Electronic Supplementary Information (ESI) for

Selective adsorption and irreversible trap of Mercury(II) from aqueous solution by a flower-like titanate nanomaterial

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Table S1. Kinetic parameters for adsorption of Hg(II) by TNFs.

Kinetic model	Parameters	Initial Hg(II) concentration (mg L^{-1})	
		50	100
Pseudo-first-order model	Q_e (mg g^{-1})	2.70	21.66
	k_1 (min^{-1})	0.0325	0.0061
	R^2	0.5441	0.8887
Pseudo-first-order model	Q_e (mg g^{-1})	245.70	411.53
	k_2 (g mg^{-1} min^{-1})	0.0230	0.0037
	R^2	1.0000	1.0000

Table S2. Isotherm parameters for adsorption of Hg(II) by TNFs.

Kinetic model	Parameters	Values
Langmuir model	Q_{max} (mg g^{-1})	454.55
	b (L mg^{-1})	0.58
	R^2	0.9997
Freundlich model	K_F ((mg g^{-1})·(L mg^{-1})$^{1/n}$)	109.01
	n	4.72
	R^2	0.6684

Table S3. Comparison on adsorption capacity of Hg(II) by different adsorbents.

Material	Q_e/Q_{max} (mg g^{-1})	Conditions	Notes	Reference
Activated carbon (AC)	55.6	pH 5; 30 °C	AC made from sago waste	1
Multi-walled carbon nanotubes(MWNTs)	87.7	pH 6.7; 27 °C	Without additional groups	2
Mesoporous silica	200.6 for SBA-15; 140.4 for MCM-41	pH 6; 25 °C	2-Mercaptothiazoline modified SBA-15 and MCM-41	3
Biomass	75.6	pH 6; 30 °C	*Aspergillus versicolor* biomass	4
Ion-exchange resin	358.7	pH 7; 20 °C	Ion-exchange resin, Duolite™ GT-73	5
TNFs	454.6	pH 5; 25 °C	Sodium Trititanate	This study

Table S4. HSAB hardness and hydration energy of concerned metal cations.

Metal cations	Hardness[6]	Hydration energy[7] (kJ mol^{-1})
Na^+	21.1	405
K^+	13.6	321
Mg^{2+}	32.5	1922
Ca^{2+}	19.7	1592
Hg^{2+}	7.7	1853

Table S5. Atomic percent of TNFs before and after adsorption of Hg(II).

Material	Element (%)			
	Na	O	Ti	Hg
TNFs	11.34	21.44	67.22	0
TNFs-Hg	1.52	26.58	69.06	2.84

