Supporting Information

Pd$_2$Au$_{36}$(SR)$_{24}$ cluster: structure studies

Bei Zhang$^a$, Sameh Kaziz$^b$, Houhua Li$^c$, Dawid Wodka$^a$, Sami Malola$^{a,†}$, Olga Safonova$^a$, Maarten Nachtegaal$^e$, Clément Mazet$^c$, Igor Dolamic$^a$, Jordi Llorca$^f$, Elina Kalenius$^{d,‡}$, Latévi Max Lawson Daku$^a$, Hannu Hakkinen$^{a,†}$, Thomas Bürgi$^{a,*}$ and Noelia Barrabés$^{a,*}$$^†$

$^a$Department of Physical Chemistry, University of Geneva, 30 Quai Ernest-Ansermet, 1211 Geneva 4, Switzerland
$^b$Department of Industrial Engineering, National High School of Engineers of Tunis, Tunis, Tunisia
$^c$Department of Organic Chemistry, University of Geneva, 30 Quai Ernest-Ansermet, 1211 Geneva 4, Switzerland
$^d$Department of Physics and $^{†,‡}$Department of Chemistry, Nanoscience Center, University of Jyväskylä, FI-40014 Jyväskylä, Finland
$^e$Paul Scherrer Institute, 5232 Villigen, Switzerland
$^f$Institute of Energy Technologies and Centre for Research in Nano Engineering, Technical University of Catalonia, Barcelona, Spain
Experimental Methods

All chemicals were purchased from standard suppliers and used as received. Nanopure water (>18 MΩ) was used.

Synthesis and Isolation of Pd$_2$Au$_{36}$(SCH$_2$CH$_2$Ph)$_{24}$ (enantiomer 2). Pd$_2$Au$_{36}$(SC$_2$H$_4$Ph)$_{24}$ enantiomer 2 is synthesized and separated according to previous method reported by our group.$^1$
Figure S1. (a) MALDI, (b) UV-vis and (c) CD spectra of Pd\textsubscript{2}Au\textsubscript{36}(SC\textsubscript{2}H\textsubscript{4}Ph)\textsubscript{24} enantiomer 2.

Figure S2. Positive polarization ESI-MS spectrum of [Pd\textsubscript{2}Au\textsubscript{36}(SC\textsubscript{2}H\textsubscript{4}Ph)\textsubscript{24} + Cs]\textsuperscript{+}. black: experimental, red: theoretical isotropic distribution
Scheme S1. Optimized structures for two staples doped Pd$_2$Au$_{36}$(SCH$_2$CH$_2$Ph)$_{24}$ models. R group is omitted for the sake of simplicity. Key: red = Pd; yellow = Au; green = S

Figure S3. Theoretical (a) optical absorption and (b) CD spectra of two staple doped models
Figure S4. Theoretical CD spectra of different doped Pd atoms locations in Pd$_2$Au$_{36}$(SCH$_2$CH$_2$Ph)$_{24}$

Figure S5. Theoretical and Experimental CD spectra of Au$_{36}$(SCH$_2$CH$_2$Ph)$_{24}$
Table S1. Pd K-edge EXAFS Analysis for the Pd$_2$Au$_{36}$(SC$_2$H$_4$Ph)$_{24}$ staple and core doped mixture

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Scheme S2. Optimized staples doped Pd$_2$Au$_{36}$(SCH$_2$CH$_2$Ph)$_{24}$ models for EXAFS fitting. R group is omitted for the sake of simplicity. Key: red = Pd; yellow = Au; green = S
**Figure S6.** EXAFS spectra of Pd$_2$Au$_{36}$(SC$_2$H$_4$Ph)$_{24}$ in R space: experimental and theoretical surface doped model

**Figure S7.** Simulated Pd K-edge EXAFS spectra in R space for two staple doped Pd$_2$Au$_{36}$(SC$_2$H$_4$)$_{24}$ models.

**References**

Optimized Coordination for core doped Pd$_2$Au$_{36}$(SC$_2$H$_4$Ph)$_{24}^{(2)}$

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3 Au     18.3444  19.2245  16.2862
4 Au     17.1998  21.6848  17.0878
5 Au     19.6451  21.3982  15.1241
6 Au     22.3317  20.4114  18.8988
7 Au     15.7264  19.2076  17.4877
8 Au     19.7203  20.9871  17.9474
9 Au     17.4077  20.3172  19.5254
10 Au    15.6832  18.4004  20.4913
11 Au    16.7901  16.98  16.0009
12 Au    21.1805  19.2071  16.3991
13 Au    20.3981  18.4778  19.0637
14 Au    20.0206  20.7047  20.6792
15 Au    21.0612  23.0091  19.3276
16 Au    19.725  16.7862  16.8614
17 Au    19.709  15.8822  19.6124
18 Au    19.403  23.5038  16.8775
19 Au    18.0885  18.8017  13.4757
20 Au    15.1249  16.6039  18.4878
21 Au    22.0176  21.9826  16.6011
22 Au    18.496  18.2198  21.1238
23 Au    15.0811  14.5057  16.009
24 Au    18.3064  22.911  19.6021
25 Au    17.5252  23.6864  14.5956
26 Au    17.0998  15.7993  20.5159
27 Au    18.4097  14.5146  14.8989
28 Au    12.9978  18.6768  19.0886
29 Au    21.0596  23.8117  14.2767
30 Au    17.6924  14.9926  17.7087
31 Au    18.5931  13.1877  20.1868
32 Pd    15.9226  21.5994  21.3726
34 Au    19.9887  23.6757  22.0782
35 Pd    24.0324  19.9722  16.6912
36 Au    19.2744  15.5146  22.602
37 Au    14.0073  16.0966  21.2962
38 Au    24.0998  22.8054  18.4897
39 Au    22.8088  17.2983  20.0827
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41 S 16.3808 13.5775 14.3511  
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48 S 23.1889 23.1915 14.9069  
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50 S 25.6036 21.2954 17.651  
51 S 12.2512 17.5285 20.9263  
52 S 13.5498 15.0774 17.635  
53 S 14.8487 19.803 22.1827  
54 S 15.6206 14.5381 21.8334  
55 S 19.9653 25.8765 21.4262  
56 S 18.9234 25.8193 16.9562  
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