Supplementary material

Isosteric Heat of Adsorption The isosteric heat of adsorption can be calculated by Eq. S1 based on the Clausius–Clapeyron equation and DA equation.

$$\frac{\Delta H}{RT^2} = \frac{d \ln P}{dT} \qquad (S1)$$

Where ΔH (kJ·mol^{-1}) is the isosteric enthalpy of adsorption, R (8.314J·mol^{-1}·K^{-1}) is the gas constant, T (K) is the temperature, P (kPa) is the equilibrium pressure.

For the heterogeneous adsorption system, the isosteric enthalpy curve changes with the surface loading. In addition, the isosteric enthalpy can be used to examine the molecular scale interactions between adsorbate molecules and adsorbent. The dependence of isosteric enthalpy on adsorption capacities was present in Fig. S3. The isosteric enthalpies of adsorption changed with equilibrium adsorption capacities but all the values lied in the order of -10^4 J·mol^{-1}. This results implied that ND-100 has the energetically heterogeneous surface.

Table S1 Fitting parameters of Langmuir, Freundlich, and DA models for methyl acetate, ethyl acetate, propyl acetate, isopropyl acetate, ethyl propionate on ND-100

model	parameters	methyl acetate			ethyl acetate			isopropyl acetate			propyl acetate			ethyl propionate		
		303K	318K	333K	303K	318K	333K	303K	318K	333K	303K	318K	333K	303K	318K	333K
Langmuir	q_0/(mg·g^{-1})	555.5	464.1	378.6	499.1	423.6	355.9	495.5	415.3	373.3	477.7	414.4	334.0	500.4	428.1	354.4
	b	0.329	0.270	0.255	0.888	0.799	0.713	1.522	1.570	1.292	3.026	2.757	2.847	3.654	2.962	2.299
	R^2	0.980	0.987	0.972	0.979	0.973	0.979	0.967	0.961	0.965	0.973	0.968	0.982	0.967	0.971	0.975
	rmsd/%	2.637	2.421	3.667	2.381	2.769	2.640	2.628	2.854	3.140	2.320	2.714	1.853	1.958	2.187	2.539
Freundlich	k	220.6	161.3	126.1	268.9	216.8	172.3	308.0	261.1	218.0	349.2	295.5	240.3	384.4	312.7	241.2
	n	0.272	0.307	0.319	0.244	0.263	0.282	0.231	0.226	0.257	0.216	0.231	0.225	0.174	0.203	0.241
	R^2	0.993	0.991	0.998	0.991	0.998	0.993	0.998	0.997	0.996	0.990	0.995	0.980	0.994	0.994	0.992
	rmsd/%	1.291	1.759	0.830	1.382	0.783	1.351	0.605	0.718	0.924	1.170	0.919	1.457	0.787	0.924	1.249
DA	q/(mg·g^{-1})	536.1	470.4	483.5	485.9	471.3	403.8	502.3	470.3	464.1	471.3	458.2	359.0	504.2	459.8	401.6
	E/ (kJ·mol^{-1})	8.926	9.601	9.987	9.647	10.712	11.894	10.517	12.054	12.248	10.603	11.983	14.009	12.749	13.016	13.408
	r	1.365	1.613	1.266	1.406	1.327	1.640	1.203	1.254	1.347	1.411	1.402	1.982	1.323	1.506	1.701
	R^2	0.999	0.999	0.998	0.998	1.000	0.998	1.000	0.998	0.997	0.997	0.998	0.999	0.998	0.998	0.997
	rmsd/%	0.560	0.533	0.723	0.722	0.188	0.618	0.183	0.609	0.813	0.659	0.668	0.435	0.405	0.475	0.795

