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Supporting Information

A Copper(II) Coordination Compound under Water-oxidation Reaction at Neutral Conditions: Decomposition on the Counter Electrode

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Table S1 Crystallographic information of compound **1**.

Compound	**1**
net formula	$C_{30}H_{24}CuN_6O_6 \cdot 2(NO_3) \cdot 0.5(C_2H_6O) \cdot 0.75(H_2O)$
M_r/g mol^{-1}	788.66
crystal size/mm	0.27 × 0.22 × 0.09
T/K	100
crystal shape, color	Block, Green
crystal system	Monoclinic
space group	$P2_1/n$
Absorption correction	Analytical
a/Å	12.800(4)
b/Å	21.718(7)
c/Å	24.685(7)
β/Å	94.90(3)
V/Å^3	6837(4)
Z	8
D_x/Mg m^{-3}	1.532
μ/mm^{-1}	0.71
F(000)	3244
Measured reflections	59580
Independent reflections	17274
Reflections with $I > 2\sigma(I)$	7995
Parameters	1026
R_{int}	0.134
θ range/°	3.0–24.5
T_{min}, T_{max}	0.880, 0.950
h,k,l	−16 → 15, -27 → 27, -34 → 28
$R[F^2 > 2\sigma(F^2)]$	0.092
$R_w(F^2)$	0.252
S	1.01
Shift/error$_{max}$	< 0.001
Max electron density/e Å^{-3}	1.07
Min electron density/e Å^{-3}	−0.56
CCDC	2171141

Table S2 Selected bond lengths and angles in the crystal structure of compound **1**.

Bond	**Length/Å**	**Bond**	**Angle/°**
Cu1–O11	1.961(3)	O11–Cu1–O22	178.52(14)
Cu1–O22	1.969(3)	O11–Cu1–O21	88.08(14)
Cu1–O21	2.056(4)	O22–Cu1–O21	90.67(14)
Cu1–O23	2.107(4)	O11–Cu1–O23	92.41(14)
Cu1–O12	2.175(4)	O22–Cu1–O23	88.88(14)
Cu1–O13	2.178(4)	O21–Cu1–O23	176.80(16)
Cu2–O26	1.950(4)	O11–Cu1–O12	91.35(15)
Cu2–O24	1.966(4)	O22–Cu1–O12	87.92(14)
Cu2–O16	1.990(4)	O21–Cu1–O12	92.54(15)
Cu2–O15	1.991(4)	O23–Cu1–O12	90.61(13)
Cu2–O14	2.254(4)	O11–Cu1–O13	87.85(15)
Cu2–O25	2.276(4)	O22–Cu1–O13	92.99(15)
N11–O11	1.342(5)	O21–Cu1–O13	92.57(16)
N12—O12	1.338(5)	O23–Cu1–O13	84.29(14)
N13—O13	1.329(6)	O12–Cu1–O13	174.80(13)
N14–O14	1.316(6)	O26–Cu2–O24	174.43(17)
N15—O15	1.335(5)	O26–Cu2–O16	89.65(16)
N16—O16	1.345(6)	O24–Cu2–O16	95.32(16)
N21–O21	1.339(6)	O26–Cu2–O15	91.59(15)
N22—O22	1.336(5)	O24–Cu2–O15	83.50(15)
N23—O23	1.344(5)	O16–Cu2–O15	178.22(17)
N24–O24	1.338(5)	O26–Cu2–O14	91.78(17)
N25—O25	1.326(7)	O24–Cu2–O14	85.95(14)
N26—O26	1.341(7)	O16–Cu2–O14	87.41(15)
		O15–Cu2–O14	93.82(15)
		O26–Cu2–O25	90.23(18)
		O24–Cu2–O25	92.02(16)
		O16–Cu2–O25	92.84(16)
		O15–Cu2–O25	85.88(15)
		O14–Cu2–O25	177.97(15)

