Superhydrophobic and Stable Mesoporous Polymeric Adsorbent for Siloxane Removal: D4 Super-Adsorbent

Tahereh Jafari,[a]‡ Iman Noshadi,[b,c]‡ Nasser Khakpash [a] and Steven. L. Suib* [a,d]

[a] Institute of Materials Science, University of Connecticut, U-3060, 91 North Eagleville Road, Storrs, Connecticut 06269, United States
[b] Department of Chemical & Biomolecular Engineering, 191 Auditorium Road, Unit 3222, Storrs, CT 06269-3222, United States
[c] Harvard-MIT Health Sciences and Technology, Massachusetts Institute of Technology, 77 Massachusetts Ave, Cambridge, MA 02139, United States
[d] Department of Chemistry, University of Connecticut, U-3060, 55 North Eagleville Road, Storrs, Connecticut 06269, United States s here.
‡These authors contributed equally.
*Correspondence and requests for materials should be addressed to S.L.S. (email:steven.suib@uconn.edu).

Electronic Supplementary Information

Biogas composition at the entrance of the biogas polishing system at 30°C and 25-30 mbar (Table S1), properties of linear and cyclic siloxanes (Table S2) and some high capacity current alternative for siloxane removal (Table S3), the siloxane adsorption capacity of PDVB and PDVB-HT (Table S4).

Molecular configuration of D4 (Figure S1), schematic view of siloxane adsorption set-up (Figure S2), GC/MS pattern of standard concentration of D4 in hexane which was used to derive calibration curve (Figure S3), GC/MS pattern of amount of D4 in trap which was sampled at different time interval when PDVB-VI-x under 50% RH was loaded (Figure S4), GC/MS pattern of amount of D4 in trap which was sampled at different time interval when AC under 50% RH was loaded (Figure S5) and GC/MS pattern of saturated AC and PDVB-VI-x, washed by hexane (Figure S6).

Table S1. Biogas composition at the entrance to the biogas polishing system at 30ºC and 25-30 mbar(g)[2].

Compound/trace	Units	Range
CH_4	%	55.1-57.8
CO_2	%	28.5-32.5
N_2	%	7.5-12
O_2	%	1.8-2.9
Relative humidity (RH)	%sat	100
H_2S	ppm	104-1.854
Organic sulfur	mg/m^3_{STP}	0.8-2.2
Alkanes	mg/m^3_{STP}	55.2-92.4
Aromatic compound	mg/m^3_{STP}	6.7-13.5
D3	mg/m^3_{STP}	0-0.8
D4	mg/m^3_{STP}	4-6.5
D5	mg/m^3_{STP}	6.5-9

Table S2. Properties of linear and cyclic siloxanes.

Siloxane type	Abbrv	Molecular weight (g/mol)	Vapor Pressure (torr)	Boiling point (oC)	Water solubility (mg/L) at 25^{o}C
Hexamethyldisiloxane	L2	162	31	100	0.93
Octamethyltrisiloxane	L3	237	3.9	153	0.04
Decamethyltetrasiloxane	L4	311	0.43	194	--
Dodecamethylpentasiloxane	L5	385	0. 1022	230	--
hexamethylcyclotrisiloxane	D3	222	10	134	1.56
Octamethycyclotetrasiloxane	D4	296	1.3	175	0.06
Decamethylcyclopentasiloxane	D5	371	0.4	210	0.02
Dodecamethylcyclohexasiloxane	D6	445	0. 0494	245	0.005

Table S3. Some high capacity current alternatives for siloxane removal.

Material	Capacity (mg/g-adsorbent)	Siloxane type	Surface area (m^2/g)	Reference
AC impregnated by KOH	878	L2	N/A	[17]
AC fiber cloths	365	D4	1576	[23]
ACs	1732	D4	2142	[5]

Table S4. The siloxane adsorption capacity of PDVB and PDVB-HT.