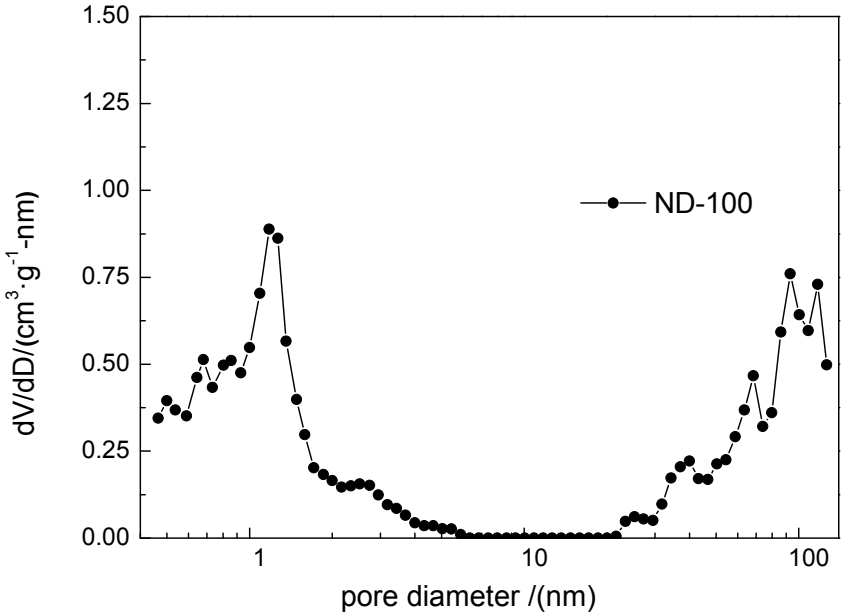
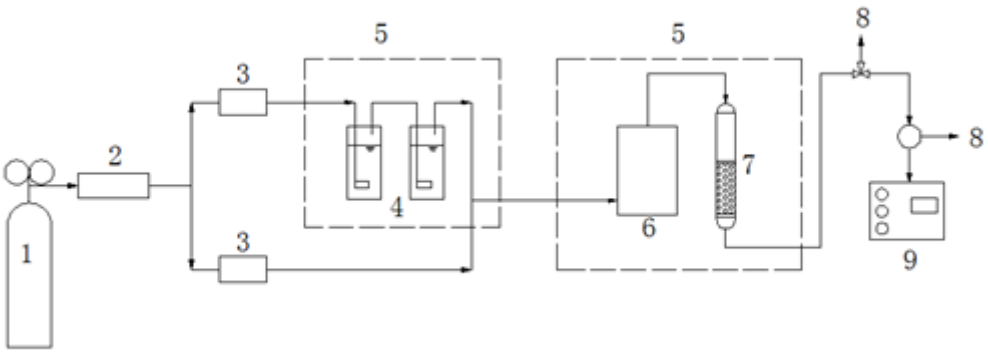


Fig. S1 the pore size distributions of ND-100



1. N_2 2. desicator 3. mass flow meter 4. evaporator 5. water bath

6. buffle bottle 7. adsorbtion column 8. outlet 9. gas chromatography

Fig. S2 Adsorption schematic diagram

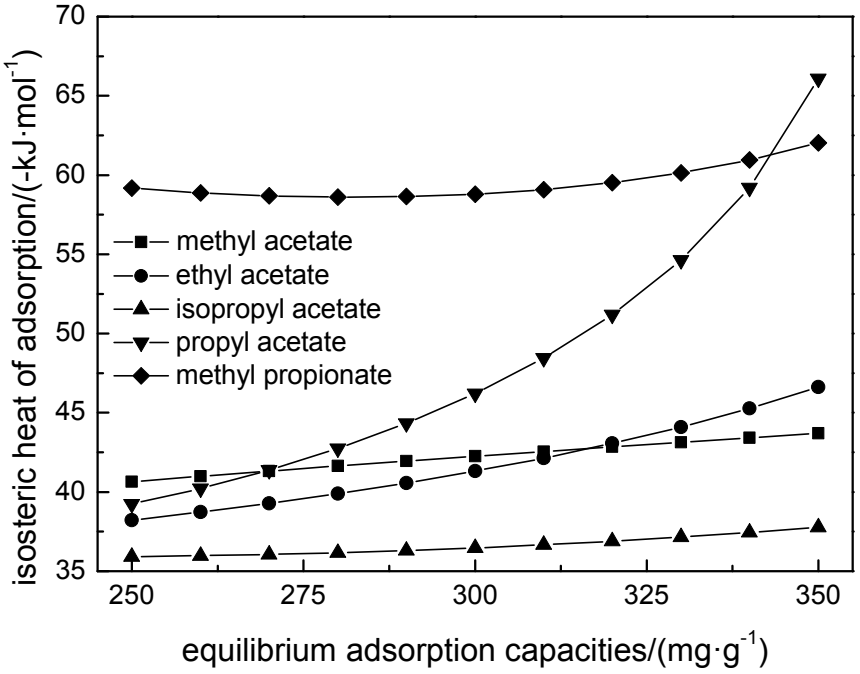


Fig. S3 The curves of isosteric enthalpy vs. adsorption capacities for five ester VOCs (methyl acetate, ethyl acetate, propyl acetate, isopropyl acetate, methyl propionate) onto ND-100.

