Supporting information

The adsorption kinetics and mechanism of odorous gases onto textile fibers

Wenli Bai,[a] Hao Yu,[b] Longlong Liu,[c] Esfandiar Pakdel,[a] Bin Tang,[a] Hongli Su,[a] Christopher Hurren,[a] Lei Liu,[c] Jinfeng Wang,[b,*] and Xungai Wang [d,*]

[a] Institute for Frontier Materials, Deakin University, Geelong/Melbourne, Victoria 3216, Australia.

[b] National Local Joint Laboratory for Advanced Textile Processing and Clean Production, Wuhan Textile University, Wuhan 430073, China.

[c] Center for Computational Chemistry, College of Chemistry and Chemical Engineering, Wuhan Textile University, Wuhan 430073, China.

[d] JC STEM Lab of Sustainable Fibers and Textiles, School of Fashion and Textiles, The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong.

*Corresponding authors. E-mail address: jinfeng.wang@wtu.edu.cn (Jinfeng Wang); xungai.wang@polyu.edu.hk (Xungai Wang).

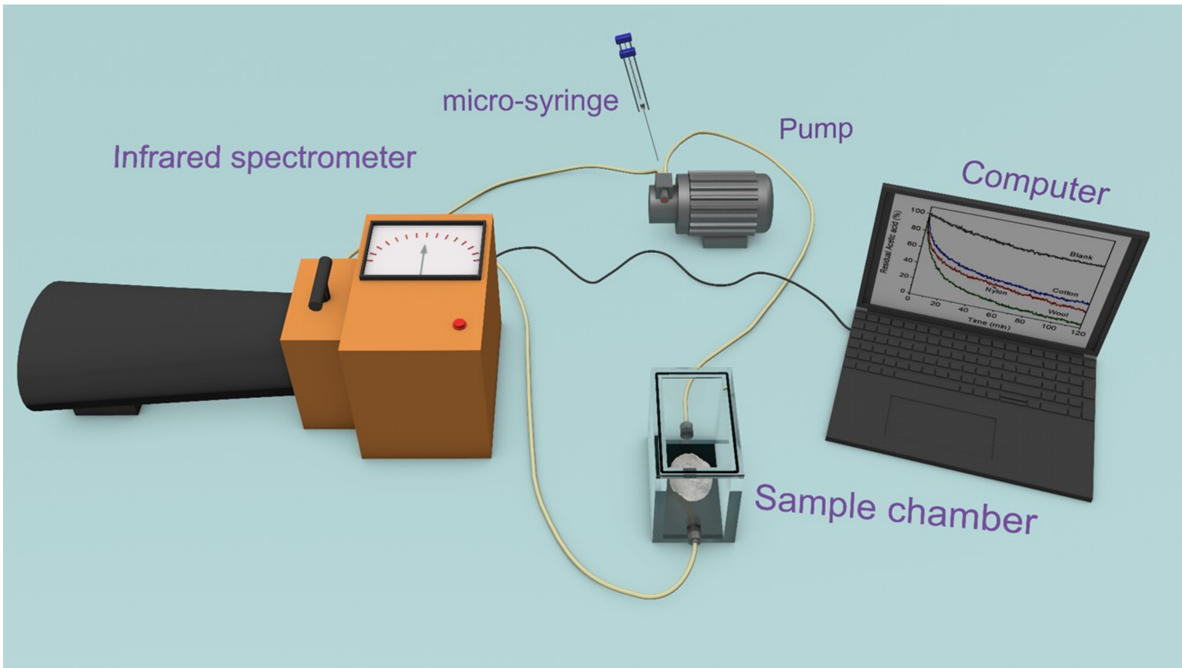

Fig. S1 Diagram of the odor detection system.

Table. S1 Correlation coefficient R^2 from diffusion kinetic models for the acetic acid adsorption onto wool, cotton and nylon fibers.

R^2	D-W diffusion model			W-M diffusion model		
	Wool	Cotton	Nylon	Wool	Cotton	Nylon
0-10 min	0.9947	0.9872	0.9863	0.9950	0.9912	0.9854
0-120 min	0.9019	0.9062	0.9131	0.8251	0.8802	0.8721

Table. S2 Correlation coefficient R^2 from adsorption reaction models for the acetic acid adsorption onto wool, cotton and nylon fibers.

R^2	Pseudo-first-order model			Pseudo-second-order model		
	Wool	Cotton	Nylon	Wool	Cotton	Nylon
0-10 min	0.9801	0.9741	0.9565	0.9734	0.9565	0.6909
0-120 min	0.9134	0.9249	0.9296	0.9993	0.9985	0.9974

Table. S3 Correlation coefficient R^2 from diffusion kinetic models for the ammonia adsorption onto wool, cotton and nylon fibers.

R^2	D-W diffusion model			W-M diffusion model		
	Wool	Cotton	Nylon	Wool	Cotton	Nylon
0-10 min	0.9601	0.9456	0.8404	0.9634	0.9529	0.8455
0-120 min	0.6405	0.5638	0.7144	0.7101	0.6802	0.9241

Table. S4 Correlation coefficient R^2 from diffusion kinetic models for the ammonia adsorption onto wool, cotton and nylon fibers.