Table S3 Hydrogen bond interactions in the crystal structure of compound **1.**

D*–H···*A	***D*–H**	**H···*A***	***D*···*A***	***D*–H···*A***
C21–H21···O14^{i}	0.95	2.36	3.153(7)	141
C51–H51···N23^{ii}	0.95	2.68	3.420(7)	136
C51–H51···O23^{ii}	0.95	2.43	3.359(7)	166
C101–H101···O2*B*	0.95	2.61	3.283(10)	129
C101–H101···O3*B*	0.95	2.49	3.436(9)	173
C22–H22···O3*D*^{a}	0.95	2.55	3.35(2)	142
C22–H22···O2*E*b	0.95	2.45	3.18(2)	134
C22–H22···O3*E*^{b}	0.95	2.64	3.222(17)	120
C42–H42···O11^{ii}	0.95	2.44	3.099(6)	126
C52–H52···O23^{ii}	0.95	2.53	3.481(6)	175
C72–H72···O2*W*b^{iii}	0.95	2.50	3.170(9)	128
C102–H102···O3*B*	0.95	2.24	3.118(9)	153
C23–H23···O3*C*^{iv}	0.95	2.61	3.284(8)	128
C43–H43···O1*C*^{v}	0.95	2.61	3.506(9)	157
C43–H43···O2*C*^{v}	0.95	2.58	3.364(10)	140
C53–H53···O2*W*b^{v}	0.95	2.44	3.132(10)	130
C73–H73···O15	0.95	2.35	3.075(7)	132
C93–H93···O1*D*a	0.95	2.54	3.33(2)	141
C93–H93···O1*E*^{b}	0.95	2.52	3.159(16)	125
C24–H24···O2*A*^{iv}	0.95	2.46	3.147(8)	129
C54–H54···O3*D*a^{vi}	0.95	2.47	3.37(2)	157
C54–H54···O2*E*b^{vi}	0.95	2.35	3.266(18)	161
C74–H74···O21^{iv}	0.95	2.24	3.041(8)	142
C94–H94···O3*C*^{vii}	0.95	2.65	3.358(8)	132
C104–H104···O1*B*^{vii}	0.95	2.31	3.222(10)	160
C25–H25···O2*B*	0.95	2.42	3.341(11)	163
C55–H55···O3*D*a^{vi}	0.95	2.11	3.05(2)	173
C55–H55···O2*E*b^{vi}	0.95	2.50	3.44(2)	173
C75–H75···O22	0.95	2.60	3.317(8)	133
C75–H75···O13	0.95	2.32	3.179(7)	150
C105–H105···O1*B*^{vii}	0.95	2.33	3.225(10)	158
C26–H26···O26^{viii}	0.95	2.52	3.133(8)	123
C56–H56···O1*B*^{vii}	0.95	2.60	3.530(11)	168
C76–H76···O3*A*^{vii}	0.95	2.57	3.145(12)	119
C106–H106···N1*D*^{vi}	0.95	2.46	3.280(9)	145
C106–H106···O1*D*a^{vi}	0.95	2.61	3.39(3)	140
C106–H106···O3*D*a^{vi}	0.95	2.39	3.31(2)	165
C106–H106···O1*E*b^{vi}	0.95	2.49	3.111(17)	123
C106–H106···O2*E*b^{vi}	0.95	2.62	3.56(2)	171
O1*F*–H1*F*···O2*C*	0.84	2.38	3.104(15)	144
O1*F*–H1*F*···O1*W*b	0.84	2.22	2.888(18)	136
C1*F*–H13*A*···O1*W*^{b}	0.99	2.51	3.07(3)	115

C2*F*–H2*FC*···O1*D*a[ix]	0.98	2.49	3.03(4)	115
O1*G*a–H1*G*a···O1*A*[iv]	0.84	2.06	2.879(14)	164
C1*G*a–H1*GA*a···N24	0.99	2.62	3.44(2)	141
C2*G*a–H2*GC*a···O2*C*[vii]	0.98	2.33	3.289(19)	165
O1*W*b–H11*W*b···N1*C*	0.89	2.56	3.233(15)	133
O1*W*b–H11*W*b···O2*C*	0.89	2.09	2.860(15)	145
O1*W*b–H11*W*b···O3*C*	0.89	2.45	2.957(15)	117
O1*W*b–H11*W*b···O1*F*	0.89	2.34	2.888(18)	120
O1*W*b–H21*W*b···O2*B*	0.92	2.25	3.086(15)	152
O2*W*b–H12*W*b···O2*C*	0.86	1.70	2.533(15)	162
O2*W*b–H22*W*b···O3*W*b[vii]	0.86	2.39	3.23(2)	165
O3*W*b–H23*W*b···O1*A*[iv]	0.86	2.53	3.18(3)	133

