Supplementary Materials

Sustainable Hydrogenation of Vinyl Derivatives Using Pd/C Catalysts

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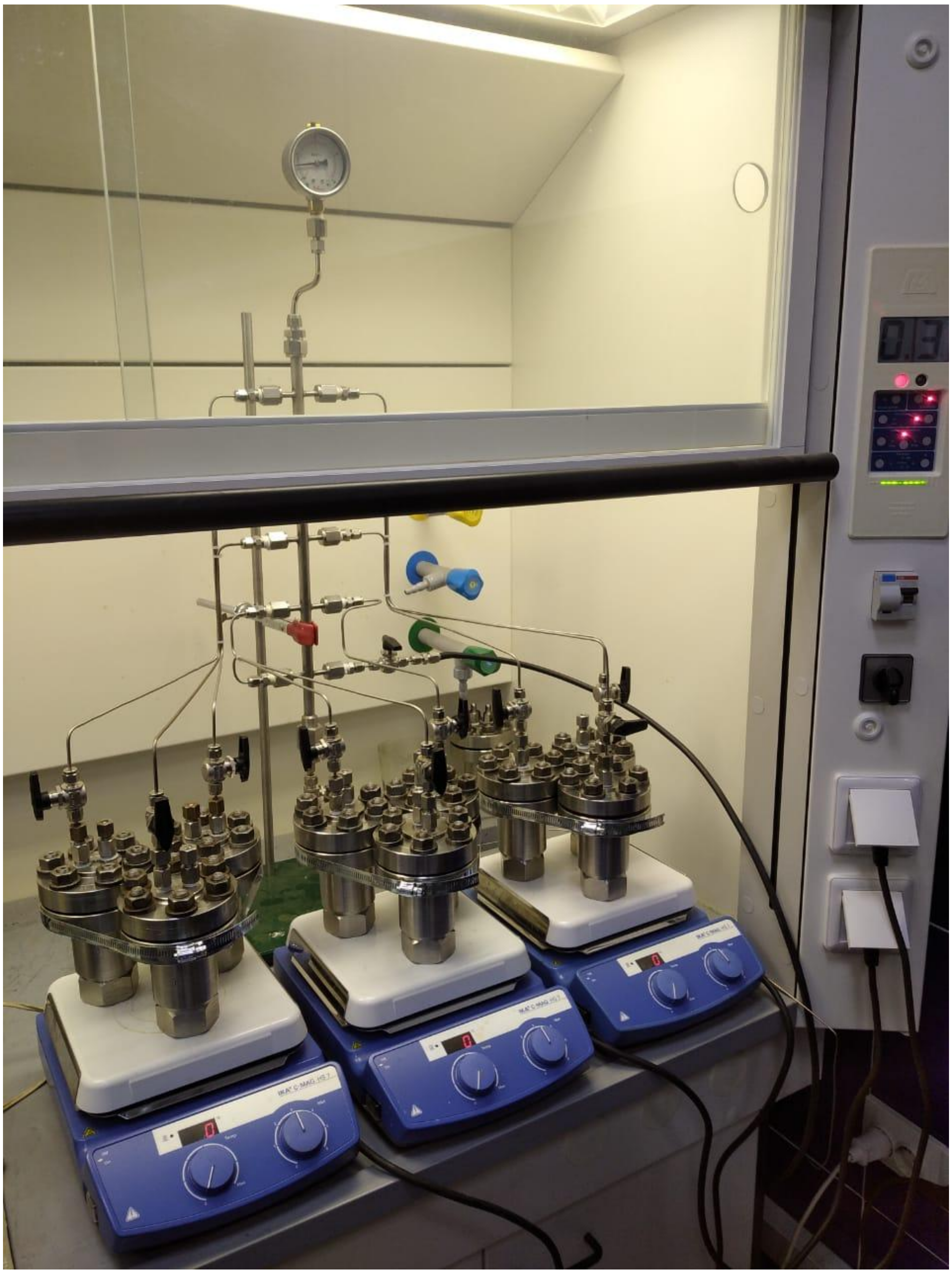


Figure S1. Multi-reactor setup used for liquid-phase hydrogenation of vinyl derivatives under hydrogen pressure.