R^2	Pseudo-first-order model			Pseudo-second-order model		
	Wool	Cotton	Nylon	Wool	Cotton	Nylon
0-10 min	0.9385	0.9251	0.8277	0.9880	0.9845	0.9210
0-120 min	0.6213	0.4434	0.5301	0.9966	0.9964	0.9808

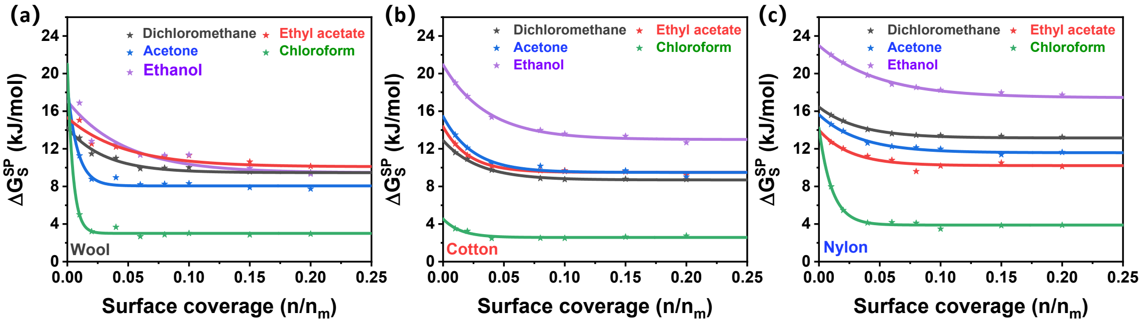

Fig. S2 Specific free energy profiles of the adsorption of polar probes onto the three fiber types: wool (a), cotton (b) and nylon (c).

Table. S5 IGC surface physicochemical properties of wool, cotton and nylon fiber at 0.1 surface coverage.

Parameters	Wool	Cotton	Nylon
S_{BET}/m^2·g^{-1}	2.24	0.78	0.56
γ_S^D/mJ·m^{-2}	49.0949	40.7655	37.1437
γ_S^{SP}/mJ·m^{-2}	7.9391	5.9396	9.5827
γ_S^T/mJ·m^{-2}	57.0340	46.7051	46.7264
γ_S^{SP}/γ_S^T	0.1392	0.1272	0.2050
K_a	0.1206	0.1079	0.1044
K_b	0.2382	0.2525	0.4157
K_a/K_b	0.5063	0.4273	0.2511
K_b/K_a	1.9751	2.3401	3.9818

The influence of fiber diameter on the odor adsorption performance was investigated using three wool fiber samples (0.4 g) with different average diameters. Wool fibers with average diameters of 13.3 µm, 17.3 µm and 20.9 µm were named as Wool-13, Wool-17 and Wool-21, respectively. The same amount of acetic acid (10 µL) was used in the adsorption test for all the three wool fiber samples. Fig. S3a shows the concentration change of acetic acid with the presence of different wool fiber samples. It can be observed the finest sample wool-13 adsorbed the highest amount of acetic acid, and the coarse fiber showed the lowest adsorption. The acetic acid equilibrium adsorption capacity was measured to be 2.20 $mg \cdot g^{-1}$, 2.09 $mg \cdot g^{-1}$, and 1.94 $mg \cdot g^{-1}$ for wool-13 µm, wool-17 µm and wool-21 µm, respectively (Fig. S3b). Wool with smaller diameters have a larger surface area for the same mass of fibers, which could improve its adsorption capacity. However, a diameter increase of 62% only leads to a slight reduction in adsorption capacity, from 2.20 $mg \cdot g^{-1}$ to 1.94 $mg \cdot g^{-1}$. Therefore, fiber composition plays a key role for its adsorption behavior when their diameters are comparable.

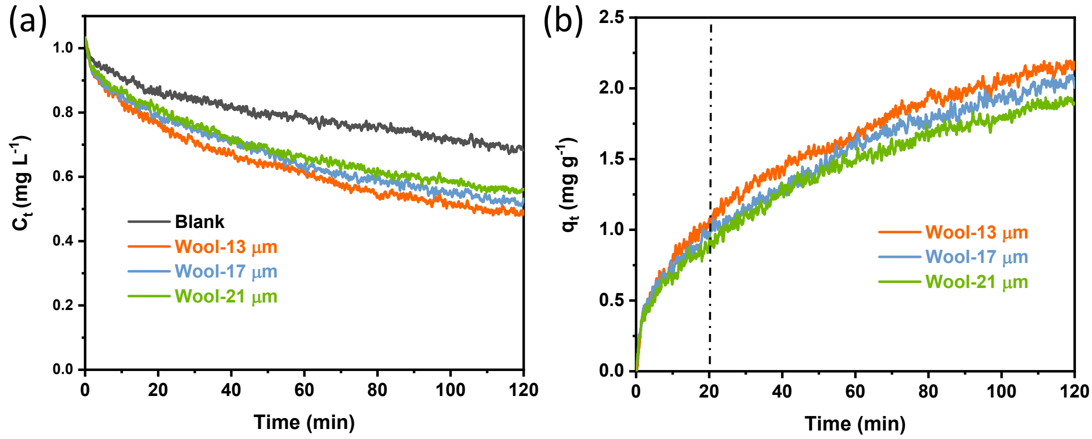

Fig. S3 Acetic acid concentration change in the odor detection system with the presence of wool fibers (0.4 g) with different diameter (a); The effect of time on the adsorption quantity of acetic acid onto wool fibers with different diameter at room temperature (b).