Symmetry codes: (i) *x*−1/2, −*y*+1/2, *z*−1/2; (ii) −*x*+1, −*y*, −*z*+1; (iii) −*x*+1/2, *y*−1/2, −*z*+1/2; (iv) *x*+1/2, −*y*+1/2, *z*+1/2; (v) −*x*+3/2, *y*−1/2, −*z*+1/2; (vi) *x*+1, *y*, *z*;(vii) −*x*+1, −*y*+1, −*z*+1; (viii) −*x*+2, −*y*+1, −*z*+1; (ix) *x*+1/2, −*y*+1/2, *z*−1/2.

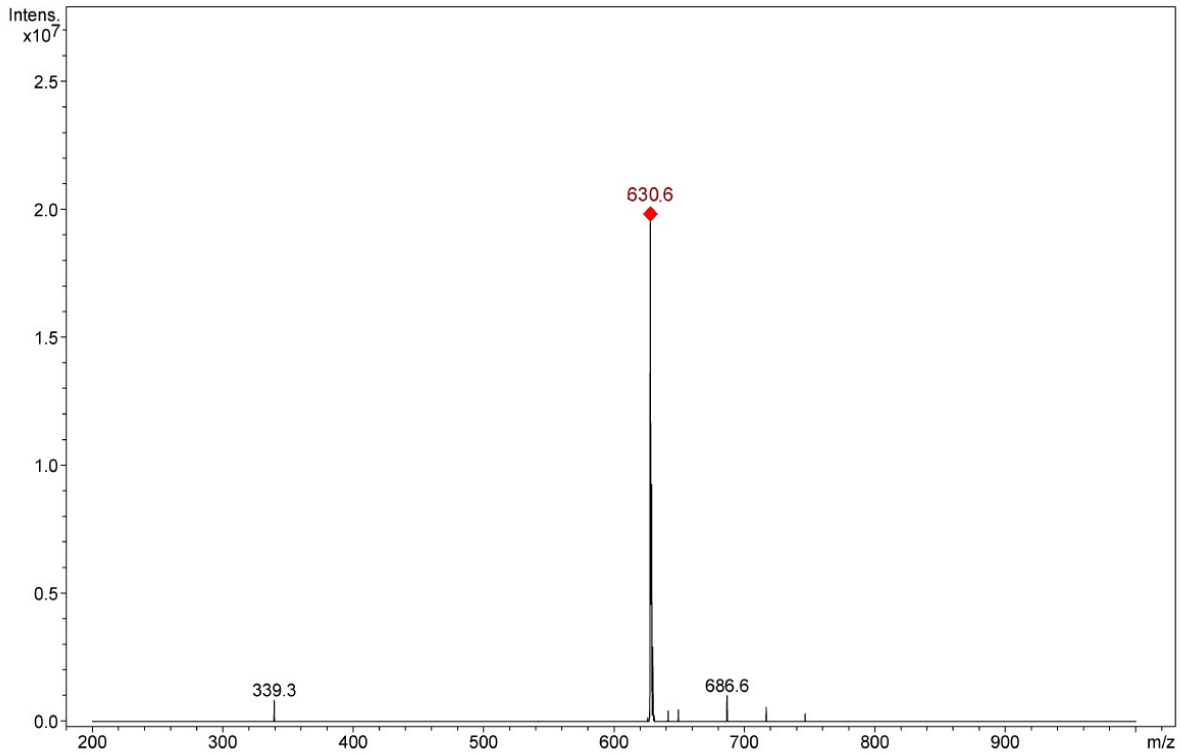

Figure S1 Electrospray ionization (ESI) mass spectroscopy of compound **1** in water.

