

## Supporting Information<sup>†</sup>

# Inverse-Micelle-Encapsulated Water-Enabled Bond Breaking of Dialkyl-Diselenide/Disulfide: a Critical Step for Synthesizing High-Quality Au Nanoparticles

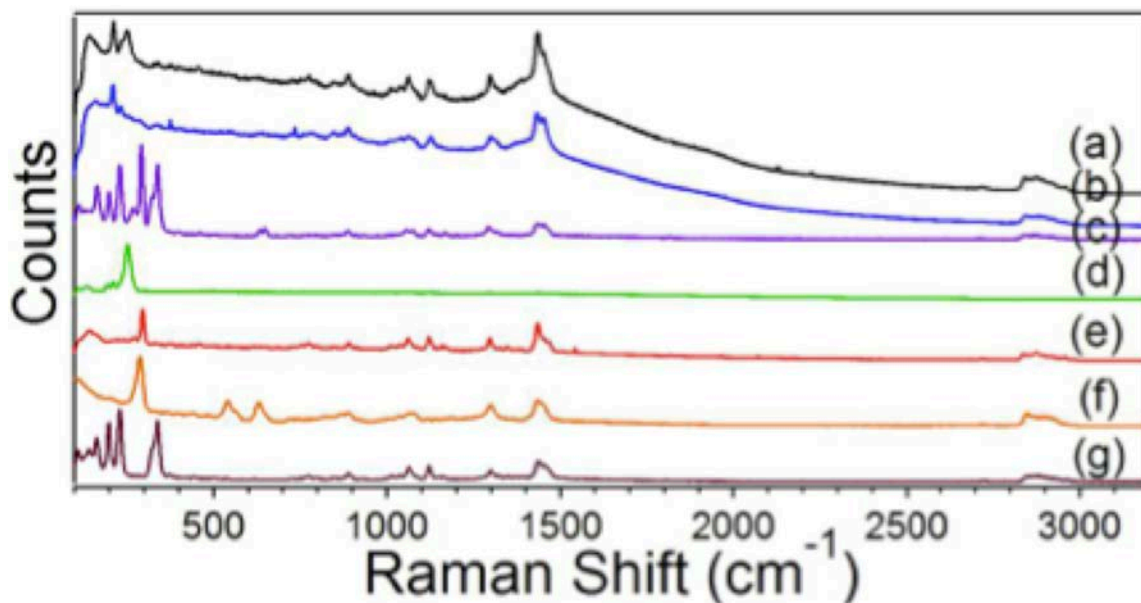
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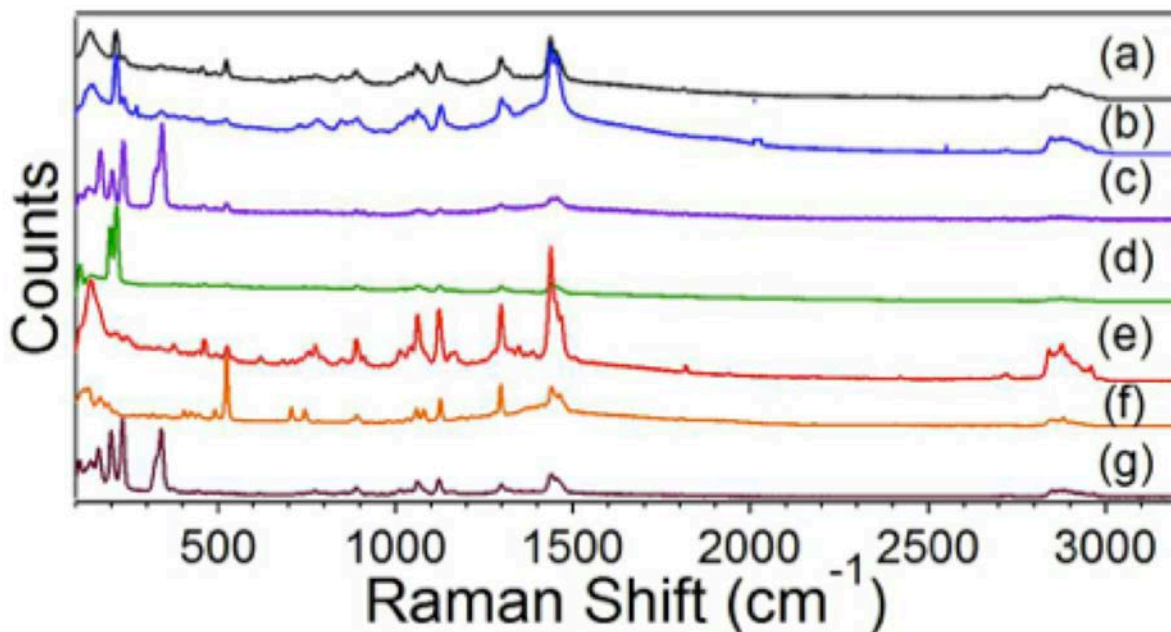
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### Figures:

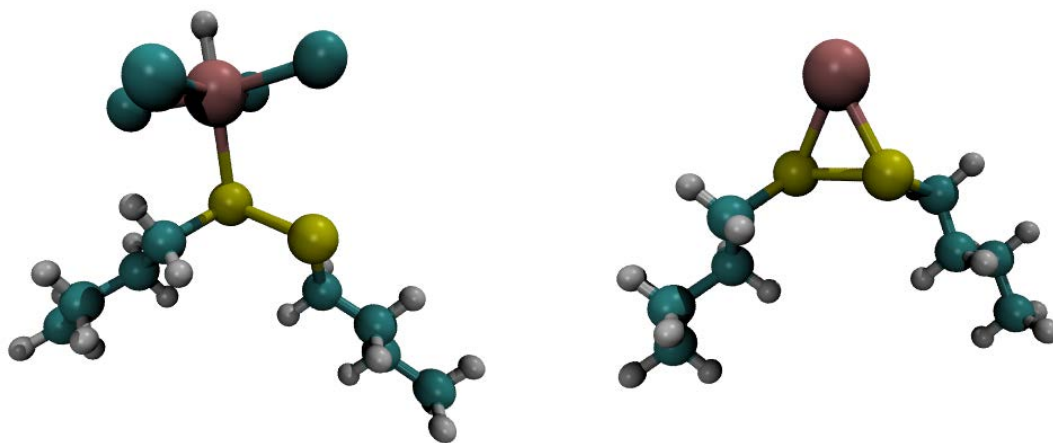


**Figure S1.** Full Raman spectra of the intermediate solutions with the same Au:Se ratio = 1:1 but different TOAB: Au ratios: (a) 3:1 (TAuSe-311), (b) 2:1 (TAuSe-211), and (c) 1:1 (TAuSe-111); (d) 3:1 but with [TOA][AuBr<sub>4</sub>] : 2TOAB : 0.5(C<sub>12</sub>H<sub>25</sub>Se)<sub>2</sub> (TAuSe-311C), and of reference materials: (e) 3TOAB : 0.5(C<sub>12</sub>H<sub>25</sub>Se)<sub>2</sub> (TAuSe-301), (f) (C<sub>12</sub>H<sub>25</sub>Se)<sub>2</sub> (TAuSe-001), and (g) 3TOAB : 1HAuCl<sub>4</sub> (TAuSe-310).

<sup>†</sup> Certain commercial equipment, instruments, or materials are identified in this paper in order to specify the experimental procedure adequately. Such identification is not intended to imply recommendation or endorsement by the National Institute of Standards and Technology, nor is it intended to imply that the materials or equipment identified are necessarily the best available for the purpose.



**Figure S2.** Full Raman spectra of the intermediate solutions with the same Au:S ratio = 1:1 but different TOAB:Au ratios: (a) 3:1 (TAuS-311), (b) 2:1 (TAuS-211), and (c) 1:1 (TAuS-111), (d) 3:1 but with [TOA][AuBr<sub>4</sub>] : 2TOAB : 0.5 (C<sub>12</sub>H<sub>25</sub>S)<sub>2</sub> (TAuS-311C), and of reference materials: (e) 3TOAB : 0.5 (C<sub>12</sub>H<sub>25</sub>S)<sub>2</sub> (TAuS-301), (f) (C<sub>12</sub>H<sub>25</sub>S)<sub>2</sub> (TAuS-001), and (g) 3TOAB : 1HAuCl<sub>4</sub> (TAuS-310).



a

b

**Figure S3.** Geometrically optimized molecular structures by the DFT calculations: (a) [HAu(III)Br<sub>4</sub>](SeC<sub>4</sub>H<sub>9</sub>)<sub>2</sub> and (b) Au(III)(SeC<sub>4</sub>H<sub>9</sub>)<sub>2</sub>. Se is depicted in yellow, Au in the reddish color, and Br in the bluish color; the alkyl chains are bonded to the Se atoms and are clearly distinguishable.

**Table 1.** Cartesian coordinates [ $\text{\AA}$ ] of  $[\text{Au(III)Br}_4]^- (\text{SeC}_4\text{H}_9)_2$  and  $\text{Au(III)} (\text{SeC}_4\text{H}_9)_2$ . $[\text{Au(III)Br}_4]^- (\text{SeC}_4\text{H}_9)_2$ 

Au	-2.1575475297	2.7558832098	1.6946769655
Br	-0.9668121945	3.4720319520	3.7463332478
Br	-0.0973018392	3.1897519555	0.3861771740
Br	-3.4286370269	2.3462738821	-0.3927718165
Br	-4.2594142360	2.6115042407	2.9838605433
Se	-3.1091017614	-0.9945864563	2.8571951755
Se	-1.2622254670	0.2820736435	2.0936515362
C	-2.0663195153	-2.4029897464	3.8207683796
H	-1.4944563233	-1.9034272400	4.6108376339
H	-1.3774154647	-2.8682371018	3.1071359639
C	-3.0468087964	-3.4228455290	4.3989073956
H	-3.5925093588	-3.9186717974	3.5812503172
H	-3.7989798069	-2.9063827795	5.0158239387
C	-2.3370766502	-4.4832225572	5.2567095544
H	-1.8043884415	-3.9823257556	6.0802076485
H	-1.5683417766	-4.9874412796	4.6497682615
C	-3.3055802348	-5.5234525099	5.8270914447
H	-4.0664219746	-5.0497236116	6.4649478755
H	-2.7742183175	-6.2673822988	6.4365315238
H	-3.8296371825	-6.0612641500	5.0231921870
C	-1.0256268957	-0.3766482929	0.2156153113
H	-1.2352587287	0.4893670468	-0.4187891545
H	-1.8064990476	-1.1299936127	0.0696693758
C	0.3799733088	-0.9271022028	-0.0015761134
H	0.5675347490	-1.7692155523	0.6824413200
H	1.1182118833	-0.1482863544	0.2401671049
C	0.5807170386	-1.3872427836	-1.4539108539
H	0.3814870776	-0.5411672074	-2.1298565125
H	-0.1648369757	-2.1609993433	-1.6974840374
C	1.9887440926	-1.9326720577	-1.7112294040
H	2.2021939224	-2.8020519990	-1.0715280590
H	2.7534573308	-1.1691469724	-1.5058090846
H	2.1042297398	-2.2497648742	-2.7569174016
H	-2.5400592928	4.1554730388	1.5105953035

 $\text{Au(III)} (\text{SeC}_4\text{H}_9)_2$ 

Au	-1.1304697915	-0.0155770632	6.1527303617
Se	-2.6390764314	-1.5206744879	4.8559708579
Se	-0.5023868881	-0.8488045543	3.9391788294
C	-2.5475869169	-3.5263365174	5.2255003355
H	-2.9521635368	-3.6026252991	6.2441084205
H	-1.5017403434	-3.8477297987	5.1787154546
C	-3.4750269887	-4.0596721074	4.1454427921
H	-3.0750282677	-3.9612350543	3.1300969318
H	-4.4942127300	-3.6598702670	4.2086179605
C	-3.5909057028	-5.6766142549	4.4775269807
H	-3.9737671844	-5.7496135549	5.5035007570
H	-2.5750383444	-6.0857420949	4.4193849833
C	-4.5291491890	-6.2740527056	3.4559992101
H	-5.5600489619	-5.9054244650	3.5206976186
H	-4.5630439666	-7.3612396640	3.7369305129
H	-4.1578889075	-6.2459591214	2.4234015661
C	-0.80171119747	0.3626076361	2.3159053138

H	-0.1121686895	1.1921746374	2.5258000408
H	-1.8455209822	0.6942047873	2.3055162462
C	-0.3593034251	-0.5411625917	1.1789721683
H	-1.0524326295	-1.3657707730	0.9781728720
H	0.6679668041	-0.9108009928	1.2860836084
C	-0.3567680809	0.4471526567	-0.1392319964
H	0.3403541305	1.2624067260	0.0929763485
H	-1.3748340158	0.8398966990	-0.2517028186
C	0.0846284385	-0.3815445513	-1.3240257389
H	-0.6168856819	-1.1761226470	-1.6094120648
H	1.1099432598	-0.7637246381	-1.2482220292
H	0.0807730357	0.3481236046	-2.1768094653