Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information for:

Theoretical exploration of Seleno and Tellurophenols as a promising alternative to sulfur ligands in the anchoring to gold (111) materials

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Table S1. Selected geometric parameters for the *para* substituted selenophenol-gold complexes[a] (distances in Å and angles in deg).

Au_{42}-Selenophenol (SeH)	**D_{top}**	**D_{C-Se}**	**θ**	**ω**
Au_{42}-$SeHC_6H_4NH_2$	2.70	1.93	87.6	95.3
Au_{42}-$SeHC_6H_4OCH_3$	2.69	1.93	88.4	94.0
Au_{42}-$SeHC_6H_4CH_3$	2.57	1.89	88.5	90.9
Au_{42}-$SeHC_6H_5$	2.70	1.93	90.3	93.3
Au_{42}-$SeHC_6H_4F$	2.68	1.93	90.3	94.2
Au_{42}-$SeHC_6H_4Cl$	2.72	1.93	88.3	95.9
Au_{42}-$SeHC_6H_4OCOCH_3$	2.70	1.93	90.6	93.1
Au_{42}-$SeHC_6H_4CF_3$	2.70	1.93	91.1	94.3
Au_{42}-$SeHC_6H_4CN$	2.60	1.91	86.9	93.2
Au_{42}-$SeHC_6H_4NO_2$	2.75	1.92	88.6	96.7

a The nomenclature used on the column headings for the definition of the geometric parameters is detailed in Figure 2 from the manuscript.

Table S2. Selected geometric parameters for the *para* substituted telurophenol-gold complexes[a] (distances in Å and angles in deg).

Au_{42}-Telurophenol (TeH)	**D_{top}**	**D_{C-Te}**	**θ**	**ω**
Au_{42}-$TeHC_6H_4NH_2$	2.77	2.12	87.24	95.83
Au_{42}-$TeHC_6H_4OCH_3$	2.76	2.12	88.82	93.08
Au_{42}-$TeHC_6H_4CH_3$	2.75	2.12	88.83	91.21
Au_{42}-$TeHC_6H_5$	2.77	2.13	89.50	93.54
Au_{42}-$TeHC_6H_4F$	2.75	2.13	89.50	93.78
Au_{42}-$TeHC_6H_4Cl$	2.77	2.12	87.97	95.28
Au_{42}-$TeHC_6H_4OCOCH_3$	2.76	2.13	89.47	93.87
Au_{42}-$TeHC_6H_4CF_3$	2.76	2.13	89.86	94.90
Au_{42}-$TeHC_6H_4CN$	2.77	2.12	87.69	91.56
Au_{42}-$TeHC_6H_4NO_2$	2.79	2.12	88.11	96.98

a The nomenclature used on the column headings for the definition of the geometric parameters is detailed in Figure 2 from the manuscript.

Table S3. Selected geometric parameters for the anionic *para* substituted selenophenolate-gold complexes[a] (distances in Å and angles in deg).

Au_{42}-Selenophenolate (Se^-)	**D_1**	**D_2**	**$D_{C\text{-}Se}$**	**α**	**β**
Au_{42}-$SeC_6H_4NH_2$	2.61	2.59	1.96	67.7	89.9
Au_{42}-$SeC_6H_4OCH_3$	2.60	2.63	1.96	67.3	88.1
Au_{42}-$SeC_6H_4CH_3$	2.60	2.60	1.97	67.6	90.3
Au_{42}-SeC_6H_5	2.62	2.59	1.97	67.5	90.7
Au_{42}-SeC_6H_4F	2.61	2.59	1.97	67.6	88.7
Au_{42}-SeC_6H_4Cl	2.62	2.60	1.97	67.4	89.3
Au_{42}-$SeC_6H_4OCOCH_3$	2.63	2.60	1.97	67.3	90.2
Au_{42}-$SeC_6H_4CF_3$	2.63	2.60	1.96	67.4	88.2
Au_{42}-SeC_6H_4CN	2.62	2.61	1.96	67.3	92.1
Au_{42}-$SeC_6H_4NO_2$	2.64	2.60	1.96	67.0	89.1

a The nomenclature used on the column headings for the definition of the geometric parameters is detailed on Figure 3 from the manuscript.