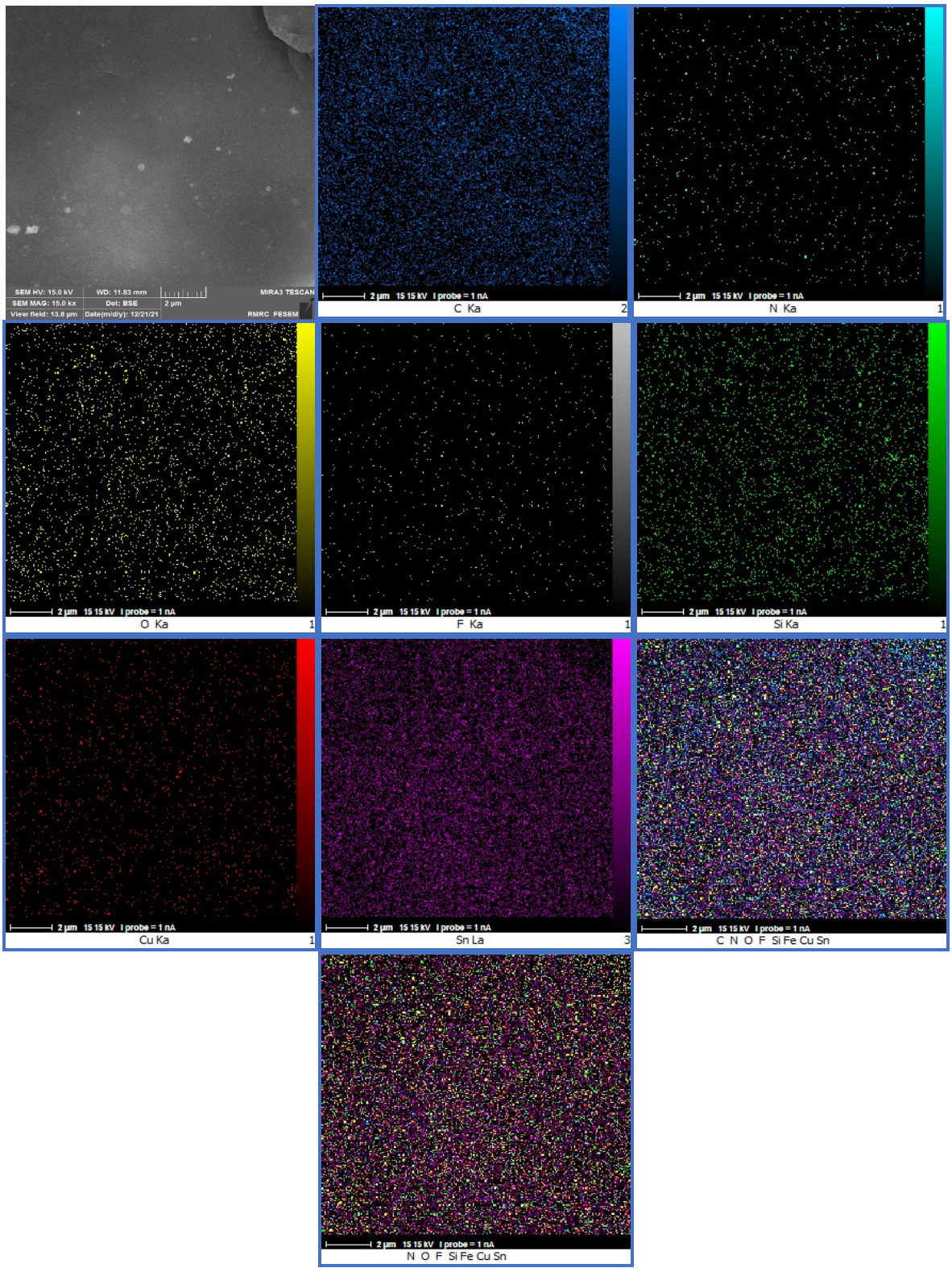

Figure S2 SEM and corresponding EDX mapping of the working electrode (FTO) in the presence of compound **1** at 0.11 V for 3 hours.

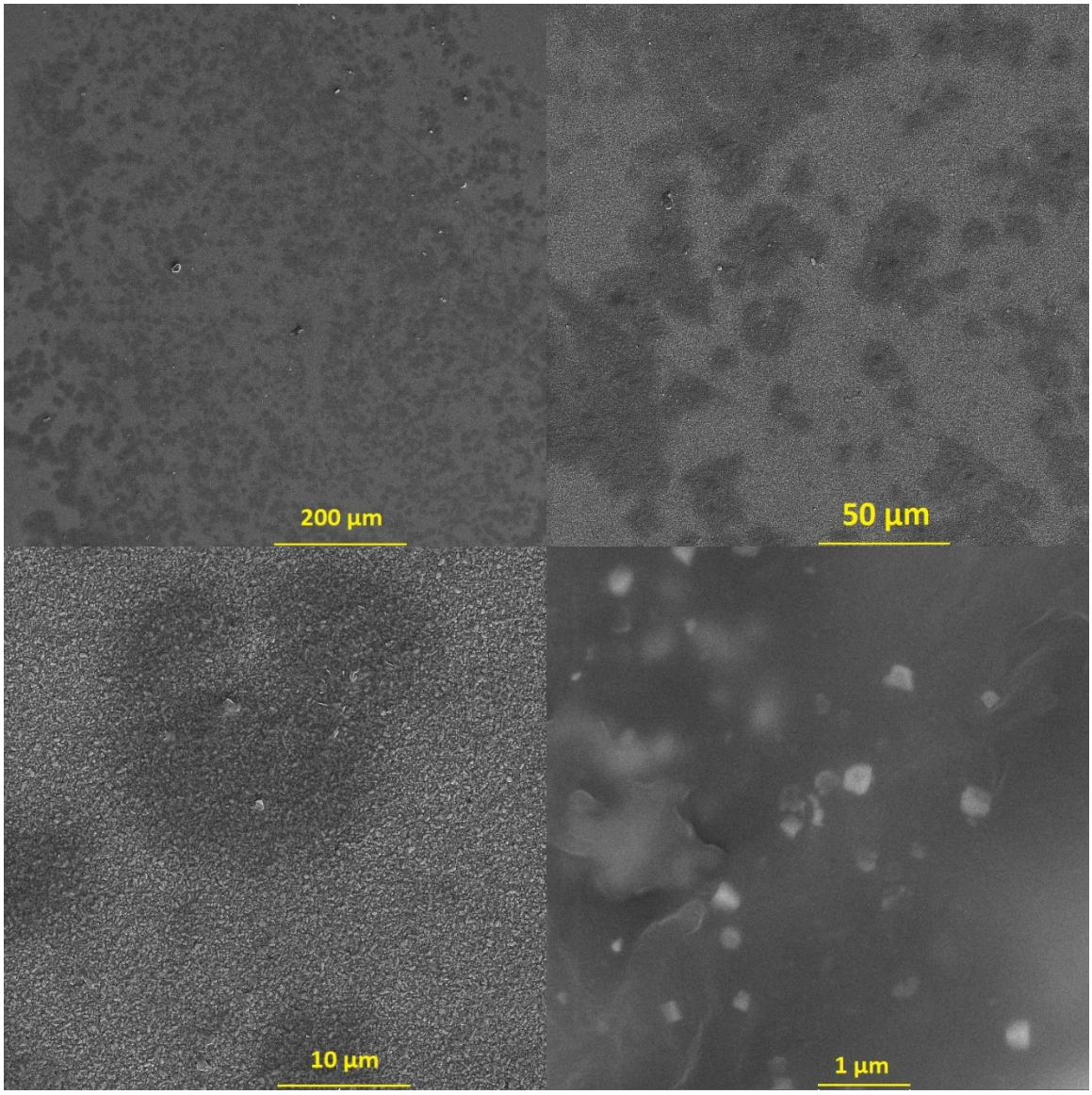

Figure S3 SEM images of the working electrode (FTO) in the presence of compound **1** at 2.41 V for 3 hours.

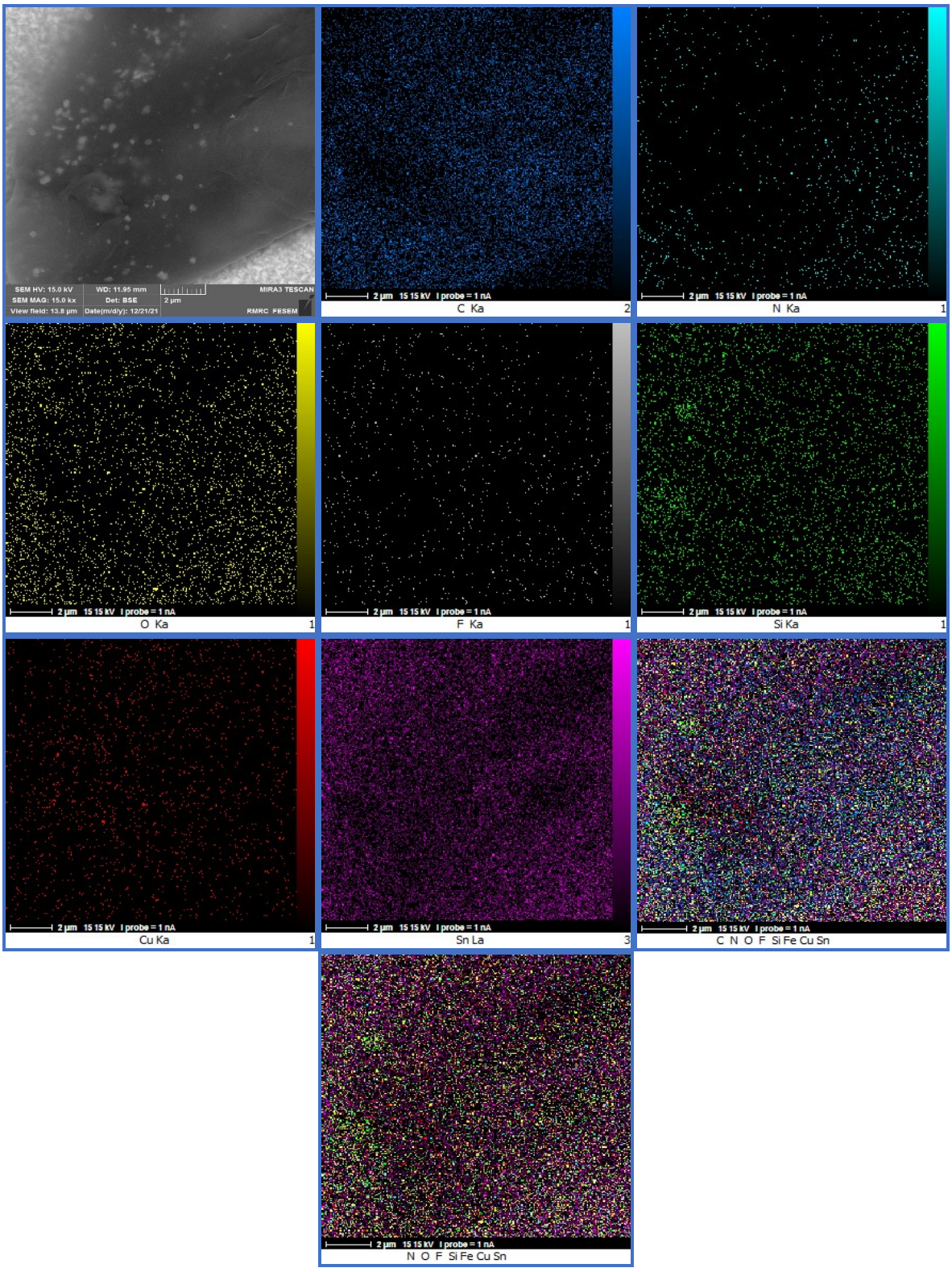

Figure S4 SEM and corresponding EDX mapping of the working electrode (FTO) in the presence of compound **1** at 2.41 V for 3 hours.

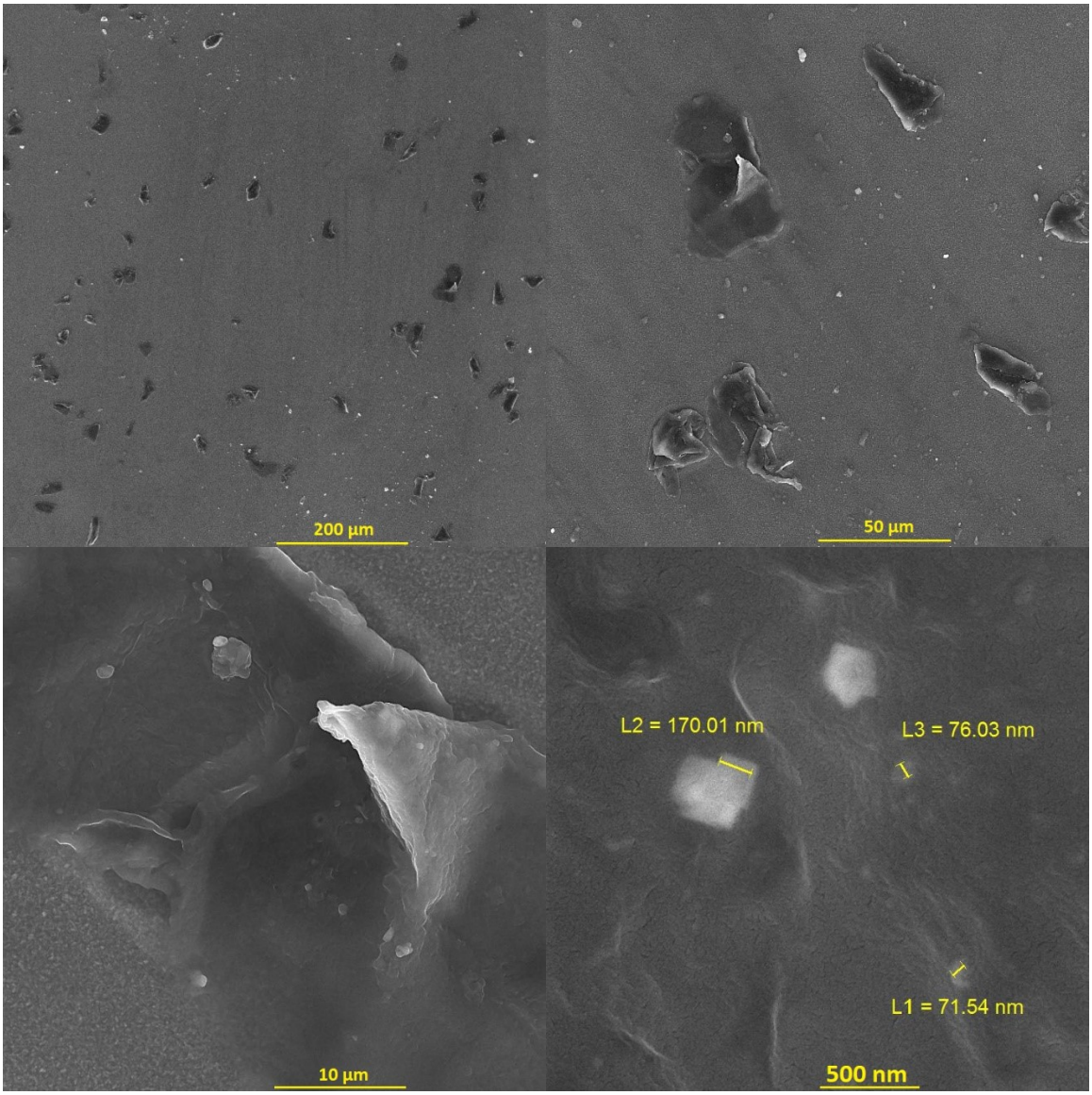

Figure S5 SEM images of the working electrode (FTO) in the presence of compound **1** at 2.31 V for 3 hours.

