

Supporting Information for:

The Role of Coordination Center in Photocurrent Behaviors of a Tetrathiafulvalene and Metal Complex Dyad

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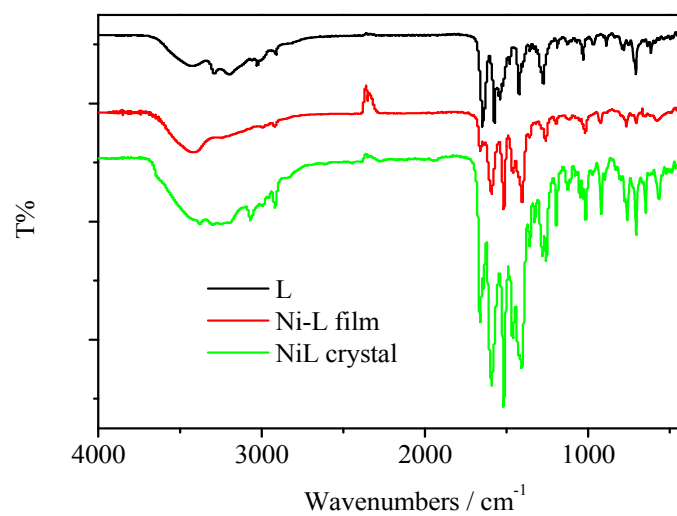
Figure SI1. FTIR of the ligand, M-L films prepared by layer-by-layer coating method and the ML crystals.

Figure SI2. EDS of the ligand (a) and crystal **1** (b) after oxidation by $\text{Fe}(\text{ClO}_4)_3$.

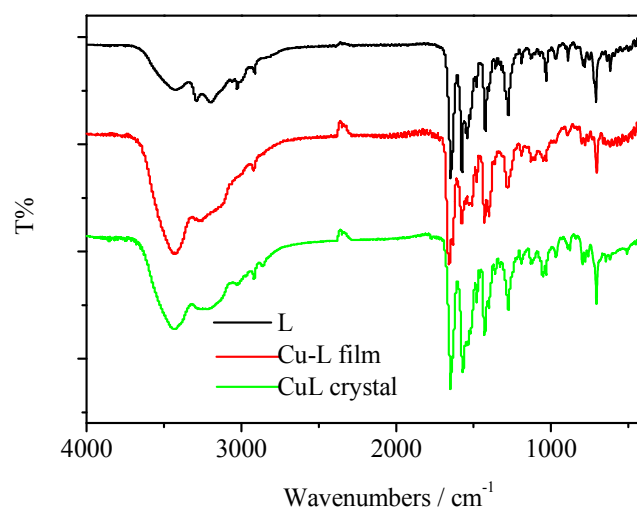
Figure SI3. Cyclic voltammogram of MVI_2 ($10^{-3} \text{ mol}\cdot\text{L}^{-1}$) in DMF

Figure SI4. Cyclic voltammogram of **L** ($10^{-3} \text{ mol}\cdot\text{L}^{-1}$) in CH_2Cl_2 – CH_3CN (1:1 by volume)

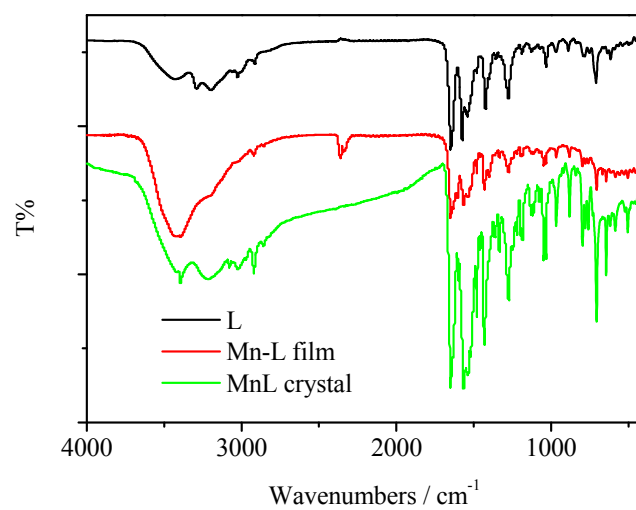
Table SI1. Selected Bond Lengths (Å) of **1–3**



(a)

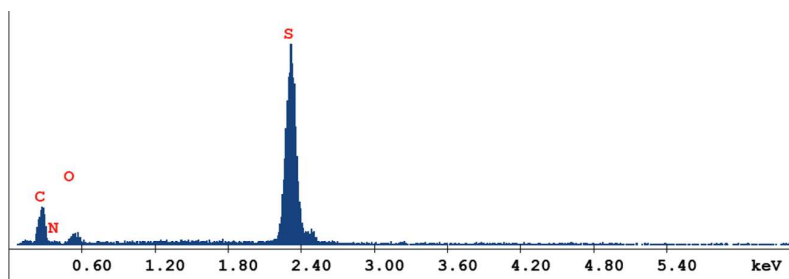


(b)



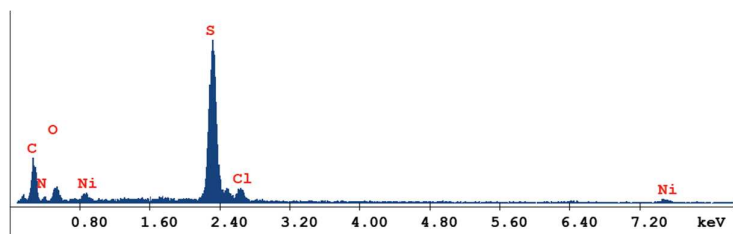
(c)

Figure SI1. FTIR of the ligand, M-L films prepared by layer-by-layer coating method and the ML crystals.



