Supplementary Information

Checking the post-processing of adsorption simulations: Henry coefficients, isosteric heats, IAST and stationarity tests validated against RASPA3

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S1 Single-component isotherms

Table S1. Absolute loadings and isosteric heats (from the block-averaged enthalpy reported by RASPA3) of CO_2 and CH_4 in silicalite-1 at 300 K. Uncertainties are RASPA3 block errors.

P (kPa)	CO_2		CH_4	
	q (mol kg^{-1})	q_{st} (kJ mol^{-1})	q (mol kg^{-1})	q_{st} (kJ mol^{-1})
1	0.0349 ± 0.0006	26.87 ± 0.10	0.0061 ± 0.0002	19.01 ± 0.05
3	0.1025 ± 0.0021	26.94 ± 0.19	0.0183 ± 0.0002	19.02 ± 0.07
10	0.3218 ± 0.0075	26.99 ± 0.29	0.0602 ± 0.0008	19.07 ± 0.06
30	0.8041 ± 0.0120	27.50 ± 0.30	0.1743 ± 0.0030	19.11 ± 0.09
100	1.6355 ± 0.0141	28.15 ± 0.51	0.5037 ± 0.0034	19.29 ± 0.08
300	2.2972 ± 0.0110	29.57 ± 0.72	1.1178 ± 0.0152	19.67 ± 0.09
1000	2.7838 ± 0.0063	30.31 ± 0.99	1.8959 ± 0.0104	20.18 ± 0.09

S2 IAST against pyIAST

S3 Stationarity test

S4 Isotherm model selection

Table S2. Binary IAST selectivities computed by AdsorpQC 1.1 and the Henry-limit ratio returned by version 1.0.0, for model isotherms with exact parameters, and the largest relative difference of the two component loadings from pyIAST 1.4.

Isotherm pair	y_1	P (bar)	S_{12} (IAST)	S_{12} (1.0.0)	max. rel. difference from pyIAST
Langmuir, equal q_{sat}	0.1	0.01	10.000	10.000	5.9e-14
Langmuir, equal q_{sat}	0.1	0.1	10.000	10.000	2.8e-15
Langmuir, equal q_{sat}	0.1	1	10.000	10.000	8.0e-14
Langmuir, equal q_{sat}	0.1	10	10.000	10.000	2.8e-13
Langmuir, equal q_{sat}	0.5	0.01	10.000	10.000	1.2e-12
Langmuir, equal q_{sat}	0.5	0.1	10.000	10.000	2.0e-14
Langmuir, equal q_{sat}	0.5	1	10.000	10.000	1.3e-15
Langmuir, equal q_{sat}	0.5	10	10.000	10.000	1.0e-13
Langmuir, equal q_{sat}	0.9	0.01	10.000	10.000	2.8e-12
Langmuir, equal q_{sat}	0.9	0.1	10.000	10.000	1.2e-13
Langmuir, equal q_{sat}	0.9	1	10.000	10.000	2.6e-13
Langmuir, equal q_{sat}	0.9	10	10.000	10.000	6.0e-14
Langmuir, q_{sat} 2 vs 6	0.1	0.01	8.841	8.889	2.7e-13
Langmuir, q_{sat} 2 vs 6	0.1	0.1	8.440	8.889	1.1e-13
Langmuir, q_{sat} 2 vs 6	0.1	1	5.876	8.889	3.5e-16
Langmuir, q_{sat} 2 vs 6	0.1	10	1.233	8.889	1.4e-12
Langmuir, q_{sat} 2 vs 6	0.5	0.01	8.760	8.889	4.4e-15
Langmuir, q_{sat} 2 vs 6	0.5	0.1	7.811	8.889	1.2e-15
Langmuir, q_{sat} 2 vs 6	0.5	1	4.388	8.889	0.0e+00
Langmuir, q_{sat} 2 vs 6	0.5	10	1.153	8.889	1.8e-16
Langmuir, q_{sat} 2 vs 6	0.9	0.01	8.681	8.889	0.0e+00
Langmuir, q_{sat} 2 vs 6	0.9	0.1	7.321	8.889	9.7e-14
Langmuir, q_{sat} 2 vs 6	0.9	1	3.719	8.889	1.3e-12
Langmuir, q_{sat} 2 vs 6	0.9	10	1.116	8.889	3.7e-14
dual-site Langmuir	0.1	0.01	11.917	11.923	4.6e-16
dual-site Langmuir	0.1	0.1	11.812	11.923	0.0e+00
dual-site Langmuir	0.1	1	9.997	11.923	4.8e-16
dual-site Langmuir	0.1	10	5.847	11.923	1.9e-16
dual-site Langmuir	0.5	0.01	11.901	11.923	1.2e-15
dual-site Langmuir	0.5	0.1	11.408	11.923	2.1e-16
dual-site Langmuir	0.5	1	8.092	11.923	2.2e-13
dual-site Langmuir	0.5	10	5.026	11.923	2.0e-15
dual-site Langmuir	0.9	0.01	11.879	11.923	5.5e-13
dual-site Langmuir	0.9	0.1	10.976	11.923	3.1e-12
dual-site Langmuir	0.9	1	7.258	11.923	4.4e-14
dual-site Langmuir	0.9	10	4.705	11.923	6.7e-14

