Electronic Supplementary Material (ESI)

N1-(3-trimethoxysilylpropyl)diethylenetriamine Grafted KIT-6
for CO2/N2 Selective Separation

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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.\textsuperscript{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\textsubscript{2}. Where, \(q_e^1\) and \(q_e^2\) are the saturation capacities (mol CO\textsubscript{2}/kg) at sites 1 and 2 respectively. In DSL equation \(b\) and \(P\) are the Langmuir parameter (bar\textsuperscript{-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:

\[
b_1 = b_o \exp\left(\frac{b_1^{(1)}}{T}\right) ; \quad b_2 = b_o \exp\left(\frac{b_2^{(2)}}{T}\right)
\tag{2}
\]

Where \(T\) is the temperature in Kelvin.

Enthalpy of adsorption is calculated at different adsorption capacities (mol CO\textsubscript{2}/kg) by Clausius–Clapeyron equation as follows:

\[
-\Delta E_{\text{ads}} = R \frac{\partial (\ln P)}{\partial (1/T)}|_q = R \left(\frac{b_1^{(1)} q_e^1 b_1 (1 + b_2)^2 + b_2^{(1)} q_e^2 b_2 (1 + b_1)^2}{q_e^1 b_1 (1 + b_2)^2 + q_e^2 b_2 (1 + b_1)^2}\right)
\tag{3}
\]

References: