Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Experimental and DFT study of the effect of mercaptosuccinic acid on cyanide-free immersion gold deposition

Bo Wu, [a] Jingmeng Huang, [a] Zeman Lv, [a] Ziya Cui, [a] Guanghui Hu, [a] Jiye Luo, [a] Mohamed S. Selim [a, b] and Zhifeng Hao*[a]

[a] *School of Chemical Engineering and Light Industry, Guangdong University of Technology, Guangzhou 510006, P. R. China.*

[b] *Petroleum Application Department, Egyptian Petroleum Research Institute, Nasr City 11727, Cairo, Egypt.*

** Correspondence to:*

haozf@gdut.edu.cn *(Zhifeng Hao)*

Figures

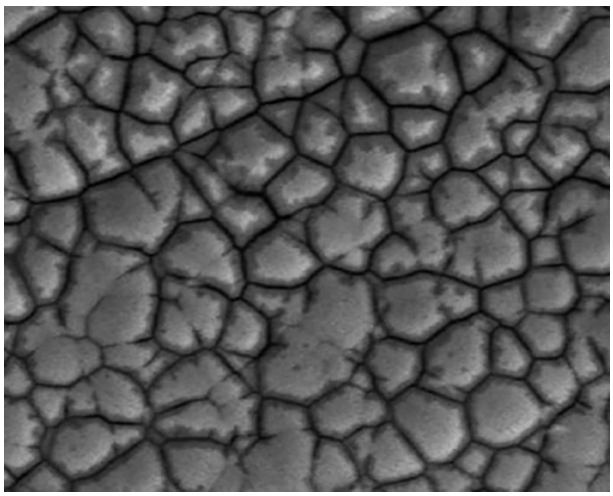

Fig. S1 Nickel deposit showing black pad (5K×)[1].

The black pad phenomenon is characterized by an uneven nickel layer and fissures or crevices between nodules, as shown in Fig. S1.

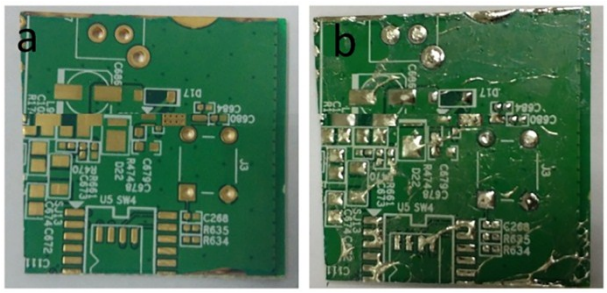

Fig. S2 Solderability test of printed circuit board: (a) before test and (b) after test.

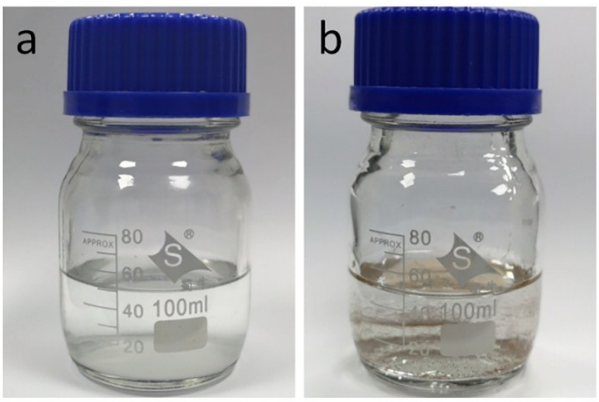

Fig. S3 Appearances of plating solutions after placing at room temperature for 200 days: (a) MSA as complexant and (b) DMH as complexant.

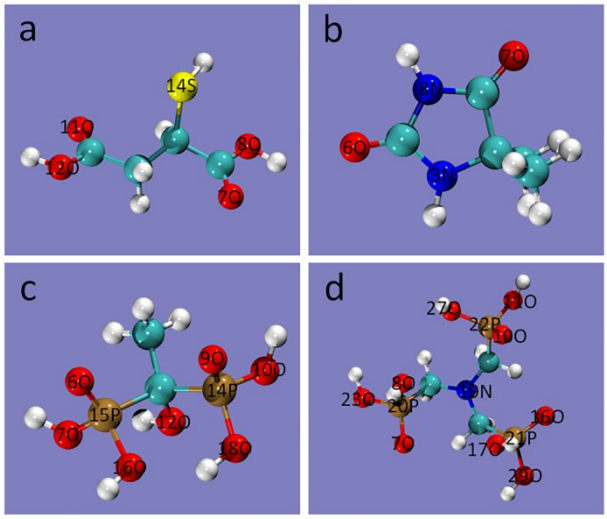

Fig. S4 Optimized molecular structure of different complexing agents with atom symbols: (a) MSA, (b) DMH, (c) HEDP, and (d) ATMP.

