

SUPPORTING INFORMATION

## Separation of CO<sub>2</sub> from Air by Temperature-Vacuum Swing Adsorption Using Diamine-Functionalized Silica Gel

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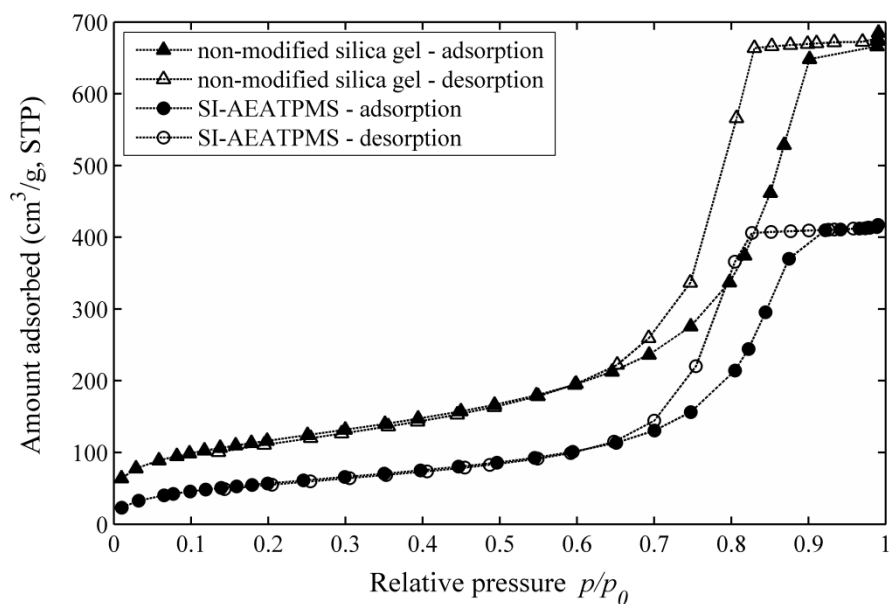
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### N<sub>2</sub> Adsorption/Desorption Isotherms



**Figure S1.** N<sub>2</sub> adsorption (closed symbols) and desorption (open symbols) isotherms for non-modified silica gel support (ZEObeads<sup>TM</sup> B2, triangles) and SI-AEATPMS sorbent material (circles).

## Energy Requirements

The energy requirements for sorbent regeneration in the TVS process were estimated using the assumptions summarized in Table S1. The work  $W_{comp}$  required for compression of the CO<sub>2</sub> from desorption pressure to ambient pressure was calculated according to Eq. (S1). The heat (low-temperature heat at below 95 °C) required for heating up the sorbent material to the desorption temperature  $Q_{sens}$  and for desorption of CO<sub>2</sub> and co-adsorbed H<sub>2</sub>O  $Q_{des}$  was calculated according to Eq. (S2) and Eq. (S3), respectively. The total required heat  $Q$  is the sum of  $Q_{sens}$  and  $Q_{des}$  (Eq. (S4)). A ratio of co-adsorbed water and adsorbed CO<sub>2</sub> of approximately 1 was assumed.<sup>1</sup>

$$W_{comp} = \frac{1}{\eta_{pump}} \cdot R \cdot T \cdot \ln\left(\frac{p_{amb}}{p_{des}}\right) \quad (S1)$$

$$Q_{sens} = \frac{1}{\Delta q_{TVS}} \cdot c_p \cdot \Delta T \quad (S2)$$

$$Q_{des} = Q_{des,CO_2} + Q_{des,H_2O} \quad (S3)$$

$$Q = Q_{sens} + Q_{des} \quad (S4)$$

Assumption	Symbol	Value	Source
Cyclic CO <sub>2</sub> capacity of sorbent (SI-AEAPTMS material used in this work)	$\Delta q_{TVS}$	0.2 mmol/g	this work
Cyclic CO <sub>2</sub> capacity of sorbent (advanced sorbent material with higher cyclic capacity)	$\Delta q_{TVS}$	2 mmol/g	2
Heat capacity of the sorbent material (silica)	$c_p$	0.9 $\frac{\text{kJ}}{\text{kg}\cdot\text{K}}$	3
Temperature difference between adsorption and desorption	$\Delta T$	65 K	this work
Heat of desorption, CO <sub>2</sub>	$Q_{des,CO_2}$	$\approx 90 \frac{\text{kJ}}{\text{mol}}$	4, 5
Heat of desorption, co-adsorbed H <sub>2</sub> O	$Q_{des,H_2O}$	$\approx 47 \frac{\text{kJ}}{\text{mol}}$	4
Amount of co-adsorbed H <sub>2</sub> O	$n_{H_2O}/n_{CO_2}$	1	1
Desorption pressure	$p_{des}$	100 mbar	this work
Vacuum pump efficiency (with respect to isothermal compression at T = 350 K)	$\eta_{pump}$	0.7	estimation

**Table S1.** Assumptions for energy requirement estimation.

## References

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