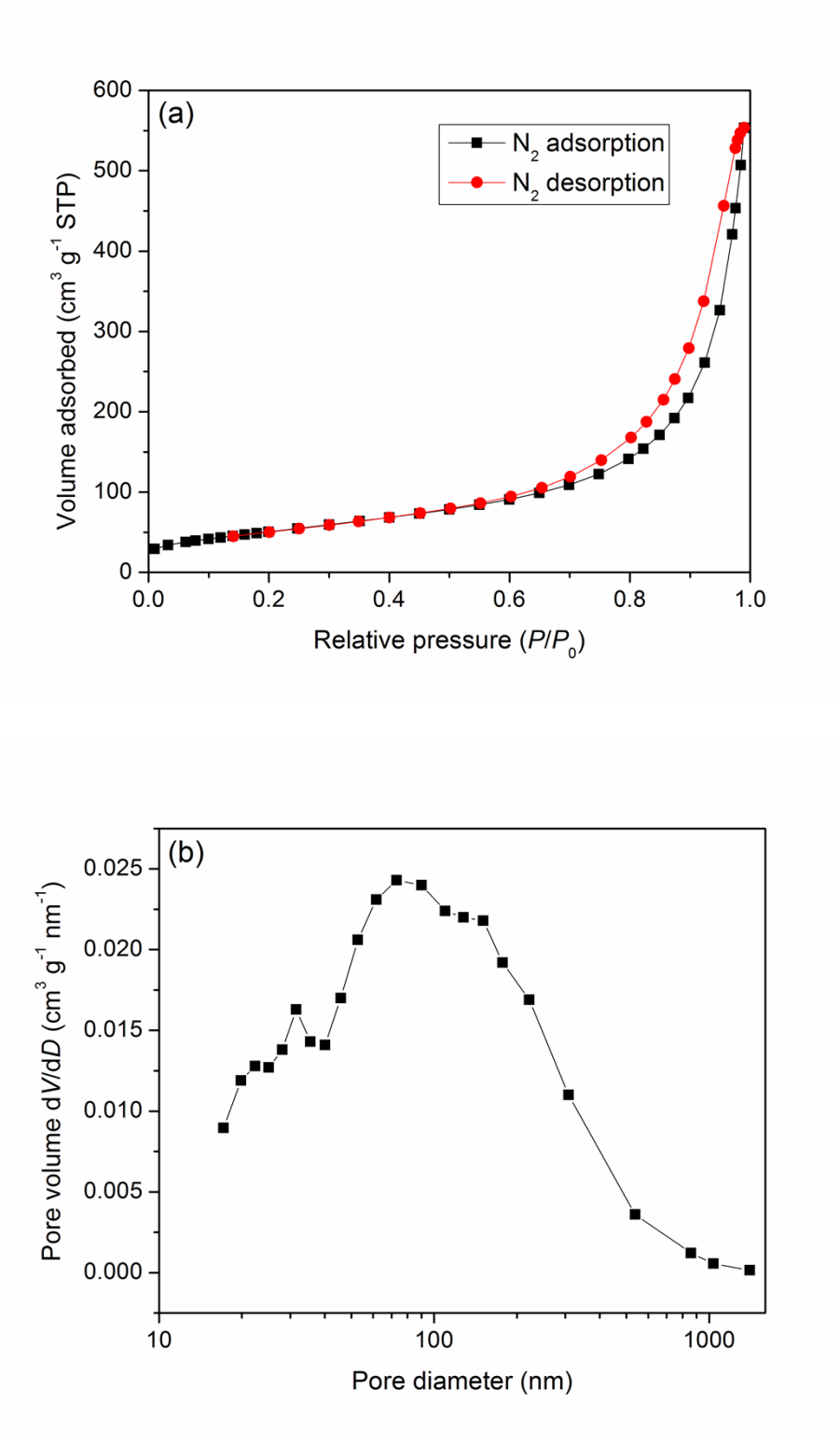

Fig. S1 (a) N_2 adsorption-desorption isotherms and (b) pore size distributions of TNFs.

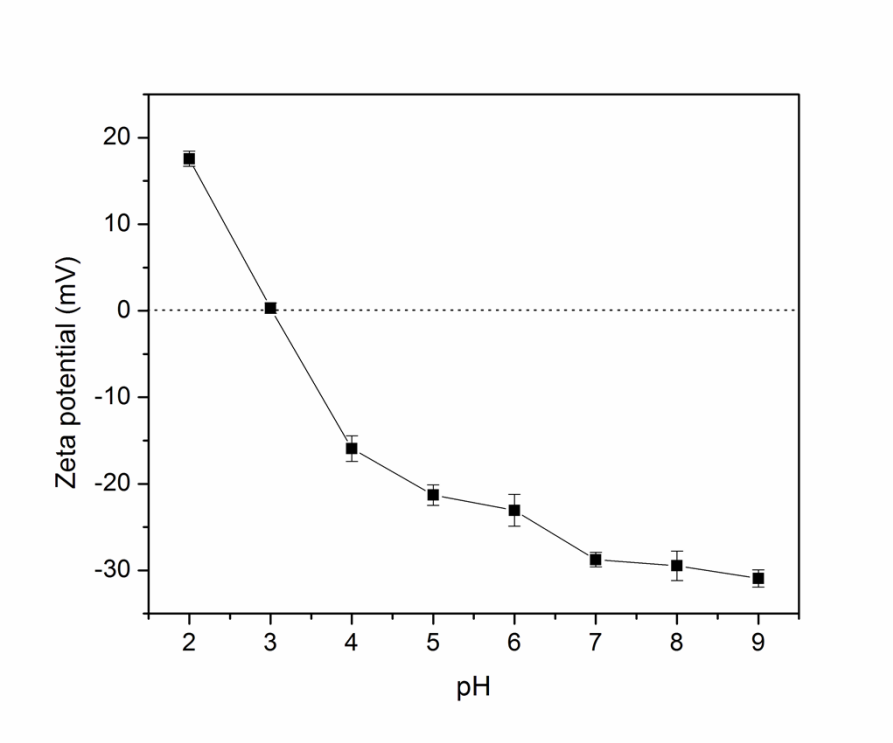

Fig. S2 Zeta potential of TNFs as different pH.