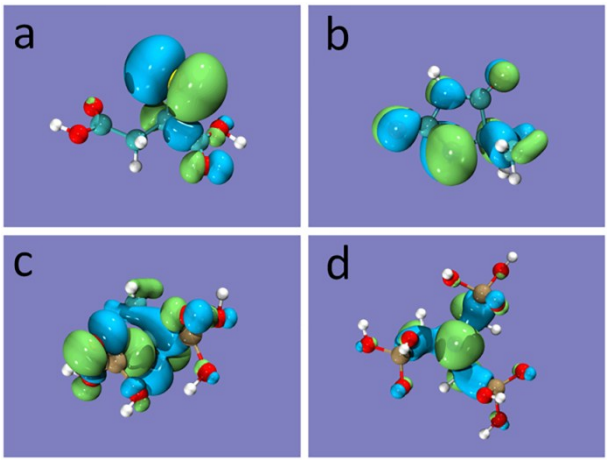

Fig. S5 Localization of HOMO (isovalues are 0.03 and -0.03 a.u.) of (a) MSA, (b) DMH, (c) HEDP, and (d) ATMP.

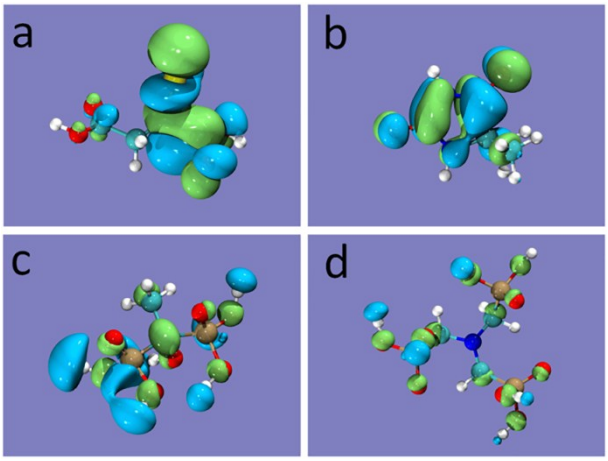

Fig. S6 Localization of LUMO (isovalues are 0.03 and -0.03 a.u.) of (a) MSA, (b) DMH, (c) HEDP, and (d) ATMP.

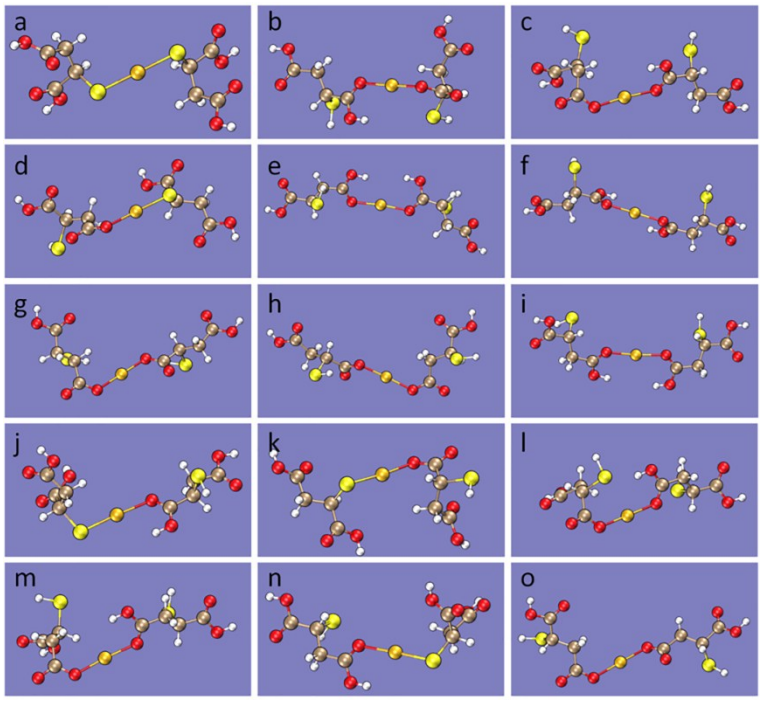

Fig. S7 Optimized structures of the gold(I) complexes with MSA: (a) S-Au-S, (b) 7O-Au-8O, (c) 7O-Au-12O, (d) 12O-Au-S, (e) 7O-Au-7O, (f) 7O-Au-11O, (g) 8O-Au-8O,(h) 8O-Au-12O, (i) 11O-Au-11O, (j) 7O-AU-S, (k) 8O-Au-S, (l) 11O-Au-8O, (m) 11O-Au-12O, (n) 11O-Au-S and (o) 12O-Au-12O.

