Electronic Supplementary Material (ESI)

N^1-(3-trimethoxysilylpropyl)diethylenetriamine Grafted KIT-6

for CO_2/N_2 Selective Separation

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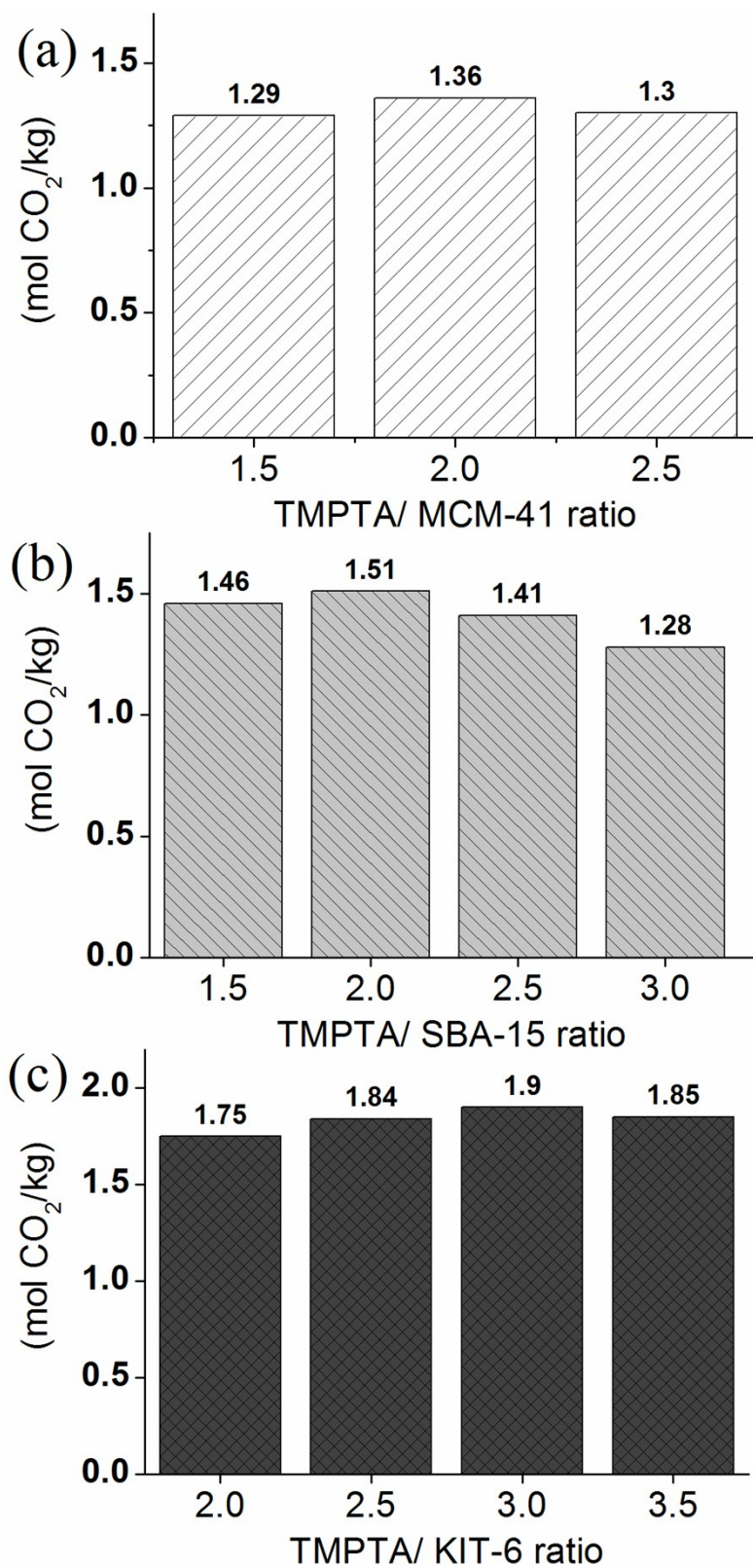*Corresponding author e-mail: rupak.k@iitg.ernet.in*