Table S4. Selected geometric parameters for the anionic *para* substituted telurophenolates-gold complexes[a] (distances in Å and angles in deg).

Au_{42}-Telurophenolate (Te^-)	**D_1**	**D_2**	**D_{C-Te}**	**α**	**β**
Au_{42}-$TeC_6H_4NH_2$	2.70	2.72	2.16	64,69	87.40
Au_{42}-$TeC_6H_4OCH_3$	2.69	2.73	2.17	64,55	85.16
Au_{42}-$TeC_6H_4CH_3$	2.70	2.72	2.17	64,65	88.74
Au_{42}-TeC_6H_5	2.70	2.71	2.17	64,70	89.51
Au_{42}-TeC_6H_4F	2.70	2.71	2.17	64,80	86.06
Au_{42}-TeC_6H_4Cl	2.70	2.71	2.17	64,71	85.19
Au_{42}-$TeC_6H_4OCOCH_3$	2.70	2.71	2.17	64,66	88.74
Au_{42}-$TeC_6H_4CF_3$	2.68	2.71	2.17	65,03	80.81
Au_{42}-TeC_6H_4CN	2.71	2.72	2.17	64,54	92.22
Au_{42}-$TeC_6H_4NO_2$	2.70	2.71	2.17	64,66	85.42

a The nomenclature used on the column headings for the definition of the geometric parameters is detailed on Figure 3 from the manuscript.

Table S5. Selected geometric parameters for the radical *para* substituted selenophenolate-gold complexes[a] (distances in Å and angles in deg).

Au_{42}-Selenophenolate ($Se^{\bullet}$)	**D_1**	**D_2**	**$D_{C\text{-}Se}$**	**α**	**β**
Au_{42}-$SeC_6H_4NH_2$	2.58	2.60	1.96	68.0	90.0
Au_{42}-$SeC_6H_4OCH_3$	2.59	2.62	1.96	67.4	87.9
Au_{42}-$SeC_6H_4CH_3$	2.60	2.58	1.97	68.0	90.2
Au_{42}-SeC_6H_5	2.59	2.59	1.97	67.9	89.6
Au_{42}-SeC_6H_4F	2.59	2.59	1.97	67.9	88.6
Au_{42}-SeC_6H_4Cl	2.60	2.60	1.97	67.7	89.1
Au_{42}-$SeC_6H_4OCOCH_3$	2.60	2.60	1.97	67.7	89.5
Au_{42}-$SeC_6H_4CF_3$	2.60	2.60	1.97	67.7	87.1
Au_{42}-SeC_6H_4CN	2.62	2.58	1.97	67.6	90.7
Au_{42}-$SeC_6H_4NO_2$	2.60	2.60	1.96	67.5	87.6

a The nomenclature used on the column headings for the definition of the geometric parameters is detailed on Figure 3 from the manuscript.

Table S6. Selected geometric parameters for the radical *para* substituted telurophenolates-gold complexes[a] (distances in Å and angles in deg).

Au_{42}-Telurophenolate ($Te^{\bullet}$)	**D_1**	**D_2**	**$D_{C\text{-}Te}$**	**α**	**β**
Au_{42}-$TeC_6H_4NH_2$	2.69	2.72	2.16	64.73	89.46
Au_{42}-$TeC_6H_4OCH_3$	2.70	2.71	2.17	64.73	88.00
Au_{42}-$TeC_6H_4CH_3$	2.69	2.72	2.17	64.70	88.89
Au_{42}-TeC_6H_5	2.70	2.71	2.17	64.76	89.03
Au_{42}-TeC_6H_4F	2.69	2.71	2.17	64.80	86.53
Au_{42}-TeC_6H_4Cl	2.70	2.71	2.17	64.68	86.99
Au_{42}-$TeC_6H_4OCOCH_3$	2.70	2.72	2.17	64.68	88.36
Au_{42}-$TeC_6H_4CF_3$	2.70	2.72	2.17	64.67	82.37
Au_{42}-TeC_6H_4CN	2.69	2.73	2.17	64.60	89.25
Au_{42}-$TeC_6H_4NO_2$	2.71	2.72	2.17	64.52	83.53

a The nomenclature used on the column headings for the definition of the geometric parameters is detailed on Figure 3 from the manuscript.