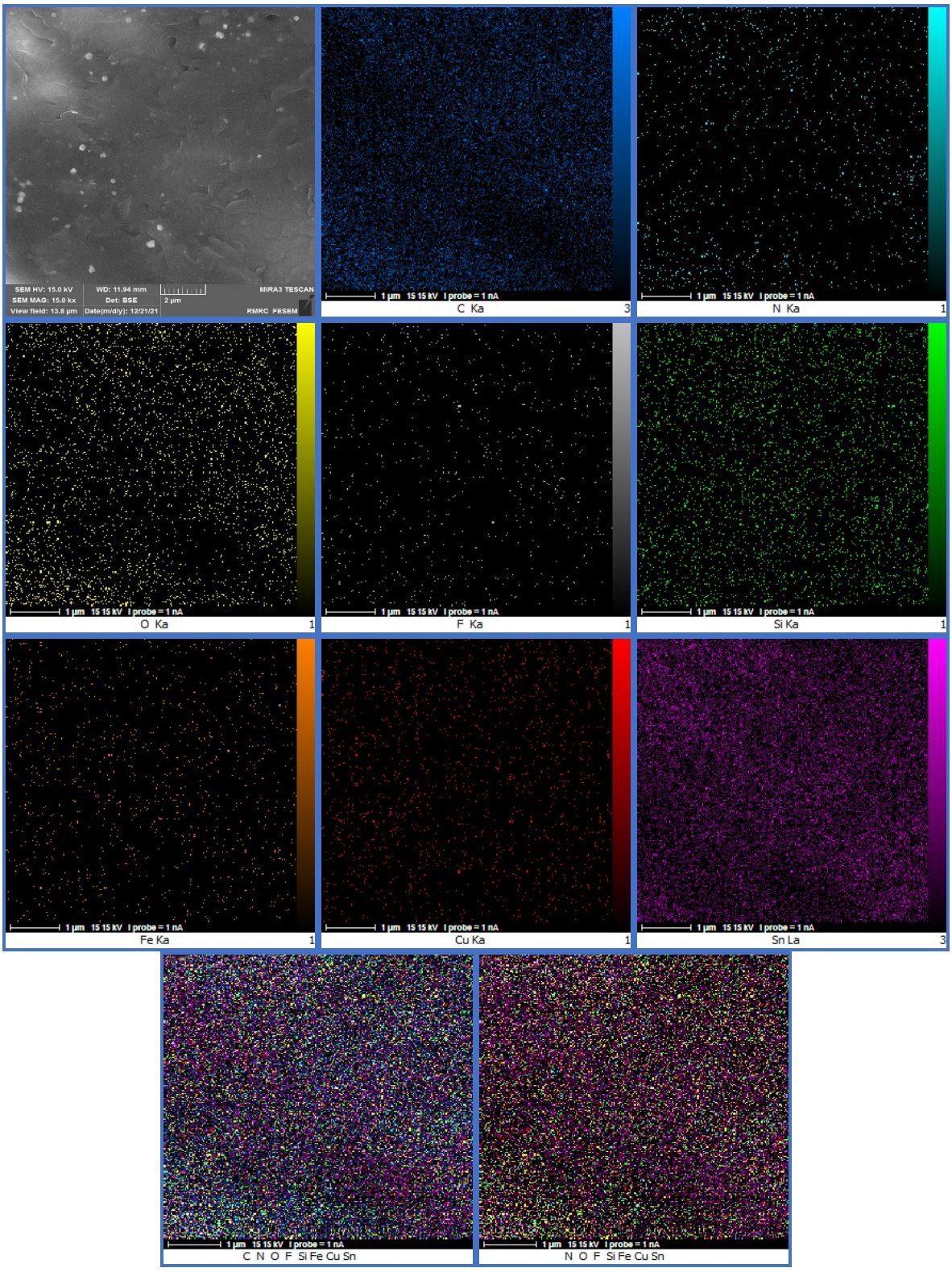

Figure S6 SEM and corresponding EDX mapping of the working electrode (FTO) in the presence of compound **1** at 2.41 V for 3 hours.