

Supporting information

Authors: Long CHENG, Li NIU, Jian GONG and Shaojun DONG*

Title: Electrochemical growth and characterization of polyoxometallates-containing monolayers and multilayers on alkanethiol monolayers self-assembled on gold electrodes

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1. XPS characterization:

A. Features of the Mo 3d spectrum:

The Mo 3d XPS signals are always present in well-defined doublet shapes for the multilayer films. The peaks of Mo 3d_{5/2} and 3d_{3/2} levels are located at 232.4 ± 0.2 and 235.6 ± 0.2 eV respectively, which are closely similar to the reported data of 232.5 and 235.6 eV for Mo 3d levels.^{28a,b,d} Therefore, these BE values are consistent with the spin orbit splitting of the Mo 3d levels in oxidation state of +6, as expected for SiMo₁₁VO₄₀⁵⁻ anion.

B. Features of the N 1s spectrum:

Unlike the O 1s and S 2p features discussed in the manuscript, N 1s XPS spectra of multilayers prepared by the electrochemical growth and the immersion growth have similar characteristics. The Mo 3p_{3/2} level is expected to be present in the same BE region of N 1s signals, but the second peak of the Mo 3p doublet lies 17.4 eV to higher BE, which goes beyond the N 1s envelop.^{28b} Deconvolution of the wide N 1s signal (Fig. S1) shows that at least four component peaks present in the multilayer film of Au/cyst/8SiMo₁₁V/7QPVP-Os. The lowest BE peak is attributed to the Mo⁶⁺ 3p_{3/2} level located at 397.0 eV which is close to the reported values of 397.7^{20a} and 396.0 eV^{28b}. The BE peak at 398.0 eV with the largest intensity is related to the N 1s signal originating from quaternized pyridine groups of QPVP-Os.^{28a} The N 1s signal at 399.7 eV is derived from 2,2'-bipyridine of Os(bpy)₂Cl₂ because an independent XPS measurement of Ru(bpy)₃Cl₂ powder gave a N 1s signal at the same BE position. The N 1s signal at the highest BE of ca. 401.2 ± 0.3 eV is assigned to the protonated amino groups of cysteamine SAM, whose BE is close to the data of 400.8,^{6b} 399.9^{28a} and 401.9^{28b} eV for protonated nitrogen species.

C. Features of the Os 4f spectrum:

In the BE window of 45.0 to 65.0 eV, weak signals of Os 4f signal appears in poorly resolved doublet shapes. The BE values of Os 4f_{7/2} and 4f_{5/2} are ca. 50.5 ± 0.5 and 53.0 ± 0.4 eV respectively. The weak intensity of Os 4f signals is in parallel with the above results of N 1s XPS signals, and also with the low amount of Os(bpy)₂Cl₂ present in QPVP-Os polymer.

D. Features of the XPS in 0~70 eV:

Fig. S2 shows the XPS in 0~70 eV for (a) Au/cyst/8SiMo₁₁V/7QPVP-Os prepared by the electrochemical growth and (b) the precipitate formed by mixing SiMo₁₁V and QPVP-Os solutions, which are nearly identical with the reported results.^{4a} This figure not only gives evidence of the presence of both Mo and Os elements in the multilayer, but also suggests that the multilayer seems to have a similar composition to the precipitate.

E. Features of the S 2p spectra:

Fig. S3 shows S 2p XPS spectra of films prepared by the immersion growth: (a) Au/Cyst, (b) Au/Cyst/SiMo₁₁V/QPVP-Os, (c) Au/Cyst/3SiMo₁₁V/2QPVP-Os. With increasing the number of multilayers, the S 2p XPS signal due to thiolates at 162.5 ± 0.3 eV becomes weaker, whereas another S 2p level due to SO₄²⁻ at 168.7 ± 0.3 eV becomes larger to some extent.