Element	Wt %	At %
C K	54.69	71.73
N K	4.65	5.23
O K	6.20	6.10
S K	34.47	16.94
Total	100.00	100.00

(a)



Element	Wt %	At %
C K	51.12	69.88
N K	4.40	5.16
O K	7.36	7.55
S K	27.73	14.20
ClK	3.18	1.47
NiK	6.21	1.74
Total	100.00	100.00

(b)

Figure SI2. EDS of the ligand (a) and crystal **1** (b) after oxidation by $\text{Fe}(\text{ClO}_4)_3$.

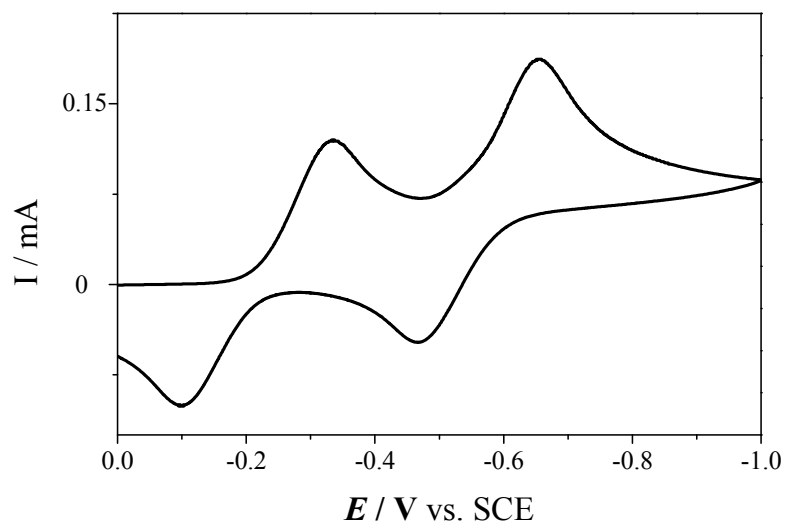


Figure SI3. Cyclic voltammogram of MVI_2 in DMF

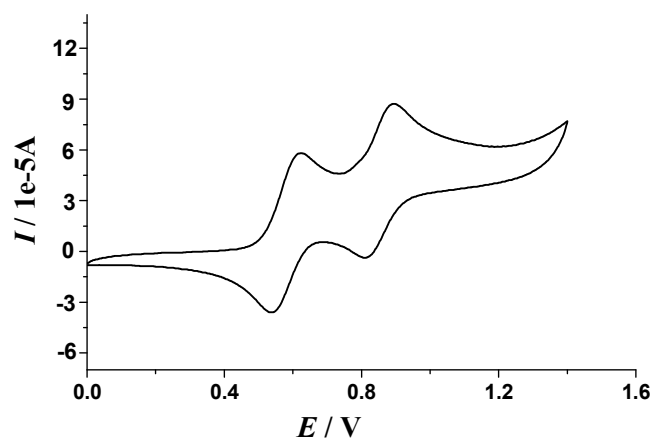


Figure SI4. Cyclic voltammogram of L ($10^{-3} \text{ mol}\cdot\text{L}^{-1}$) in CH_2Cl_2 - CH_3CN (1:1 by volume)

Table S11. Selected Bond Lengths (Å) of **1–3**

1			
Ni1–O3	2.014(4)	S2–C2	1.762(6)
Ni1–O4	2.043(5)	S3–C4	1.752(7)
Ni1–O6	2.043(4)	S3–C5	1.753(8)
Ni1–O5	2.050(4)	S4–C6	1.737(8)
Ni1–N4	2.102(5)	S4–C4	1.756(7)
Ni1–N2	2.132(5)	C1–C2	1.335(8)
S1–C1	1.742(6)	C3–C4	1.352(9)
S1–C3	1.751(7)	C5–C6	1.362(11)
S2–C3	1.746(7)		
2			
I1–Cu1	2.6473(6)	S3–C4	1.756(3)
Cu1–N2	2.056(2)	S3–C5	1.768(3)
Cu1–N4	2.062(2)	S4–C4	1.747(3)
S1–C3	1.751(3)	S4–C6	1.765(3)
S1–C1	1.757(3)	C1–C2	1.347(4)
S2–C3	1.755(3)	C3–C4	1.341(4)
S2–C2	1.757(3)	C5–C6	1.340(4)
3			
Mn1–N4	2.305(4)	S3–C5	1.759(4)
Mn1–N2	2.339(4)	S3–C4	1.761(4)
Mn1–Cl1	2.4856(11)	S4–C6	1.762(4)
S1–C3	1.752(4)	S4–C4	1.764(5)
S1–C2	1.756(4)	C1–C2	1.351(6)
S2–C3	1.751(4)	C3–C4	1.341(6)
S2–C1	1.759(4)	C5–C6	1.341(6)