TEM images of Pd/C catalysts.

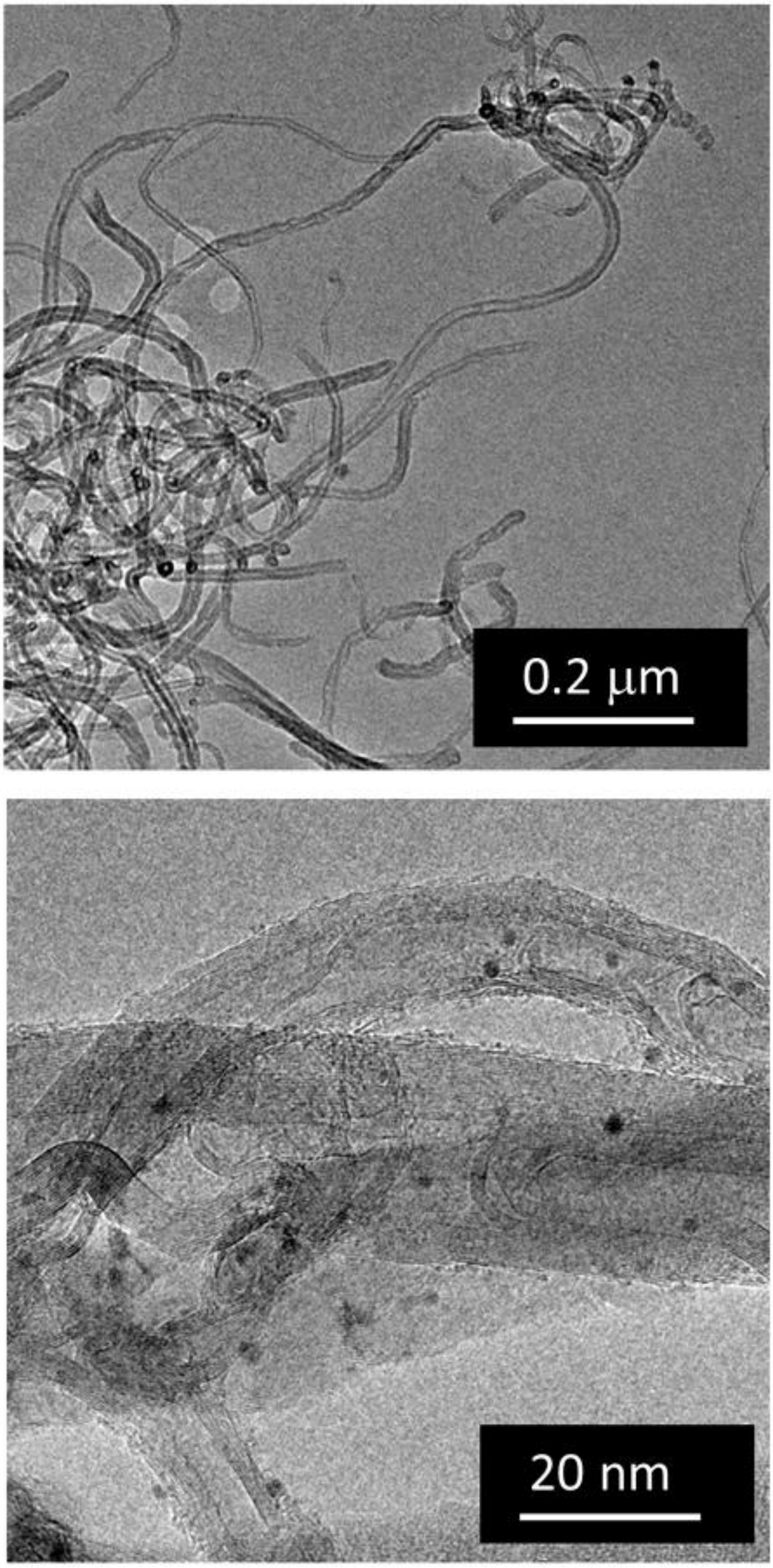


Figure S2. TEM images of 2% Pd-CCs/MWCNTs catalyst. See also Fig. 1a.