Tables

Table S1 Au^{+} and Ni^{2+} concentrations of plating bath before and after gold plating

Solution	$[Au^{+}]_0$/ mM	$[Ni^{2+}]_0$/ mM	$[Au^{+}]_1$/ mM	$[Ni^{2+}]_1$/ M	$\Delta[Au^{+}]$/ M	$\Delta[Ni^{2+}]$/ M
1	7.101	0	7.059	7.017×10^{-5}	4.213×10^{-5}	7.017×10^{-5}
2	7.102	0	7.059	7.230×10^{-5}	4.297×10^{-5}	7.230×10^{-5}
Mean value	7.102	0	7.059	7.123×10^{-5}	4.256×10^{-5}	7.123×10^{-5}

In Table S1, the subscript "0" represents the ion concentration before the reaction, and the subscript "1" represents the ion concentration after the reaction. Numbers "1" and "2" represent two baths with the same formula. Before gold plating, the nickel coating has been rinsed, so the Ni^{2+} in the gold plating solution can only be dissolved from the coating into the solution through a replacement reaction. The Au^{+} consumed by immersion gold is twice as much as Ni^{2+} generated, so based on the data above, it can be calculated that the ratio of immersion gold is 83.68%.

Table S2 Composition of the main atoms for HOMO and condensed local softness of MSA, DMH, HEDP, and ATMP

Molecule	Atom	Composition of each atom	Condensed local softness/ Hartree·e
MSA	7(O)	6.6%	0.366
	8(O)	1.3%	0.128
	11(O)	0.2%	0.193
	12(O)	0.03%	0.108
	14(S)	85.7%	1.155
DMH	3(N)	57.0%	0.570
	6(O)	16.7%	0.442
	7(O)	4.3%	0.279
	8(N)	4.9%	0.127
HEDP	6(O)	24.4%	0.410
	7(O)	2.7%	0.119
	9(O)	6.3%	0.463
	10(O)	0.8%	0.124

	12(O)	33.7%	0.309
	14(P)	3.3%	0.190
	15(P)	10.3%	0.177
	16(O)	1.0%	0.064
	18(O)	0.4%	0.125
ATMP	7(O)	1.2%	0.135
	8(O)	0.9%	0.029
	10(O)	1.0%	0.187
	11(O)	1.8%	0.070
	16(O)	1.0%	0.158
	17(O)	1.0%	0.038
	19(N)	45.4%	0.619
	20(P)	6.0%	0.072
	21(P)	5.3%	0.082
	22(P)	8.0%	0.096
	23(O)	2.5%	0.096
	25(O)	1.8%	0.101
	27(O)	0.4%	0.055

Table S3 Minima of ALIE of MSA, DMH, HEDP, and ATMP

Molecule	Number	ALIE/ a.u.	Number	ALIE/ a.u.
MSA	1	0.371	6	0.444
	2	0.419	7	0.392
	3	0.419	8	0.421
	4	0.293	9	0.292
	5	0.393	10	0.372
DMH	1	0.357	7	0.356
	2	0.353	8	0.422
	3	0.395	9	0.422
	4	0.395	10	0.424
	5	0.368	11	0.424
	6	0.367	12	0.367
HEDP	1	0.418	9	0.374
	2	0.372	10	0.376
	3	0.377	11	0.410
	4	0.428	12	0.436
	5	0.437	13	0.373
	6	0.425	14	0.406
	7	0.385	15	0.364
	8	0.372	16	0.411
ATMP	1	0.403	11	0.414
	2	0.358	12	0.411
	3	0.404	13	0.362
	4	0.414	14	0.404
	5	0.360	15	0.365
	6	0.412	16	0.361
	7	0.409	17	0.402
	8	0.312	18	0.406
	9	0.414	19	0.360
	10	0.407	20	0.358

Reference

1. G. Milad, *Circuit World*, 2010, **36**, 10-13.