Supporting Information

Aggregation-free Gold Nanoparticles in Ordered Mesoporous Carbons: Towards Highly Active and Stable Heterogeneous Catalysts

Shuai Wang[†], Qingfei Zhao[†], Huimin Wei[†], Jian-Qiang Wang[‡], Minhyung Cho[§], Hae Sung Cho[§], Osamu Terasaki[§], Ying Wan^{*†}

[†] The Education Ministry Key Lab of Resource Chemistry, Shanghai Key Laboratory of Rare Earth Functional Materials, and Department of Chemistry, Shanghai Normal University, Shanghai 200234,

P. R. China; [‡]Shanghai Synchrotron Radiation Facility (SSRF), Shanghai Institute of Applied Physics, Chinese Academy of Sciences, Shanghai, 201204, P. R. China; [§]Graduate School of EEWS (WCU), Korea Advanced Institute of Science and Technology, Daejeon, 305-701, Republic of Korea

* To whom correspondence should be addressed. Tel: 86-21-6432-2516; Fax: 86-21-6432-2511; E-mail: ywan@shnu.edu.cn

Preparation of low-polymerized phenolic resins.

8.0 g of phenol was melted at 42 - 45 °C in a flask and mixed with 1.7 g of 20 *wt*% NaOH aqueous solution under stirring. After 10 min, 14.16 g of formalin (37 *wt*% formaldehyde) was added. Then the mixture was heated to 70 °C. Upon further stirring for 1 h at this temperature, the mixture was cooled to room temperature. The PH value was adjusted with 2 M HCl solution until it reached a value of ~ 7.0. Subsequently, water was removed by vacuum evaporation below 50 °C.

SI Table S1. Oxidation of benzyl alcohol in water using Au based or bimetallic Au-Pd based supported catalysts.

Catalyst	Au:substrate /mol: mol	Solvent	T / $^{\circ}C$	P /atm	t / h	Conv. %	Sel. % (acid)	TON/h ⁻¹ (initial rate/total Au concentration)	Ref.
Au/SBA-15	1:400	water	80 (MW)		1	100	91	not provided	1
Au-Pd/SBA-15	1:120 ^a	decane/ water	80	1	8	40	97 (aldehyde)	12 ^a	2
Au60-Pd40/C	1:20000	cyclo- hexane /water	60	1.5	4	90	98 (aldehyde)	7600 ^b	3
Au/PVP	1:50	water	RT	1	6	95	91	not provided	4
Au/PoPD	1:33.3	water	RT	1	24	99	99	not provided	5
Au/C	1:1600	water	90	10	1	> 99	> 99	4512 ^c	this work
Au/C	1:1600	water	60	1	12	> 99	> 99	384 ^d	this work

a: Not provided. Calculated on the basis of the experimental data, and assumed that gold species were completely loaded on the support. Measured after 2 h of reaction.

b: Not provided. Calculated on the basis of the experimental data. Measured after 30 min of reaction.

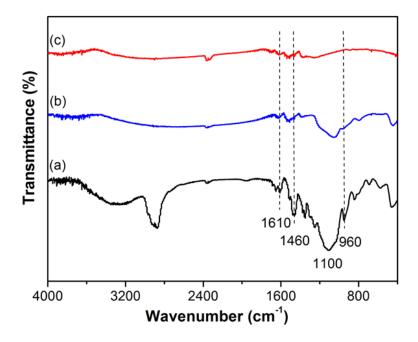
c: Measured after 10 min of reaction.

d: Measured after 30 min of reaction.

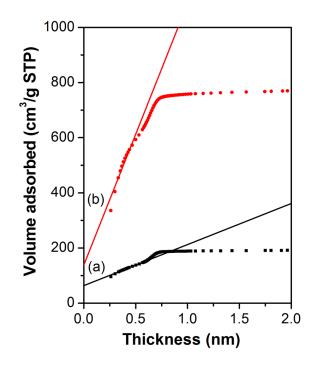
Reference:

- (1) Liu, Y.; Tsunoyama, H.; Akita, T.; Tsukuda, T. J. Phys. Chem. C 2009, 113, 13457.
- (2) Ma, C. Y.; Dou, B. J.; Li, J. J.; Cheng, J.; Hu, Q.; Hao, Z. P.; Qiao, S. Z. Appl. Catal., B 2009, 92, 202.
- (3) Villa, A.; Janjic, N.; Spontoni, P.; Wang, D.; Su, D. S.; Prati, L. Appl. Catal., A 2009, 364, 221.
- (4) Tsunoyama, H.; Sakurai, H.; Negishi, Y.; Tsukuda, T. J. Am. Chem. Soc. 2005, 127, 9374.
- (5) Han, J.; Liu, Y.; Guo, R. Adv. Funct. Mater. 2009, 19, 1112.

