Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information

Single-step synthesis of prominently selective and easily regenerable POSS functionalized with highly-loaded sulfur and carboxylic acids

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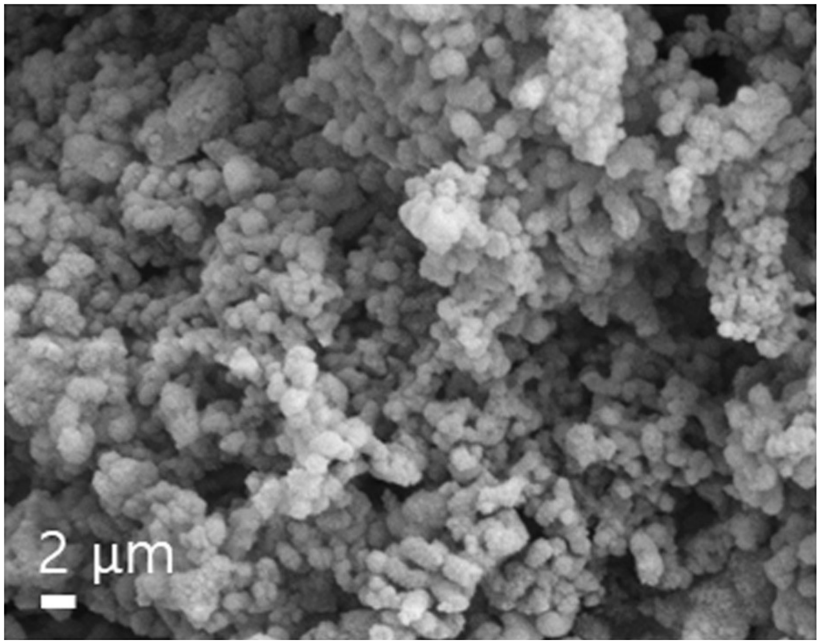

Figure S1: FESEM image of the octavinyl-POSS.