Materials	Regular gas stream
PDVB	1951±74
PDVB-HT	1965±36

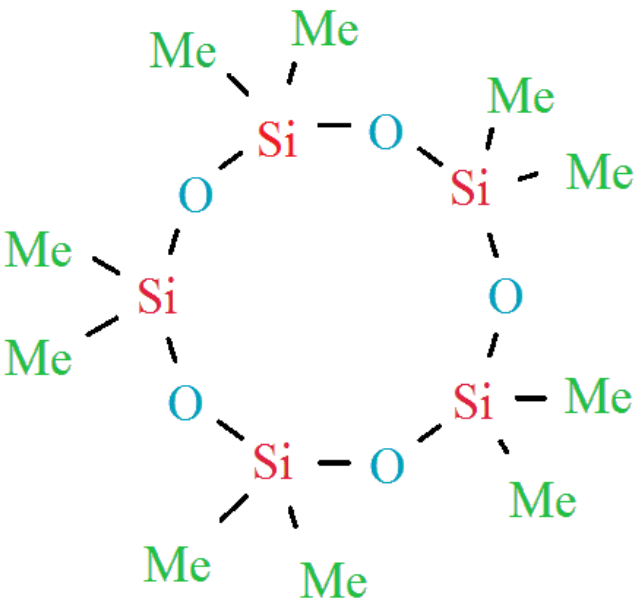

Figure S1. Molecular structure of octamethylcyclotetrasiloxane (D4).

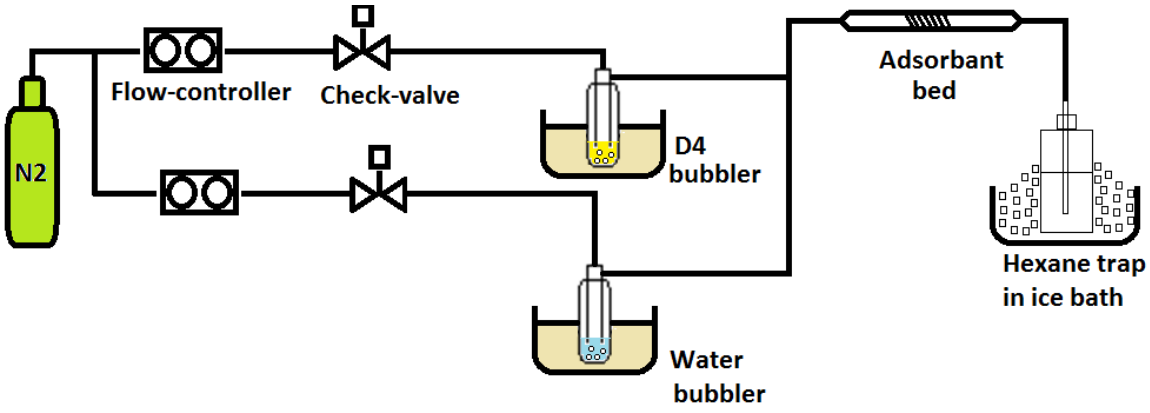

Figure S2. Experimental set-up for siloxane adsorption.