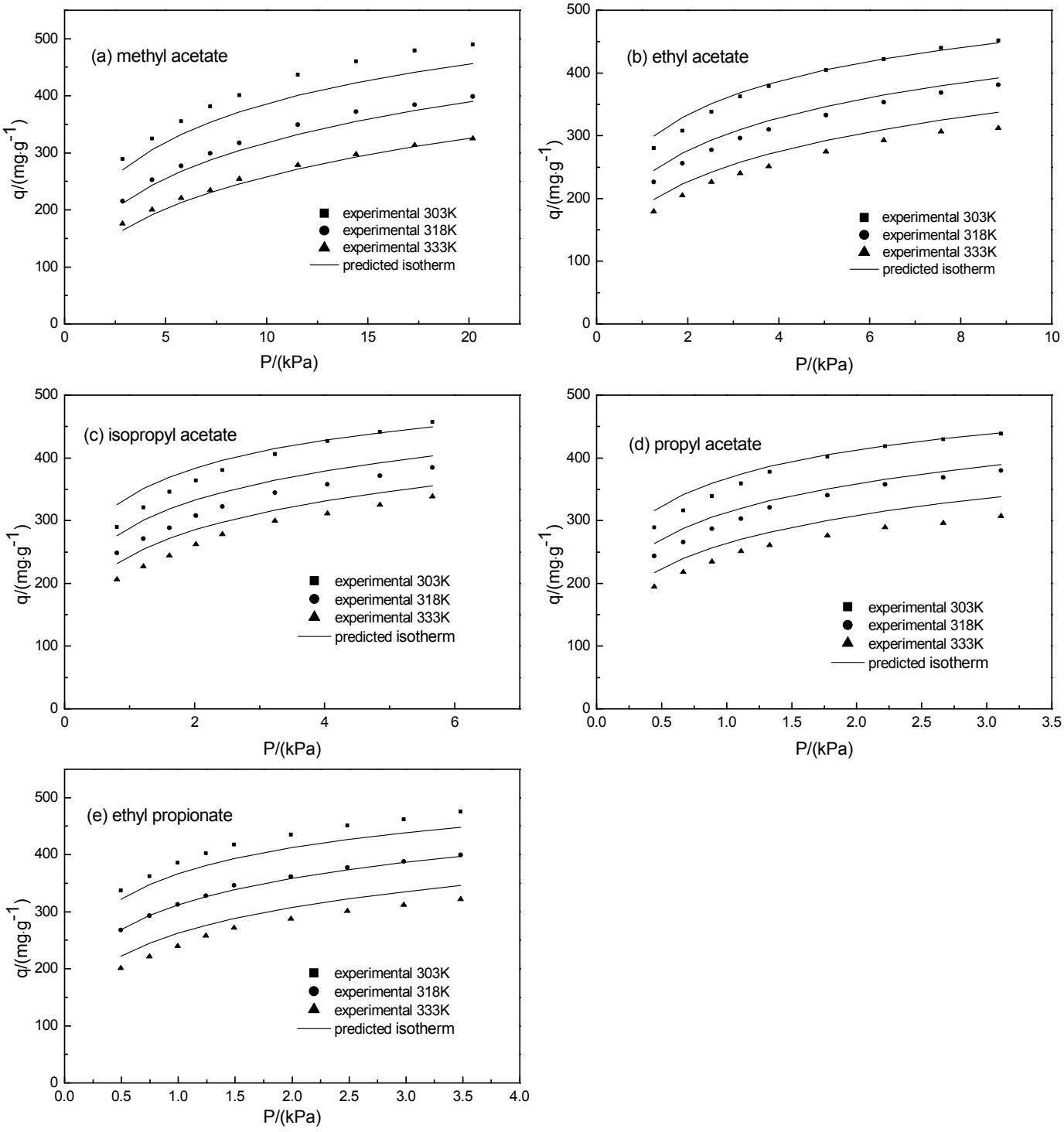


Fig. S4 Comparison of the predictive and experimental adsorption capacities of esters on ND-100 at 303K, 318K, and 333K: (a) methyl acetate, (b) ethyl acetate, (c) isopropyl acetate, (d) propyl acetate, and (e) ethyl propionate.