Fig. S1 Effect of aminosilane (TMPTA) to OMSs ratio on CO_2 adsorption.
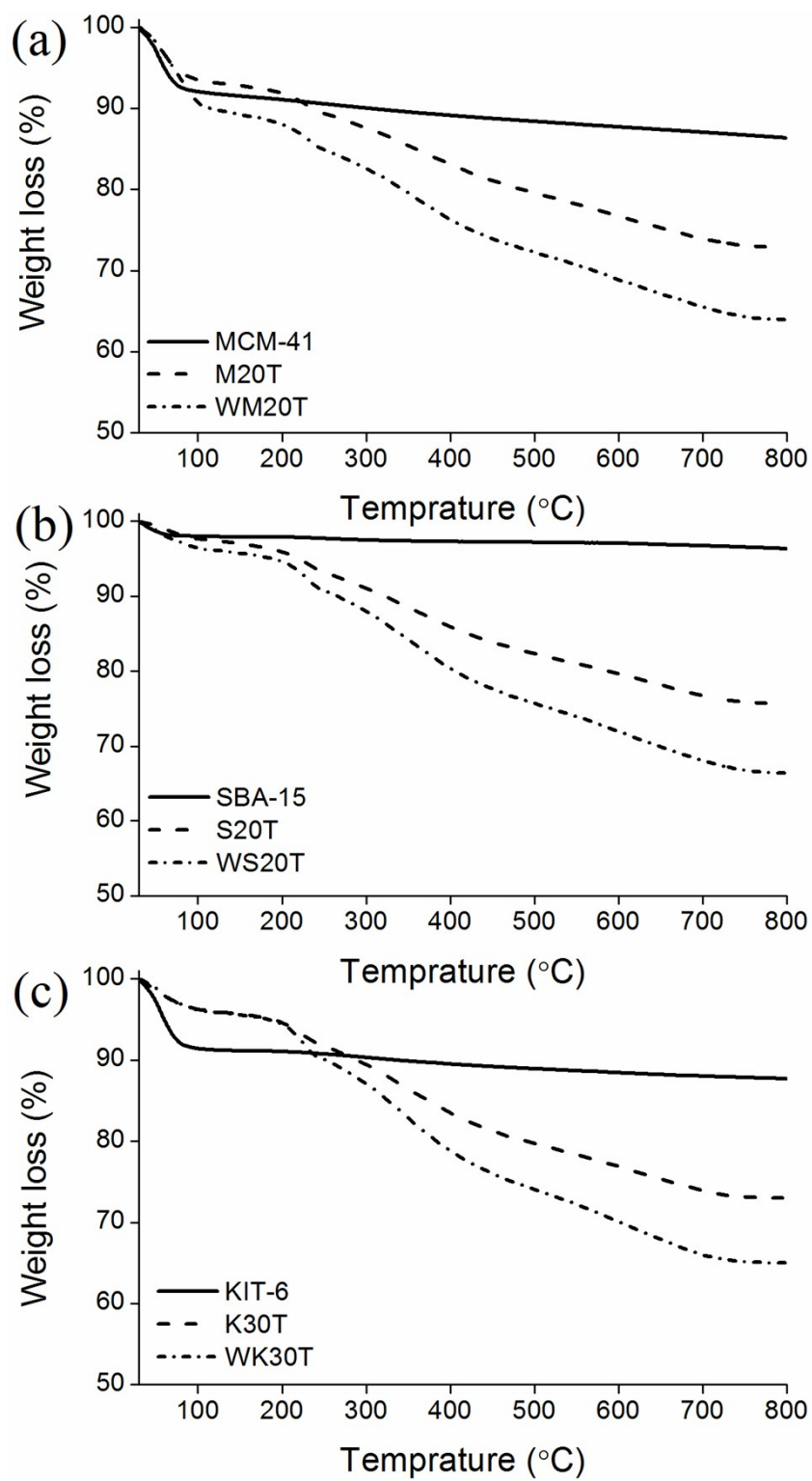
Fig. S2 Thermogravimetric (TG) analysis curves of pure and TMPTA grafted (a) MCM-41, (b) SBA-15 and (c) KIT-6.

Enthalpy of adsorption

Dual-site Langmuir (DSL) model provides excellent agreement between experimental and predicated adsorption capacity.[1,2] In present study, multi temperature DSL model (equation 1) is used to fit the experimental data of TMPTA grafted mesoporous silica for CO_2. Where, q_e^1 and q_e^2 are the saturation capacities (mol CO_2/kg) at sites 1 and 2 respectively. In DSL equation b and P are the Langmuir parameter (bar^{-1}) and pressure (bar), respectively.

$$q_e = \frac{(q_e^1 \, b_1 \, P)}{(1 + b_1 P)} + \frac{(q_e^2 \, b_2 \, P)}{(1 + b_2 P)} \tag{1}$$

The Langmuir parameters follow the temperature dependence as per equation 2:

$$b_1 = b_o \, exp^{\left(b_1^{(1)}/T\right)}; \qquad b_2 = b_o \, exp^{\left(b_2^{(2)}/T\right)} \tag{2}$$

Where T is the temperature in Kelvin.

Enthalpy of adsorption is calculated at different adsorption capacities (mol CO_2/kg) by Clausius–Clapeyron equation as follows:

$$-\Delta E_{ads} = R \left.\frac{\partial (lnP)}{\partial (1/T)}\right|_q = R \left(\frac{b_1^{(1)} q_e^1 \, b_1 (1 + b_2)^2 + b_1^{(1)} q_e^2 \, b_2 (1 + b_1)^2}{q_e^1 \, b_1 (1 + b_2)^2 + q_e^2 \, b_2 (1 + b_1)^2} \right) \tag{3}$$

References:

1. P. Mishra, S. Edubilli, B. Mandal, and S. Gumma, *J. Phys. Chem. C* 2014, **118**, 6847–6855.

2. P. M. Mathias, R. Kumar, J. D. Moyer, Jr., J. M. Schork, S. R. Srinivasan, S. R. Auvil, and O. Talu, *Ind. Eng. Chem. Res.* 1996, **35**, 2477–2483.