2. FTIR-RA spectra:

Fig. S4 shows FTIR-RA spectra of multilayers at various stages of film formation: (a) Au/Cyst, (b) Au/Cyst/SiMo₁₁V, (c) Au/Cyst/3SiMo₁₁V/2QPVP-Os and (d) Au/Cyst/7SiMo₁₁V/6QPVP-Os.

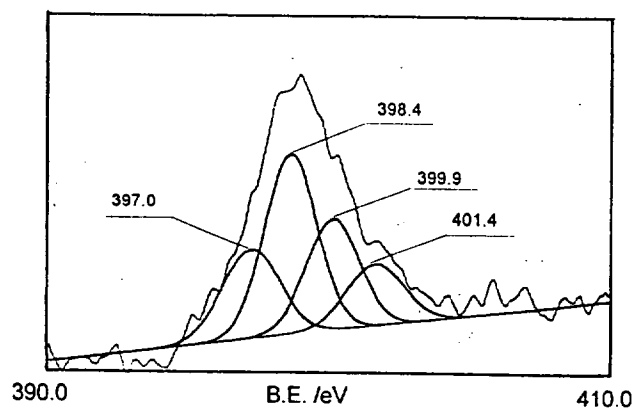


Fig. S1

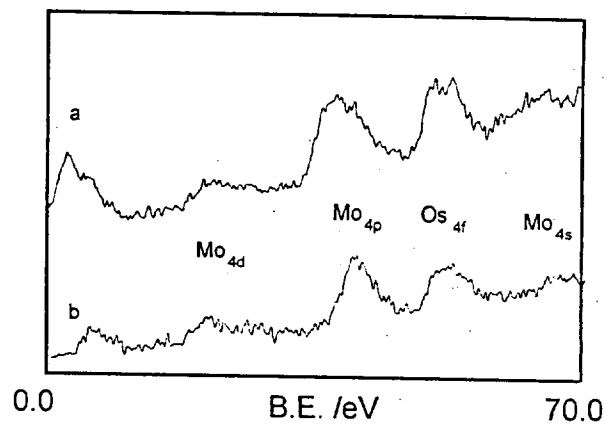


Fig. S2

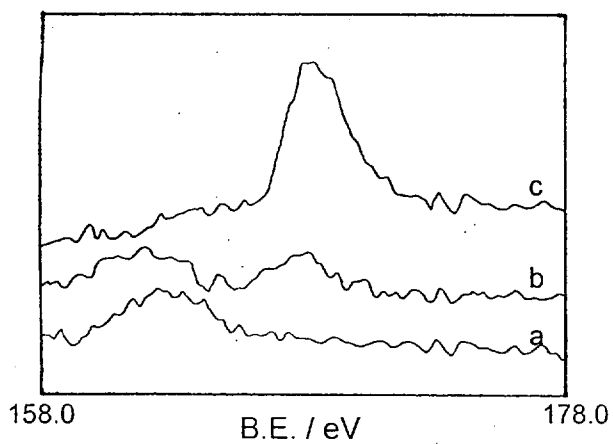


Fig. S3

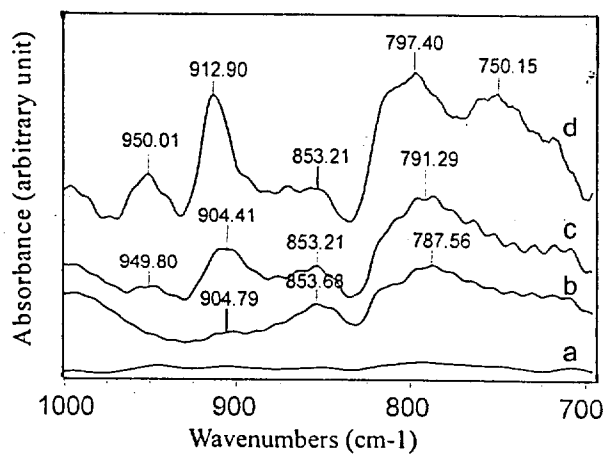


Fig. S4

Table II. Atomic coordinates for the PE-1 adduct.