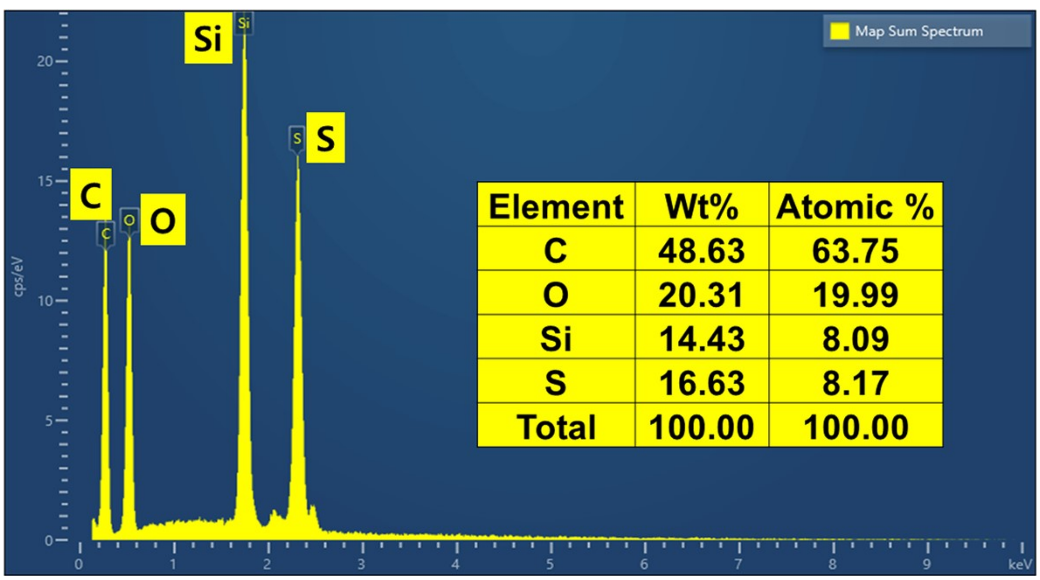

Figure S2: EDX of the as-developed POSS-S-COOH

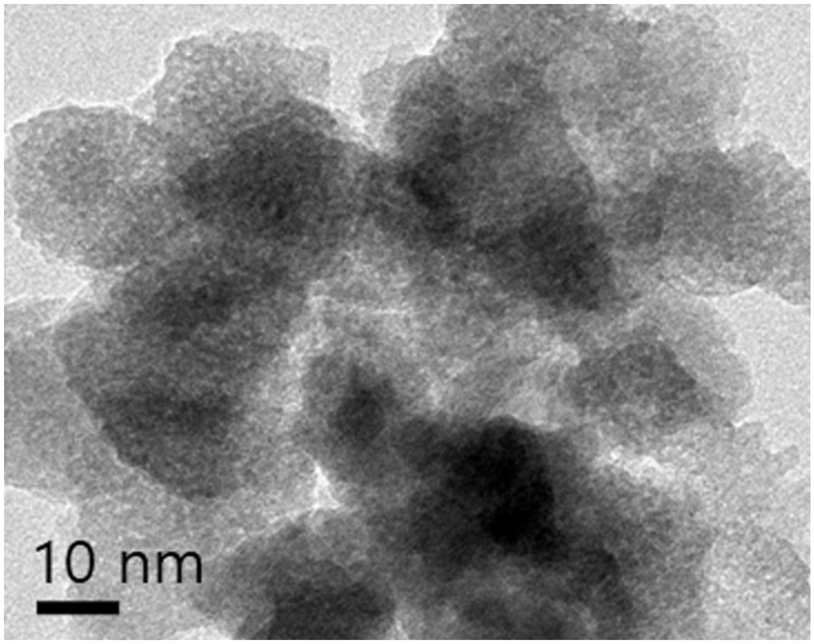

Figure S3: TEM image of the octavinyl-POSS.

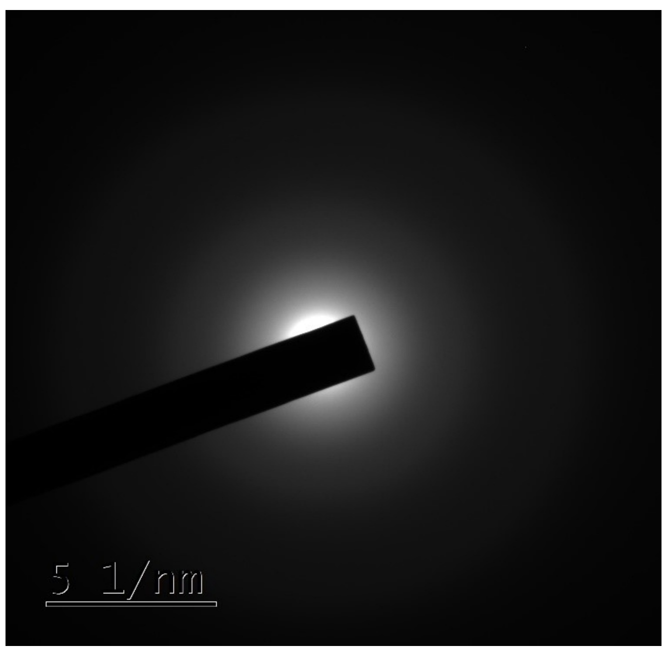

Figure S4: SAED pattern of the as-developed POSS-S-COOH.

