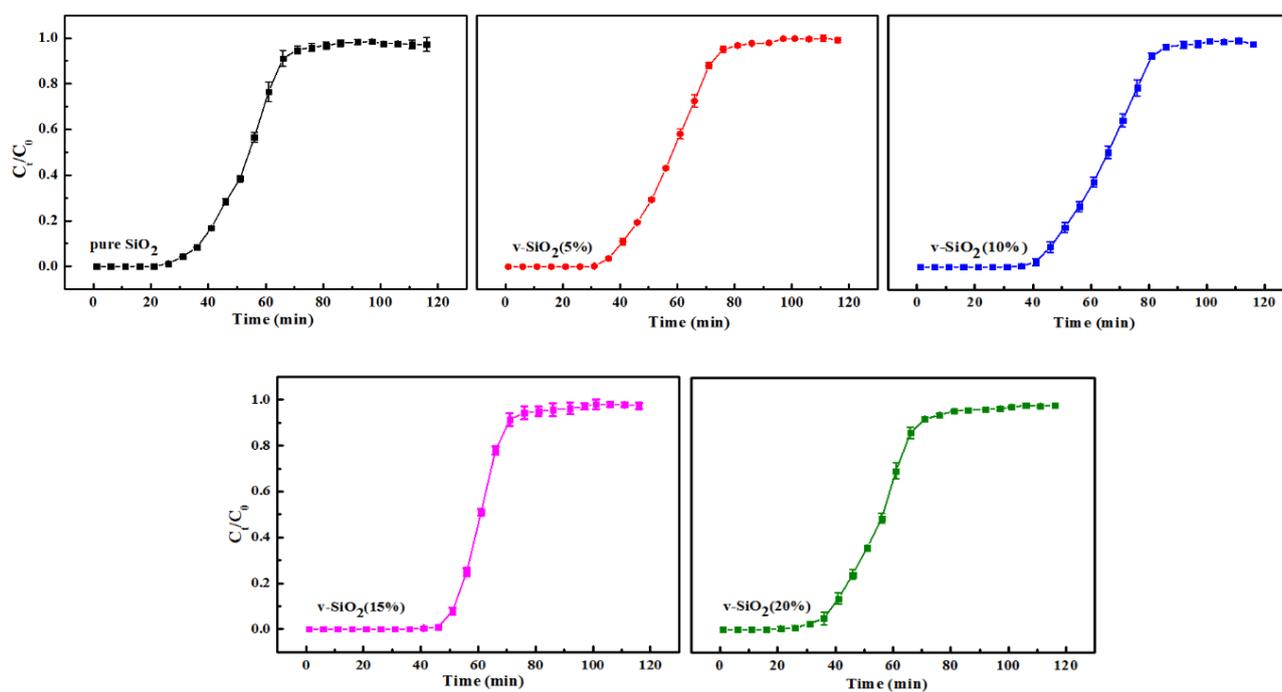


Figure S2. Adsorption breakthrough curves of *p*-xylene on the synthesized adsorbents under dry condition on replicates.