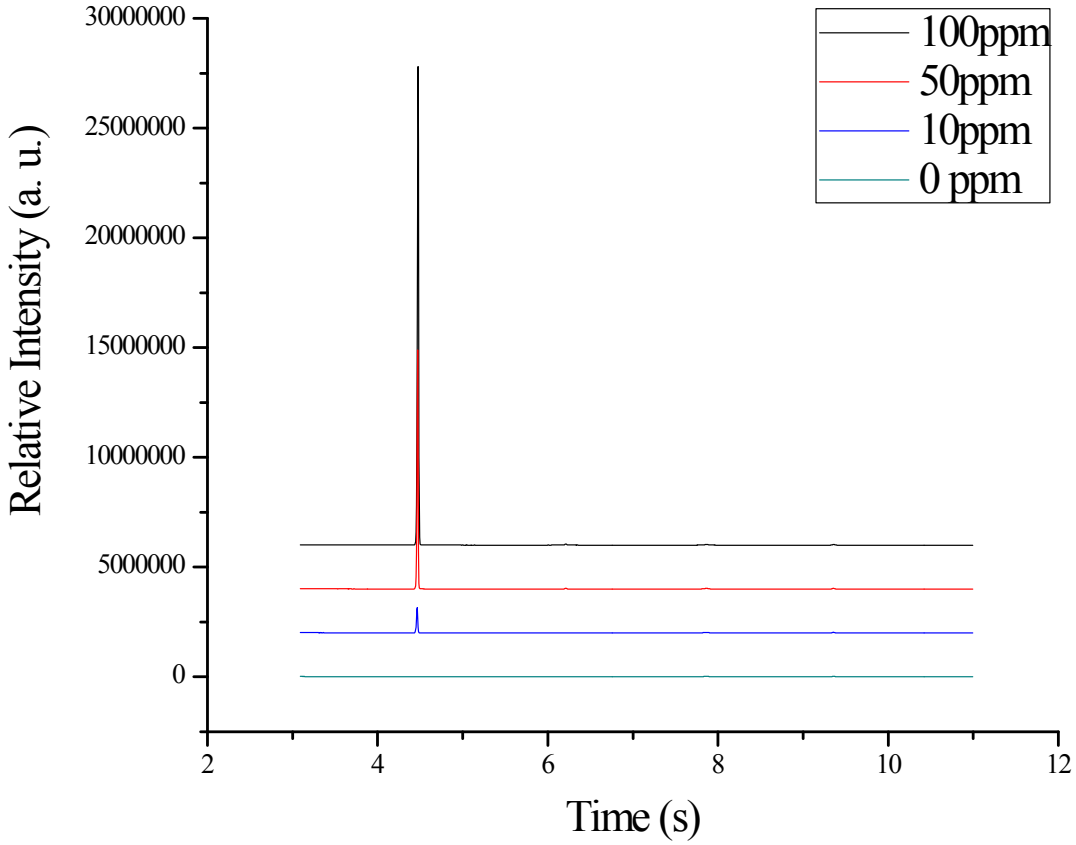

Figure S3. GC/MS pattern of standard concentration of D4 in hexane which was used to derive the calibration curve (D4 peak appears at 4.5 s).