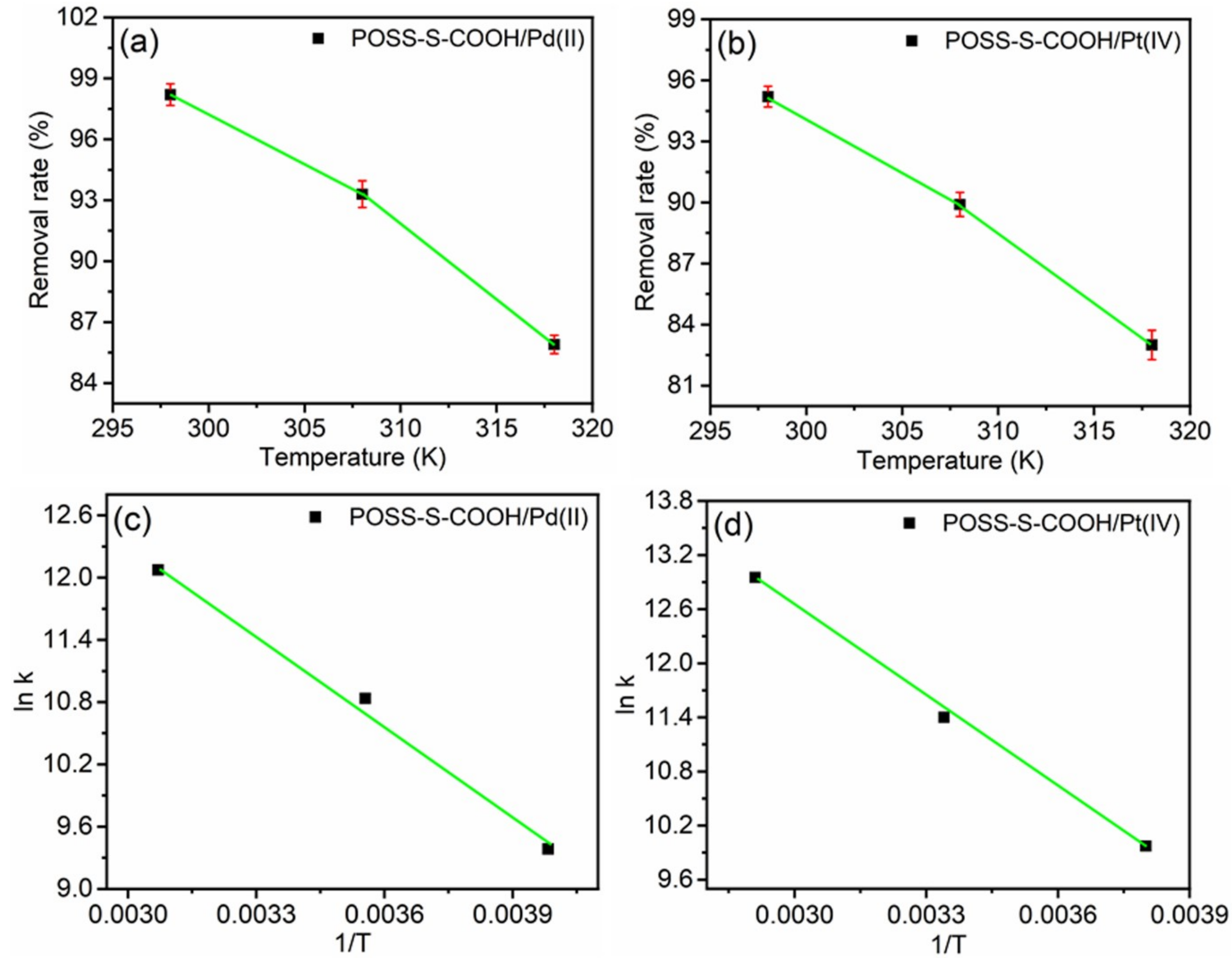

Figure S5: (a, b) Influence of temperature on the removal rates and (c, d) van't Hoff isotherms for the adsorptions of Pd(II) and Pt(IV) using POSS-S-COOH.