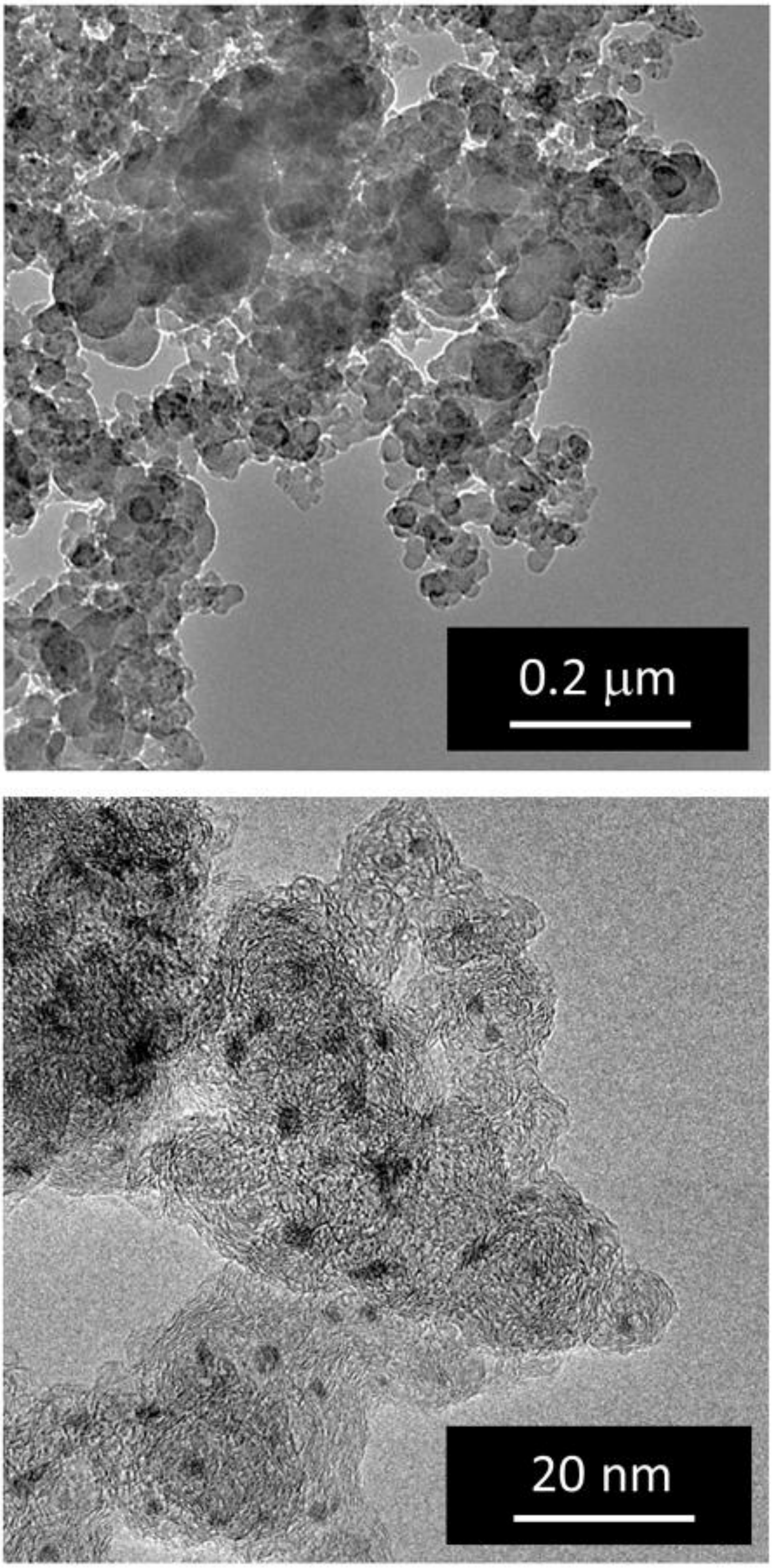


Figure S3. TEM images of 2% Pd-CCs/P278-E catalyst. See also Fig. 1b.