Table S3. Fraction of synthetic loading series failed (`FAIL`) and flagged (`FAIL` or `WARNING`) by the stationarity tests of AdsorpQC 1.0.0 and 1.1 (1000 series per row). The drift is the total change over the run as a fraction of the mean.

Regime	samples	drift	FAIL (1.0.0)	FAIL (1.1)	flagged (1.0.0)	flagged (1.1)
high loading (AR(1), CV 5%)	40	0%	0.045	0.009	0.472	0.090
high loading (AR(1), CV 5%)	40	5%	0.172	0.077	0.652	0.229
high loading (AR(1), CV 5%)	40	20%	0.980	0.899	1.000	0.979
high loading (AR(1), CV 5%)	40	50%	1.000	1.000	1.000	1.000
high loading (AR(1), CV 5%)	400	0%	0.000	0.000	0.026	0.025
high loading (AR(1), CV 5%)	400	5%	0.002	0.002	0.768	0.759
high loading (AR(1), CV 5%)	400	20%	1.000	1.000	1.000	1.000
high loading (AR(1), CV 5%)	400	50%	1.000	1.000	1.000	1.000
low loading (Poisson, mean 2)	40	0%	0.786	0.005	0.923	0.040
low loading (Poisson, mean 2)	40	5%	0.838	0.005	0.950	0.052
low loading (Poisson, mean 2)	40	20%	0.850	0.004	0.955	0.062
low loading (Poisson, mean 2)	40	50%	0.913	0.036	0.969	0.197
low loading (Poisson, mean 2)	400	0%	0.495	0.002	0.797	0.045
low loading (Poisson, mean 2)	400	5%	0.510	0.004	0.815	0.058
low loading (Poisson, mean 2)	400	20%	0.781	0.050	0.919	0.272
low loading (Poisson, mean 2)	400	50%	0.999	0.676	1.000	0.934

Table S4. Fraction of simulated isotherms (500 per row; 1% Gaussian noise) for which each model was selected by AIC and by AIC_c.

Generating model	points	criterion	Langmuir	Sips	Toth	dual-site Langmuir
Dual-Site Langmuir	7	AIC	0.000	0.002	0.086	0.912
Dual-Site Langmuir	7	AIC_c	0.000	0.002	0.686	0.312
Dual-Site Langmuir	12	AIC	0.000	0.000	0.048	0.952
Dual-Site Langmuir	12	AIC_c	0.000	0.000	0.096	0.904
Langmuir	7	AIC	0.592	0.138	0.158	0.112
Langmuir	7	AIC_c	0.912	0.050	0.036	0.002
Langmuir	12	AIC	0.726	0.104	0.114	0.056
Langmuir	12	AIC_c	0.862	0.074	0.052	0.012