atom	x	y	z	B _{eq}
P(1)	0.5435(1)	0.1828(1)	0.2500	2.16(3)
O(1)	0.4614(2)	0.0827(2)	0.1304(2)	2.53(5)
N(1)	0.5200(4)	0.3066(4)	0.2500	2.40(9)
C(1)	0.3552(3)	-0.0360(3)	0.1812(3)	2.19(7)
C(2)	0.2620(3)	-0.1422(3)	0.1094(3)	2.82(8)
C(3)	0.1656(4)	-0.2511(3)	0.1807(3)	3.58(9)
C(4)	1.0000	0.0000	0.0000	15.9(8)
C(5)	1.0000	0.0000	0.124(2)	15.3(4)
C(6)	1.0000	0.0000	0.2500	18.2(9)
H(1)	0.2720	-0.1393	0.0075	3.6182
H(2)	0.0982	-0.3363	0.1180	3.6182

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^* \cos \gamma + 2U_{13}aa^*cc^* \cos \beta + 2U_{23}bb^*cc^* \cos \alpha)$$

Table III. Anisotropic displacement coefficients for the PE-1 adduct.

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
P(1)	0.0285(8)	0.0257(7)	0.0244(6)	0.0111(7)	0.0000	0.0000
O(1)	0.035(1)	0.026(1)	0.022(1)	0.005(1)	0.001(1)	0.000(1)
N(1)	0.026(2)	0.028(2)	0.037(2)	0.014(2)	0.0000	0.0000
C(1)	0.032(2)	0.026(2)	0.024(2)	0.013(2)	0.003(2)	0.002(2)
C(2)	0.041(2)	0.030(2)	0.029(2)	0.013(2)	-0.003(2)	-0.005(2)
C(3)	0.052(3)	0.028(2)	0.038(2)	0.007(2)	-0.005(2)	-0.005(2)

The general temperature factor expression:

$$\exp(-2\pi^2(a^2U_{11}h^2 + b^2U_{22}k^2 + c^2U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table IV. Observed and calculated structure factors for the PE-1 adduct

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
0	2	1700	1748	5	5	5	51	49	4	1	3	252	240	2
0	4	301	297	2	5	7	49	48	4	1	4	556	545	2
0	6	177	203	3	5	8	52	52	5	1	5	247	253	2
0	8	545	546	3	5	9	61	67	4	1	6	329	326	2
0	10	209	187	4	6	1	219	225	3	1	7	99	92	4
1	2	519	522	2	6	2	211	211	3	1	8	163	169	3
1	3	603	606	2	6	3	225	216	3	1	9	71	67	3
1	4	86	101	3	6	4	357	361	3	1	10	138	151	5
1	5	462	458	2	6	5	95	95	5	2	0	598	567	2
1	6	158	164	3	6	6	171	173	4	2	1	618	627	2
1	7	410	408	3	6	7	199	198	4	2	2	132	147	2
1	8	215	202	3	6	8	55	59	5	2	3	142	124	2
1	9	347	354	3	6	9	120	113	5	2	4	84	80	3
1	10	100	118	5	6	10	117	110	6	2	5	155	150	3
1	11	185	185	4	7	0	117	115	4	2	6	40	47	4
2	0	506	474	2	7	2	182	181	3	2	7	231	242	3
2	1	786	772	2	7	3	345	349	3	2	8	144	141	4
2	3	81	83	3	7	4	107	93	5	2	9	232	242	4
2	4	248	249	2	7	5	414	416	3	2	10	193	190	4
2	5	30	30	4	7	7	203	208	4	3	0	539	561	2
2	6	89	92	4	7	8	93	88	4	3	1	525	510	2
2	7	75	74	4	7	9	107	104	4	3	2	225	251	2
2	8	69	77	3	8	1	172	165	3	3	3	307	298	2
3	0	107	97	2	8	2	83	85	4	3	4	223	224	2
3	1	698	699	2	8	3	161	157	4	3	6	359	372	3
3	2	75	94	3	8	4	148	150	4	3	7	111	112	4
3	3	146	138	2	8	5	161	158	4	3	8	367	374	3
3	4	149	147	2	8	6	91	93	4	3	10	207	204	4
3	5	152	155	3	8	7	136	137	5	3	11	62	54	5
3	6	220	222	3	8	8	83	83	4	4	0	188	183	2
3	7	115	121	4	9	0	114	108	5	4	2	112	126	3
3	8	195	186	3	9	1	208	223	4	4	3	575	563	3
3	9	88	83	4	9	3	139	141	4	4	4	141	135	3
3	10	87	88	4	9	4	74	76	4	4	5	325	325	3
4	0	275	276	2	9	5	190	197	4	4	6	295	296	3
4	1	324	340	2	9	7	54	48	5	4	7	69	74	3
4	2	36	49	3	10	0	157	145						