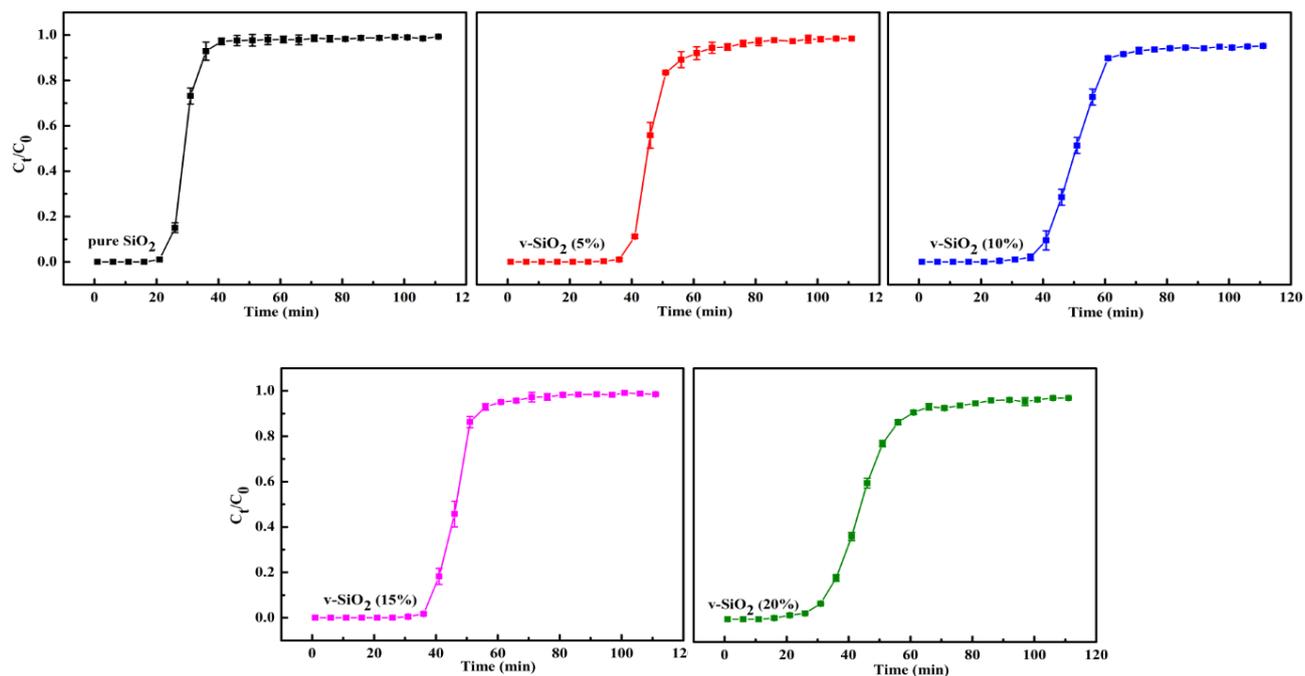


Figure S3. Adsorption breakthrough curves of *p*-xylene on the synthesized adsorbents under wet condition on replicates.

Analysis of desorption process for *p*-xylene on pure SiO₂ and vinyl-functionalized SiO₂ under dry condition

To further understand the desorption process on different adsorbents, the desorption data has been analyzed. Results have been presented in the **Figure S4**. We introduce two important parameters for discussions, D_e and D_t . The D_e represents the final desorption ratio defined as equilibrium desorption ratio. The D_t represents the desorption ratio within a certain time defined as the desorption ratio. The dimensionless value D_t/D_e represents the desorption equilibrium conversion ratio. The time to reach the equilibrium desorption status is mainly affected by the mass transfer rate and the interaction between the adsorbate and the adsorbent. The v-SiO₂ (15%) and v-SiO₂ (20%) possess stronger affinity to the adsorbate (i.e., *p*-xylene). However, the time for the equilibrium desorption on these adsorbents is shorter than those of pure-SiO₂ and v-SiO₂(5%). This result indicated that the desorption process is mainly controlled by the diffusion process. It is suggested that the v-SiO₂ (15%) and v-SiO₂ (20%) with 3D cubic structure present higher mass transfer rate in the desorption process than that of pure-SiO₂ and v-SiO₂ (5%) with 2D hexagonal structure³.

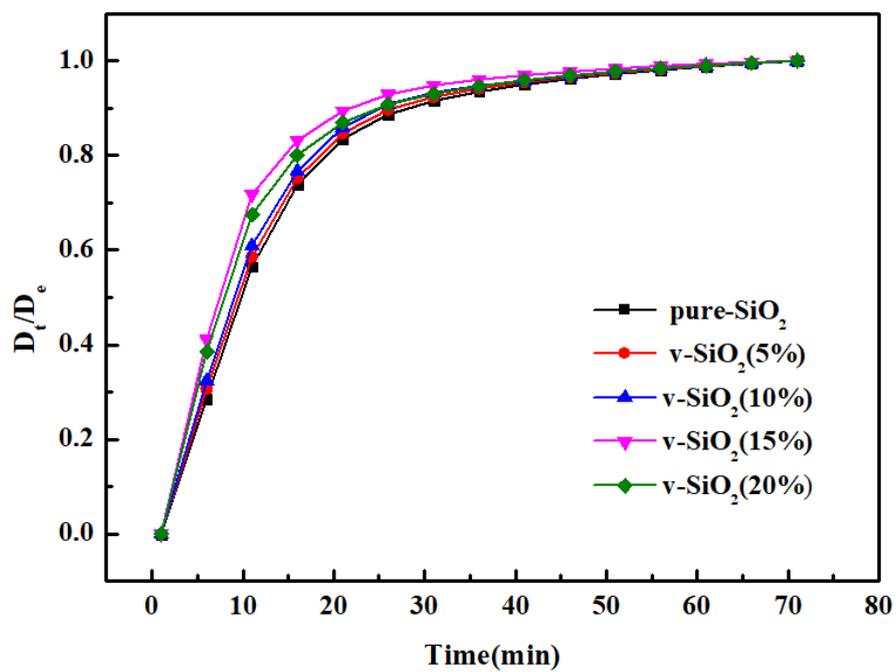


Figure S4. Desorption equilibrium curves of the pure-SiO₂ and v-SiO₂.

Reference

1. Ryoo, R.; Ko, C. H.; Kruk, M.; Antochshuk, V.; Jaroniec, M., Block-Copolymer-Templated Ordered Mesoporous Silica: Array of Uniform Mesopores or Mesopore Micropore Network *J.Phys.Chem.B* **2000**, *104*, 11465-11471.
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3. Dou, B.; Hu, Q.; Li, J.; Qiao, S.; Hao, Z., Adsorption performance of VOCs in ordered mesoporous silicas with different pore structures and surface chemistry. *J. Hazard. Mater.* **2011**, *186*, 1615-1624.