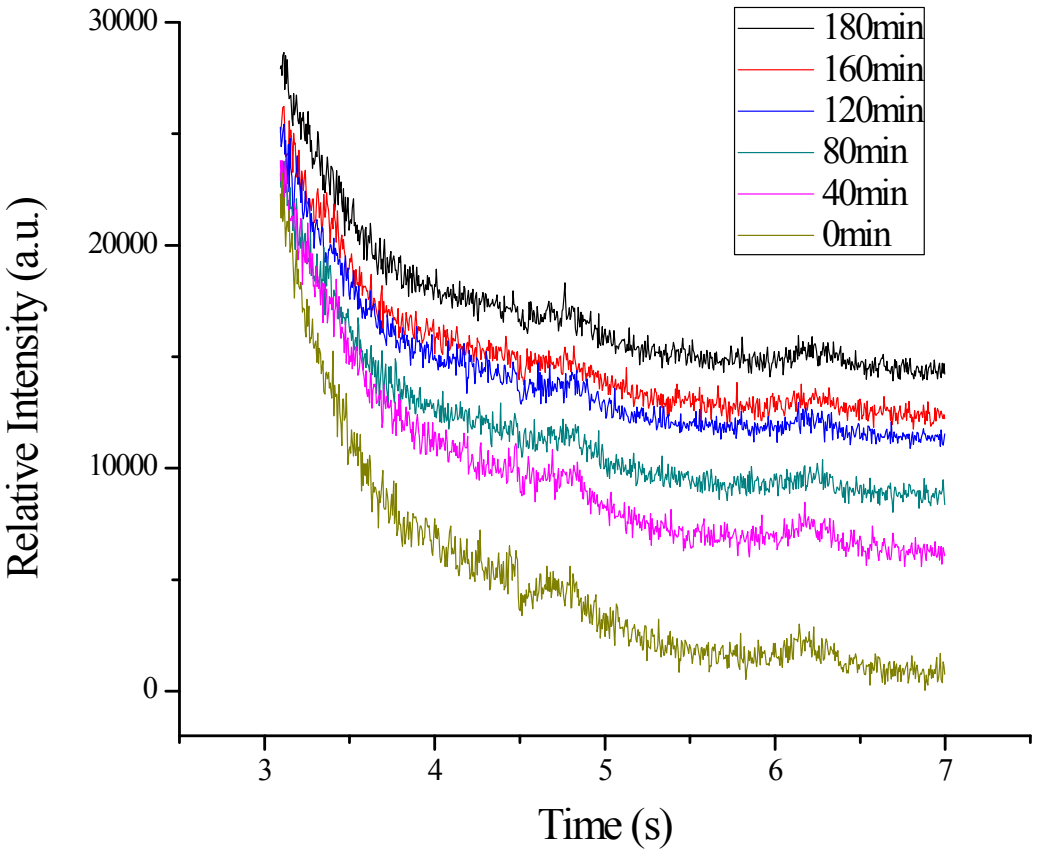

Figure S4. GC/MS pattern of amounts of D4 in trap which were sampled at different time intervals when PDVB-VI-x under 50% RH was loaded (D4 peak appears at 4.5 s).