10|F|o vs 10|F|c

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
5	1	90	101	3	3	3	90	79	4	2	0	167	166	3
5	2	126	132	4	3	4	139	140	3	2	1	212	212	3
5	3	272	264	3	3	5	129	130	4	2	2	345	356	3
5	4	70	65	3	3	6	51	55	4	2	3	111	108	4
5	5	286	287	3	3	7	246	247	3	2	4	456	469	3
5	6	172	169	4	3	8	88	86	4	2	5	121	123	4
5	7	109	113	4	3	9	82	89	4	2	6	243	245	3
5	8	228	220	4	3	10	54	64	5	2	7	64	56	4
6	0	119	121	4	4	0	60	66	3	2	8	109	103	5
6	1	274	272	3	4	1	52	47	3	2	9	62	64	4
6	2	191	194	3	4	3	265	266	3	2	10	159	144	5
6	3	193	180	4	4	5	112	115	4	3	0	117	132	4
6	4	380	392	3	4	7	112	112	5	3	1	89	93	4
6	5	120	115	5	5	0	113	117	4	3	2	167	172	3
6	6	135	148	5	5	1	160	155	3	3	3	356	355	3
6	7	103	98	4	5	2	198	194	3	3	4	57	44	4
7	0	230	237	3	5	3	103	111	5	3	5	292	297	3
7	1	212	223	3	5	4	242	246	3	3	8	54	44	5
7	2	176	170	4	5	5	137	153	4	4	0	74	80	3
7	3	68	70	4	5	6	177	163	4	4	1	131	130	4
7	4	165	150	4	5	8	133	109	5	4	2	99	103	4
7	6	202	189	4	6	0	53	34	4	4	3	53	47	4
8	1	53	55	5	6	1	353	358	3	4	4	90	84	3
8	3	141	141	4	6	2	106	100	5	4	5	46	57	5
8	5	68	67	4	6	3	249	246	3	4	6	57	51	4
8	6	51	43	5	6	4	91	87	4	4	7	119	116	5
9	1	42	26	6	6	5	136	119	4	4	9	95	89	4
10	0	56	35	6	6	7	66	55	4	5	0	269	276	3
10	1	130	125	6	7	3	175	171	4	5	1	165	161	4
^^^^^^ h = 4 ^^^^^^^					7	5	139	136	5	5	2	121	127	5
1	0	605	625	2	7	6	155	158	5	5	3	95	95	4
1	1	264	271	2	8	0	61	56	4	5	6	70	64	4
1	2	288	288	2	8	2	44	41	6	5	7	211	217	4
1	3	91	79	3	8	3	126	121	5	5	8	99	92	5
1	4	596	584	3	9	5	98	89	4	6	1	114	116	5
1	5	78	88	3	9	0	85	76	4	6	2	83	74	3
1	6	52	62	4	9	1	124	117	6	6	3	87	84	4
1	7	121	119	4	9	2	82	79	4	6	4	103	102	4
1	8	291	317	3	^^^^^^ h = 5 ^^^^^^^					6	6	89	85	4
1	9	54	57	4	1	0	238	241	2	8	0	151	153	5
2	0	67	61	3	1	1	559	552	3	8	2	112	101	4
2	1	67	70	3	1	2	298	292	2	^^^^^^ h = 6 ^^^^^^^				
2	3	64	54	3	1	3	297	299	2	1	0	134	142	3
2	4	37	39	4	1	4	113	113	4	1	1	449	461	3
2	6	150	151	4	1	6	62	64	3	1	2	173	180	3
2	8	181	177	4	1	7	84	91	3	1	3	272	278	3
2	10	84	82	4	1	8	52	43	4	1	4	242	245	3
3	0	132	130	3	1	10	65	58	4	1	5	306	312	3