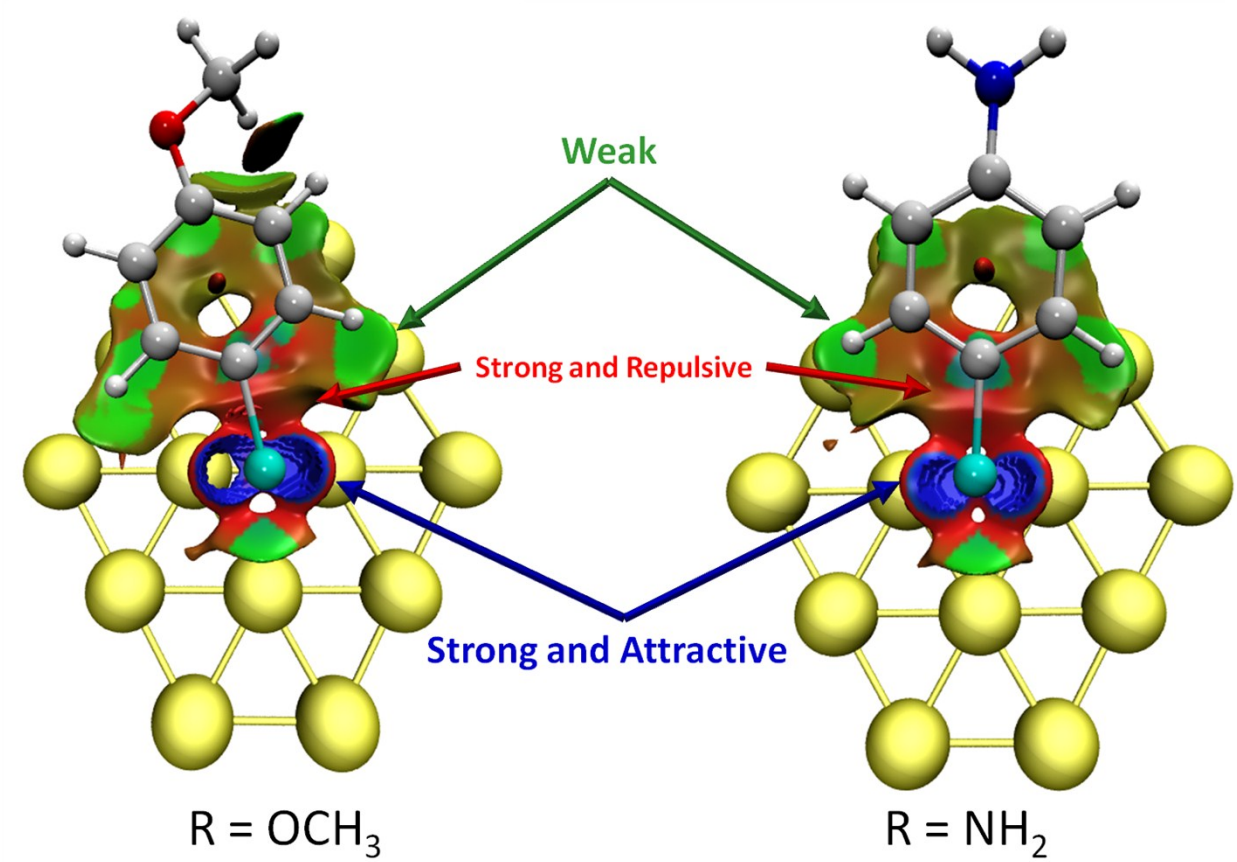

Figure S1. Graphical representation of the non-covalent interactions between the radical ligands (carbon-grey, nitrogen-blue, hydrogen-white, cyan-chalcogen spheres) and the gold surface (yellow spheres). At the left side there is the ligand with the strongest interaction strength ($-OCH_3$) and at the right side of the picture the ligand with the weakest ($-NH_2$).