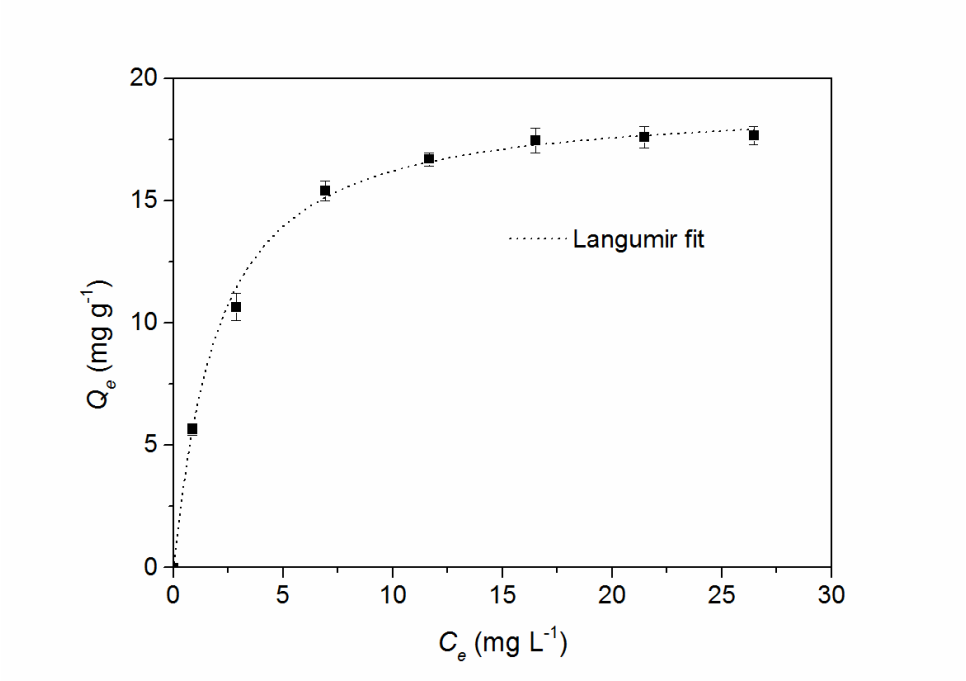

Fig. S3 Adsorption isotherm of Hg(II) by P25 at pH 5.

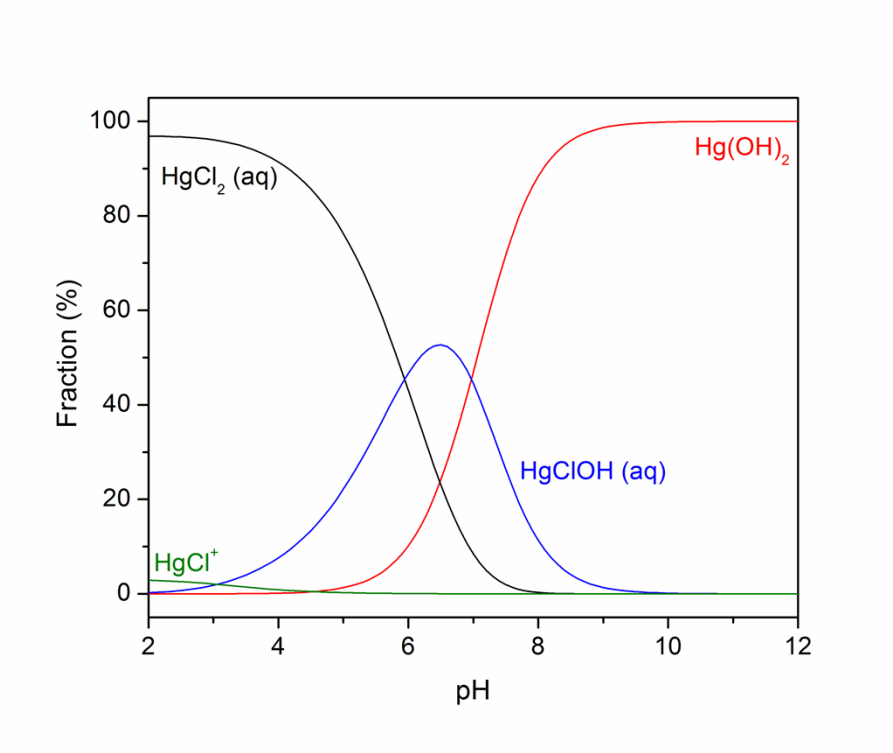

Fig. S4 Species distribution of Hg(II) as a function of pH at 25 °C simulated by Visual MINTEQ 3.0. Total Hg(II) concentration is 50 mg L^{-1}.

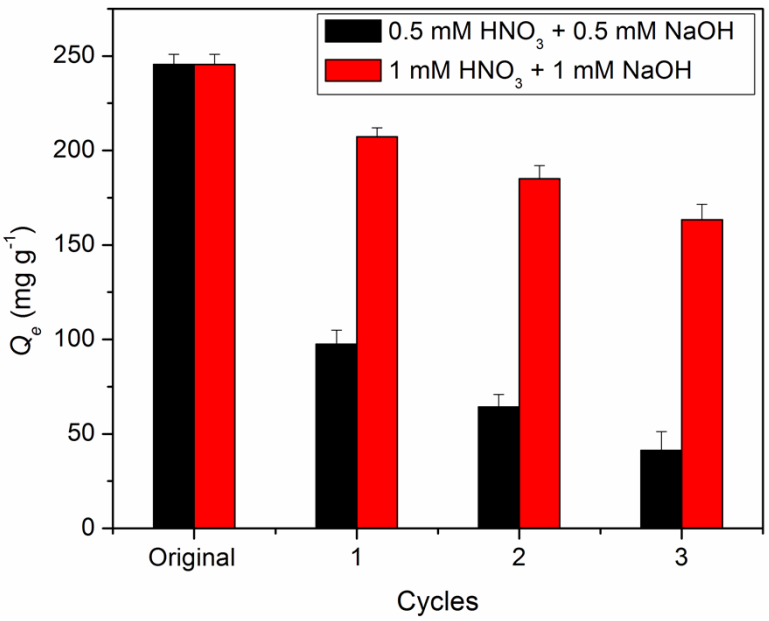

Fig. S5 Adsorption capacity of Hg(II) on regenerated TNFs over 3 desorption-regeneration cycles.

References

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