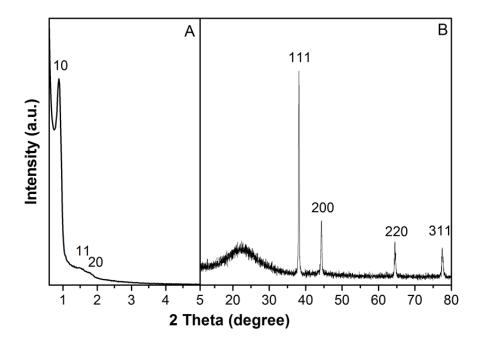
SI Figure S1. FT-IR spectra for (a) as-made gold-containing mesoporous catalysts synthesized by solvent evaporation induced self-assembly (as-made Au(SH)-SC); (b) the catalyst calcined at 600 °C (Au(SH)-SC); and (c) the Au(SH)-SC catalyst after dissolution of silica (Au(SH)-C).



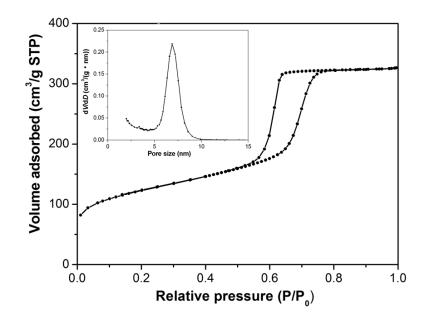
SI Figure S2. *t*-plots for (a) Au(SH)-CS and (b) Au(SH)-C.



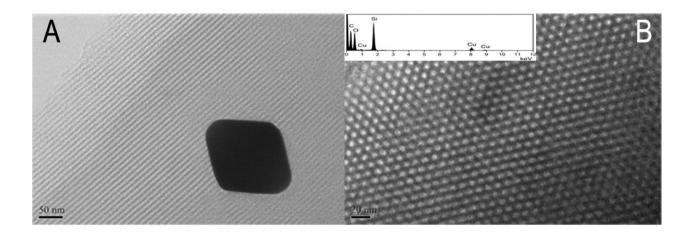
SI Figure S3. SAXRD (A) and WAXRD (B) patterns for the thiol-free sample Au(0)-SC.



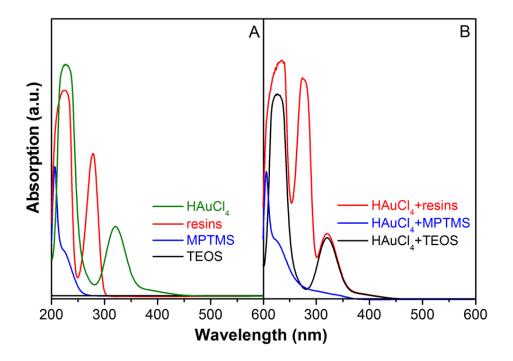
SI Figure S4. N₂ sorption isotherms and pore-size distribution curve (inset) for the thiol-free sample Au(0)-SC.



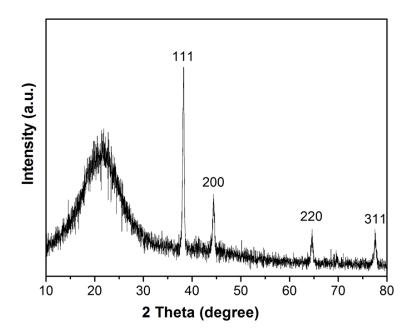
SI Figure S5. TEM images for Au(0)-SC heated at 600 °C with low (A) and high (B) magnifications . Inset (B) is EDX pattern.



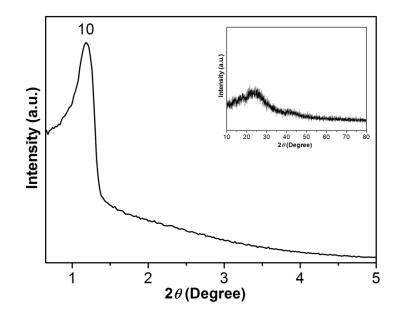
SI Figure S6. UV-vis spectra for mono-constituent (A) and bi-constituent (B) synthesis solutions in ethanol.



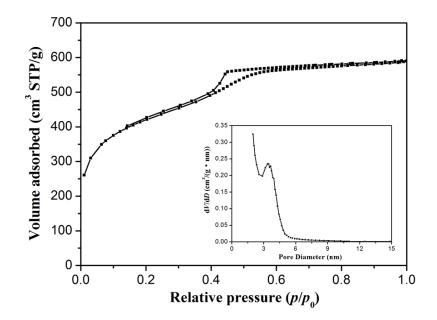
SI Figure S7. WAXRD pattern for as-made Au(0)-SC.



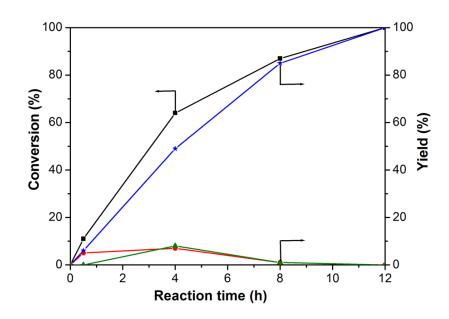
SI Figure S8. SAXRD and WAXRD (inset) patterns for the gold-free sample (SH)-C.



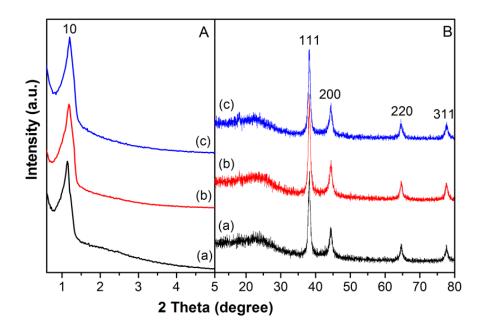
SI Figure S9. N₂ sorption isotherms and pore-size distribution curve (inset) for the gold-free sample (SH)-C.



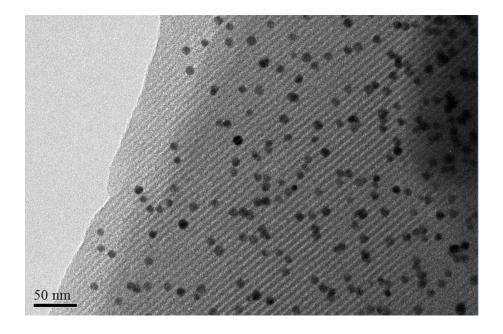
SI Figure S10. Time course plots for the conversion of benzyl alcohol (- \blacksquare -) and yields of benzoic acid (-★-), benzaldehyde (- \bullet -), and benzyl benzoate (-▲-) over the reused catalyst Au(SH)-C-R2.



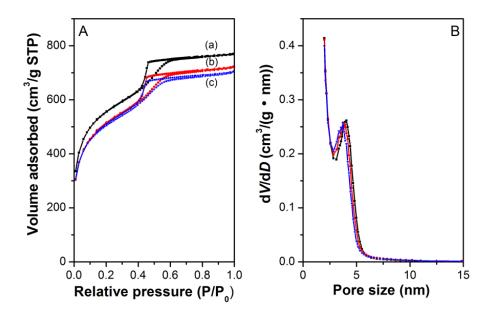
SI Figure S11. SAXRD (A) and WAXRD (B) patterns for the (a) fresh Au(SH)-C catalyst, and the catalysts after (b) the first run (Au(SH)-C-R2) and (c) third run (Au(SH)-C-R4).



SI Figure S12. TEM image for the reused catalyst Au(SH)-C-R2.



SI Figure S13. N_2 sorption isotherms (A) and pore-size distribution curves (B) for the (a) fresh Au(SH)-C-600 catalyst, and the catalysts after (b) the first run (Au(SH)-C-600-R2) and (c) third run (Au(SH)-C-R4).



SI Figure S14. TEM image (A), and WAXRD pattern (B) for the supported 5.0 nm-gold catalyst.