Table 1. Crystal data and structure refinement for 1.

Identification code	hra07
Empirical formula	$C_{23}H_{12}N_3O_6P_3$
Formula weight	519.27
Temperature	213(2) K
Wavelength	0.71073 Å
Crystal system	Hexagonal
Space group	$P6_3/m$
Unit cell dimensions	$a = 11.4883(4)$ Å $\alpha = 90^\circ$ $b = 11.4883(4)$ Å $\beta = 90^\circ$ $c = 10.0799(5)$ Å $\gamma = 120^\circ$
Volume, Z	$1152.12(8)$ Å ³ , 2
Density (calculated)	1.497 g/cm ³
Absorption coefficient	0.305 mm ⁻¹
F(000)	528
Crystal size	$0.30 \times 0.30 \times 0.30$ mm
Crystal color	Colorless block
θ range for data collection	2.05 to 28.19°
Limiting indices	$-15 \leq h \leq 15$, $-15 \leq k \leq 13$, $-11 \leq l \leq 13$
Reflections collected	3767
Independent reflections	946 ($R_{int} = 0.0865$)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	946 / 0 / 54
Goodness-of-fit on F^2	1.024
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0453$, $wR2 = 0.1202$
R indices (all data)	$R1 = 0.0540$, $wR2 = 0.1245$
Largest diff. peak and hole	0.412 and -0.588 eÅ ⁻³

Table 2. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 1. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
P(1)	6391(1)	1822(1)	2500	21(1)
O(1)	6213(1)	819(1)	1304(1)	27(1)
N(1)	5194(2)	2131(2)	2500	26(1)
C(1)	5865(3)	-2526(2)	1810(2)	42(1)
C(2)	5979(2)	-1436(2)	1085(2)	33(1)
C(3)	6096(2)	-369(2)	1818(2)	24(1)
C(5)	10000	0	0	240(14)
C(6)	10000	0	1059(23)	191(7)
C(7)	10000	0	2034(25)	233(11)

Table 4. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 1.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [(ha^*)^2 U_{11} + \dots + 2hka^*b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
P(1)	24(1)	19(1)	20(1)	0	0	11(1)
O(1)	42(1)	23(1)	19(1)	1(1)	-1(1)	18(1)
N(1)	21(1)	23(1)	33(1)	0	0	10(1)
C(1)	69(2)	27(1)	35(1)	-4(1)	0(1)	27(1)
C(2)	49(1)	27(1)	24(1)	-5(1)	1(1)	19(1)
C(3)	29(1)	21(1)	24(1)	1(1)	0(1)	12(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1.

	x	y	z	U(eq)
H(1B)	5787(3)	-3276(2)	1354(2)	51
H(2A)	5977(2)	-1430(2)	153(2)	40

Table 6. Observed and calculated structure factors for the PEO-1 adduct

Table 6.