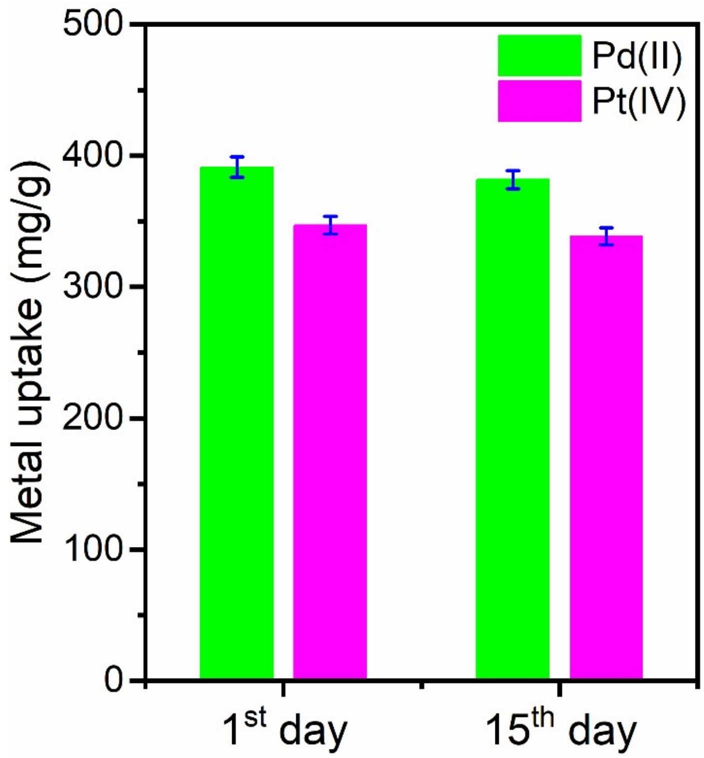

Figure S6: Acid-resistance performance of POSS-S-COOH for Pd(II) and Pt(IV) at pH 1.

Table S1: Comparison table of adsorption performances of reported adsorbents for Pt(IV)

Adsorbent	pH	q_m (mg/g)	Equilibrium time (min.)	b (L/mg)	Ref.
Bayberry tannin immobilized collagen fiber	3	41.7	60	-	1
Primary amine lignin	1	42.93	150	-	2
3'-Nitro-4-amino azobenzene modified chitosan	3	43.1	600	-	3
Polysulfone based fibre	1	45.1	40	0.020	4
Escherichia coli biomass	1	45.65	30	0.030	5
Graphene oxide	6	71.378	40	0.2695	6
Amberlite IRC 718	0.5	99.33	180	-	7
MIL-101(Cr)-NO_2	1	104.5	5	0.001	8
Ethylenediamine lignin	2	104.57	150	-	2
Glycine modified crosslinked chitosan resin	2	122.47	120	0.474	9
L-lysine modified crosslinked chitosan resin	1	129.255	70	0.303	10
Thiourea-modified chitosan microspheres	2	129.9	300	-	11
PAN/UiO-66	1	132.5	5	0.01	12
MIL-101(Cr)-NH_2	1	140.7	60	0.003	8
PU/UiO-66	1	141	5	0.008	12
UiO-66	1	144.8	5	0.01	12
UiO-66-NH_2	1	168.2	15	0.023	12

PU/UiO-66-NH_2	1	169.4	15	0.018	12
Ethylenediamine-modified magnetic chitosan	2	171	20	-	13
PAN/UiO-66-NH_2	1	172.5	15	0.02	12
DMA-paper gel	1	176	300	-	14
Cyphos IL-101-immobilized capsules	1	177.5	1440	1.422	15
PS-ATD resin	1	222.2	900	-	16
Amine modified VBC/AN/DVB	1	245	70	-	17
Cationic chitosan/E. coli fiber	1	290.98	30	-	18
PEI-coated Polysulfone E. coli biomass	1	296.2	150	0.022	4
Chitosan sorbent	2	346.3	720	1.10	19
$MnFe_2O_4$	1	371.35	30	0.251	20
Amine functionalized magnetic nanoparticles	1	380	5	0.11	21
Thiourea derivative of chitosan (TGC-3: 2: 1)	2	386.9	1440	0.135	22
EI-PVC fibers	1	410.53	200	0.18	23
PEI-loaded CHB	1	815.2	180	0.042	24
POSS-S-COOH	**1**	**597.2**	**155**	**0.033**	**This work**

Table S2: Comparison table of adsorption performances of reported adsorbents for Pd(II)