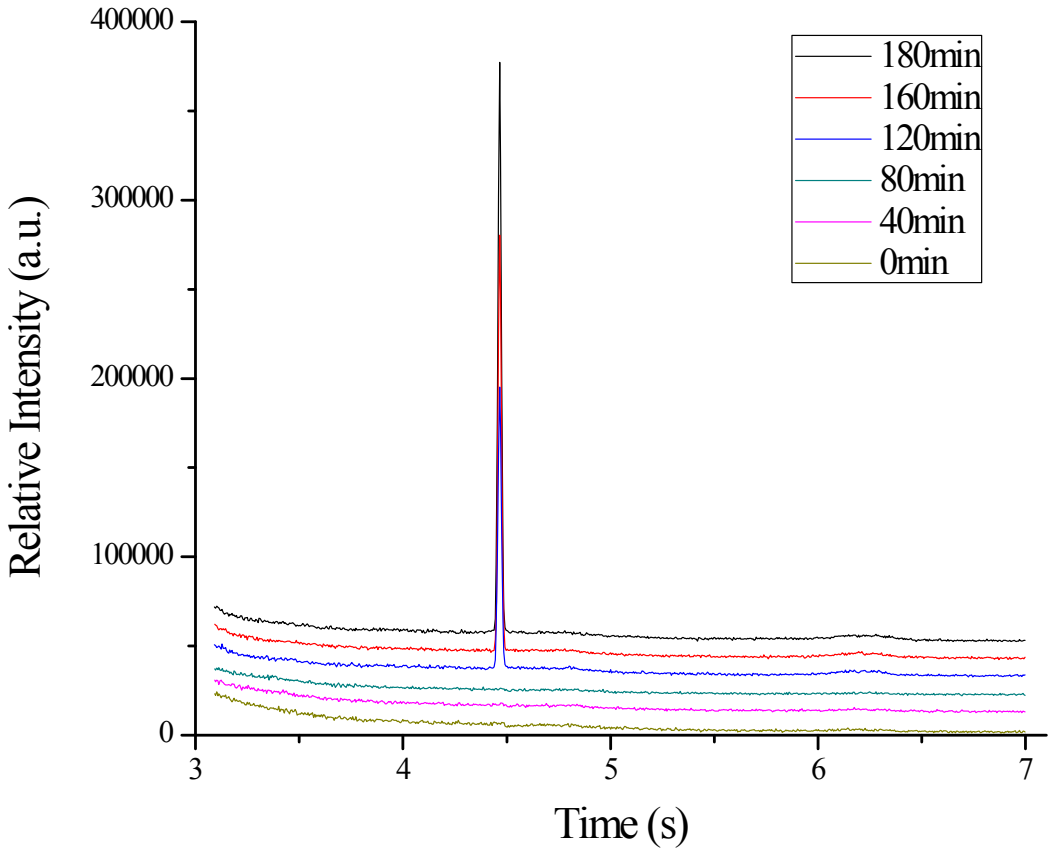

Figure S5. GC/MS pattern of amounts of D4 in trap which were sampled at different time intervals when AC under 50% RH was loaded (D4 peak appears at 4.5 s).

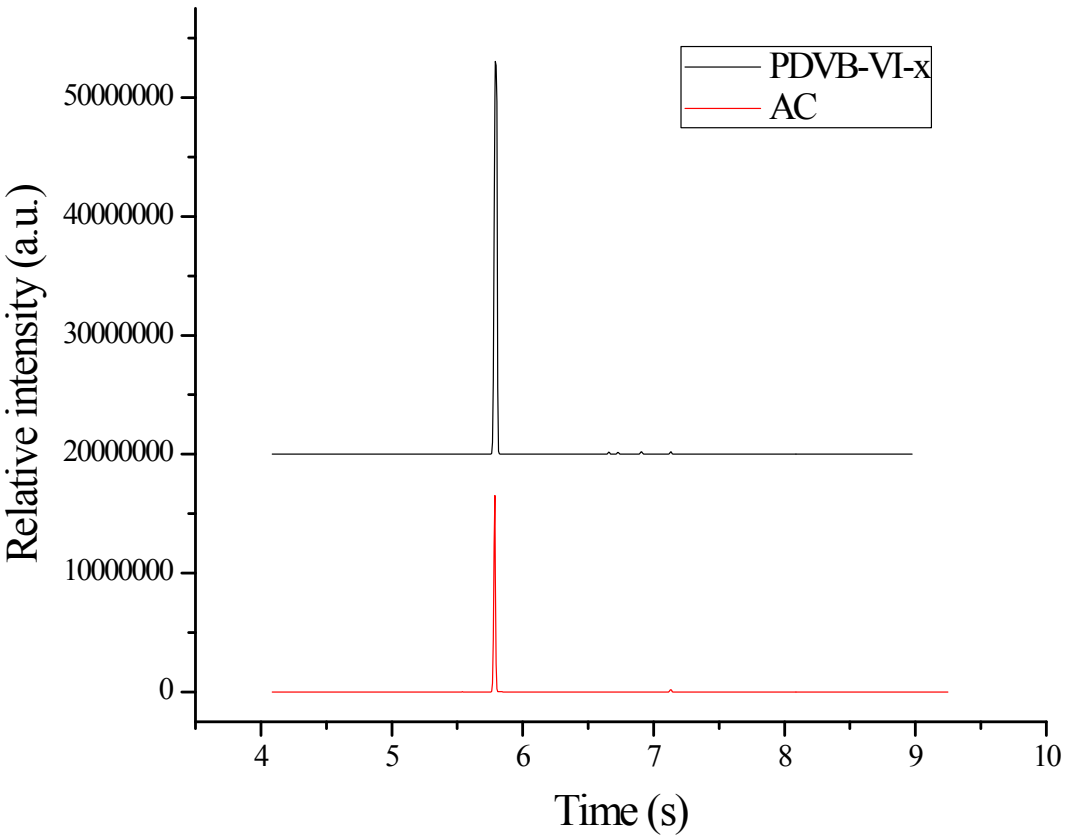

Figure S6. GC/MS pattern of saturated AC (red) and PDVB-VI-x (black), washed by hexane.