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
0	1	0	320	453	24	-1	13	0	10	9	9	-6	12	1	20	23	7	-10	11	2	139	136	3	-3	9	3	220	204	5
0	2	0	574	535	13	0	13	0	56	62	6	-5	12	1	23	24	4	-9	11	2	116	112	3	-2	9	3	111	114	2
-2	3	0	1251	1220	68	-12	14	0	115	105	9	-4	12	1	38	37	3	-8	11	2	91	92	3	-1	9	3	36	38	3
-1	3	0	608	608	21	-11	14	0	87	73	5	-3	12	1	23	20	5	-7	11	2	84	83	6	0	9	3	152	158	4
0	3	0	171	167	4	-10	14	0	33	45	6	-2	12	1	111	117	2	-6	11	2	109	114	5	-9	10	3	18	10	17
-3	4	0	284	281	15	-9	14	0	51	61	5	-1	12	1	173	171	4	-5	11	2	84	88	3	-7	10	3	23	22	5
-2	4	0	258	235	8	-8	14	0	86	75	5	0	12	1	22	19	6	-4	11	2	19	9	7	-7	10	3	130	131	4
-1	4	0	632	613	13	-7	14	0	124	126	4	-12	13	1	0	9	1	-3	11	2	10	14	9	-6	10	3	16	12	16
0	4	0	272	274	7	-6	14	0	106	90	4	-11	13	1	4	0	4	-2	11	2	11	0	10	-5	10	3	101	100	2
-4	5	0	665	625	37	-5	14	0	76	65	5	-10	13	1	4	9	3	-1	11	2	86	83	4	-4	10	3	267	271	6
-3	5	0	262	289	6	-4	14	0	237	232	9	-9	13	1	206	212	4	0	11	2	194	191	3	-3	10	3	81	73	5
-2	5	0	256	225	10	-3	14	0	21	12	21	-8	13	1	205	212	7	-11	12	2	39	36	6	-2	10	3	11	14	10
-1	5	0	189	176	5	-2	14	0	91	95	6	-7	13	1	26	33	5	-10	12	2	48	45	4	-1	10	3	11	7	10
0	5	0	392	420	10	-9	15	0	105	97	8	-6	13	1	95	98	6	-9	12	2	161	161	5	0	10	3	131	129	3
-5	6	0	216	212	5	-8	15	0	9	20	9	-5	13	1	11	9	10	-8	12	2	189	191	5	-10	11	3	18	19	11
-4	6	0	85	73	4	-7	15	0	7	19	6	-4	13	1	120	128	7	-7	12	2	70	68	8	-9	11	3	56	49	5
-3	6	0	143	138	6	-6	15	0	61	85	7	-3	13	1	145	146	4	-6	12	2	95	107	6	-8	11	3	82	82	3
-2	6	0	177	188	7	0	15	1	482	476	10	-2	13	1	96	93	3	-5	12	2	4	1	4	-7	11	3	106	100	3
-1	6	0	303	276	8	-1	2	1	756	752	12	-1	13	1	66	60	4	-4	12	2	46	43	3	-6	11	3	18	18	10
0	6	0	25	23	5	0	2	1	803	792	13	0	13	1	12	14	12	-3	12	2	21	17	8	-5	11	3	77	83	3
-6	7	0	162	174	4	-2	3	1	198	214	8	-12	14	1	147	131	9	-2	12	2	77	74	3	-4	11	3	192	187	4
-5	7	0	204	201	8	-1	3	1	645	636	15	-11	14	1	50	45	4	-1	12	2	31	34	5	-3	11	3	174	148	13
-4	7	0	148	143	10	0	3	1	674	696	12	-10	14	1	14	15	13	0	12	2	80	83	4	-2	11	3	114	109	4
-3	7	0	186	171	6	-3	4	1	18	13	8	-9	14	1	107	109	4	-12	13	2	25	29	5	-1	11	3	112	119	5
-2	7	0	130	125	5	-2	4	1	124	110	5	-8	14	1	137	126	5	-11	13	2	36	32	3	0	11	3	43	43	3
-1	7	0	13	13	13	-1	4	1	523	545	13	-7	14	1	9	12	9	-10	13	2	44	45	5	-11	12	3	88	93	10
0	7	0	153	135	7	0	4	1	319	341	6	-6	14	1	154	153	7	-9	13	2	8	5	8	-10	12	3	83	82	3
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