Adsorbent	pH	q_m (mg/g)	Equilibrium time (min.)	b (L/mg)	Ref.
3'-Nitro-4-amino azobenzene modified chitosan	4	29.33	900	0.83	3
Bayberry tannin immobilized collagen fiber	4	33.4	240	0.16	1
Escherichia coli biomass	1	38.87	10	0.48	5
Ni/Al_2O_3-E	5	40.3	30	0.0139	25
2-Mercaptobenzothiazole functionalized resin	4	50		0.24	26
DKTS modified silica gel	4	76.92			27
Graphene oxide	6	80.77	40	0.4303	6
PAN/UiO-66	1	91.5	5	0.004	12
TAOB impregnated onto GO	3	92.67	30	0.0233	28
PEI coated alumina nanopowder	6	97.7		0.03	29
L-lysine modified crosslinked chitosan resin	2	109.467	70	1.579	10
Thiourea tailored chitosan microspheres	2	112.4	150	0.978	11
UiO-66	1	113	5	0.003	12
Glycine modified crosslinked chitosan resin	2	120.39	95	0.258	9
Ethylenediamine modified magnetic chitosan	2	138	60		13
PU/UiO-66	1	140.8	5	0.002	12
PU/UiO-66-NH_2	1	157.4	15	0.471	12

UiO-66-NH_2	1	159.1	15	1.009	12
PAN/UiO-66-NH_2	1	165.8	15	0.865	12
PdCBD-cellulose	3	175.44	60	0.1161	30
Functionalized mesoporous silica	3.5	184.5	70		31
Cross-linked chitosan/montmorillonite	2	193	300		32
Aliquot 336 impregnated onto SBA-15	4	212.76	60	0.0079	33
Chitosan/graphene oxide composite	3	216.92	720	0.784	34
Polymer-impregnated alginate capsule	4.3	291.19	400	0.0076	35
POP-Py	3	708	20		36
POP-pNH_2-Py	3	743	20		36
POP-oNH_2-Py	3	752	20		36
POSS-S-COOH	**1**	**692.6**	**140**	**0.039**	**This Work**

Table S3: Selectivity parameters of Pd(II) and other used metal ions

Ions	Removal rate (%)	K_d (L/g)	K
Ni(II)	3.41	0.0529	1339.6200
Zn(II)	2.51	0.0386	1835.9041
Mg(II)	4.60	0.0723	980.1646
Cu(II)	5.75	0.0916	773.6452
Pb(II)	4.11	0.0643	1102.1135
Cd(II)	3.12	0.0484	1464.1715
Fe(III)	5.87	0.0936	757.1143
Co(II)	2.55	0.0392	1807.8036
Pd(II)	97.93	70.8659	

Table S4: Selectivity parameters of Pt(IV) and other used metal ions

Ions	Removal rate (%)	K_d (L/g)	K
Ni(II)	4.83	0.0762	355.5092
Zn(II)	3.34	0.0518	522.9691
Mg(II)	4.65	0.0731	370.5855
Cu(II)	6.51	0.1045	259.2325
Pb(II)	3.31	0.0513	528.0663
Cd(II)	2.82	0.0436	621.3257
Fe(III)	6.41	0.1028	263.5195
Co(II)	2.84	0.0438	618.4886
Pt(IV)	94.75	27.0898	

Table S5: Geometry parameters of PGMs-adsorbed POSS-S-COOH

$E_{\text{Total.POSS-S-COOH/Pd(II)}}$ (Ha)	-9148.369
$E_{\text{Total.POSS-S-COOH/Pt(IV)}}$ (Ha)	-9158.895
$E_{\text{POSS-S-COOH}}$ (Ha)	-9129.054
$E_{\text{Pd(II)}}$ (Ha)	-18.584
$E_{\text{Pt(IV)}}$ (Ha)	-30.297
$E_{\text{b.POSS-S-COOH/Pd(II)}}$ (Ha)	0.507
$E_{\text{b.POSS-S-COOH/Pt(IV)}}$ (Ha)	0.486
Dipole moment (POSS-S-COOH/Pd(II)) (D)	17.633
Dipole moment (POSS-S-COOH/Pt(IV)) (D)	21.292

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