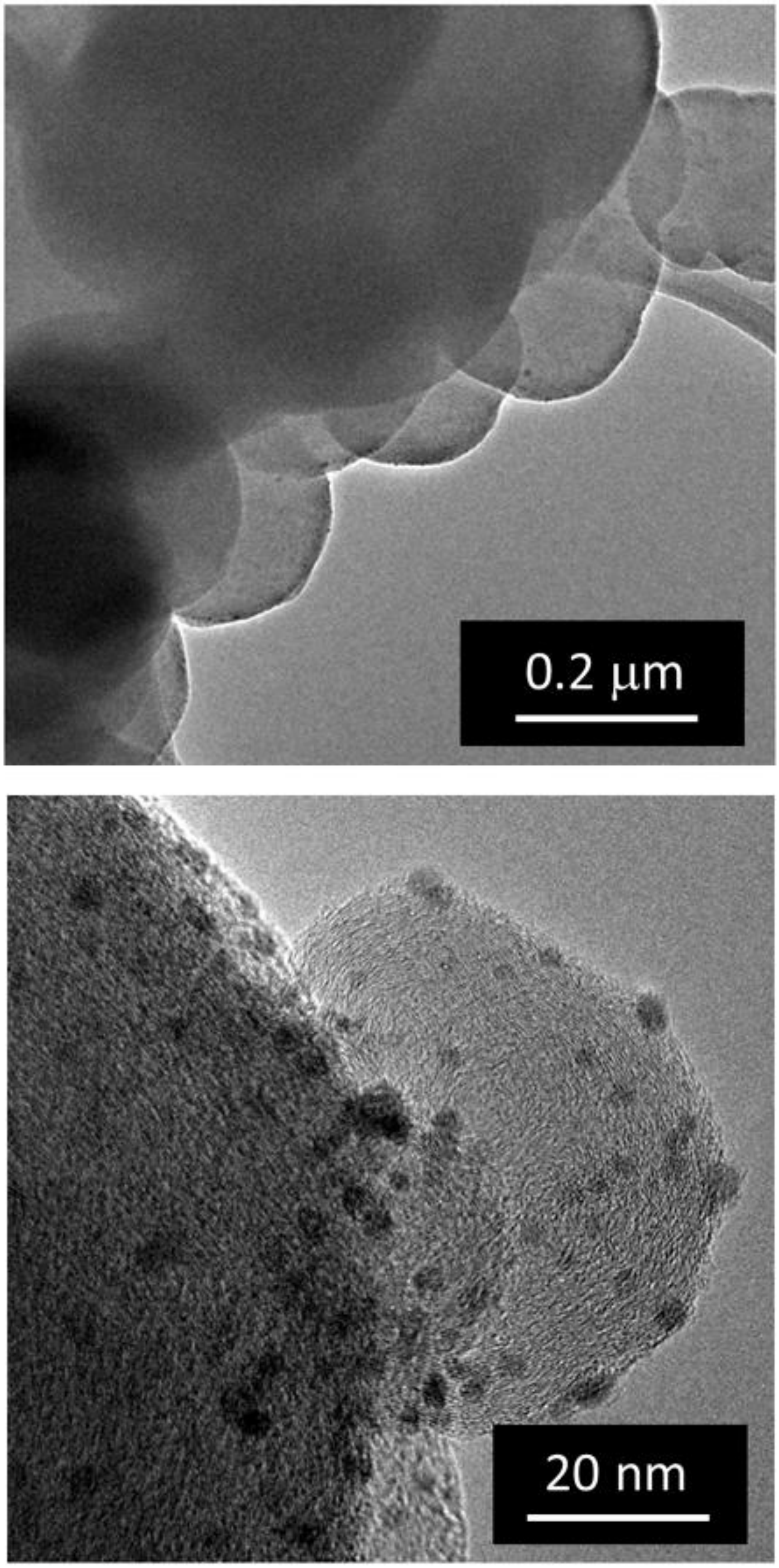


Figure S4. TEM images of 2% Pd-CCs/T900 catalyst. See also Fig. 1c.

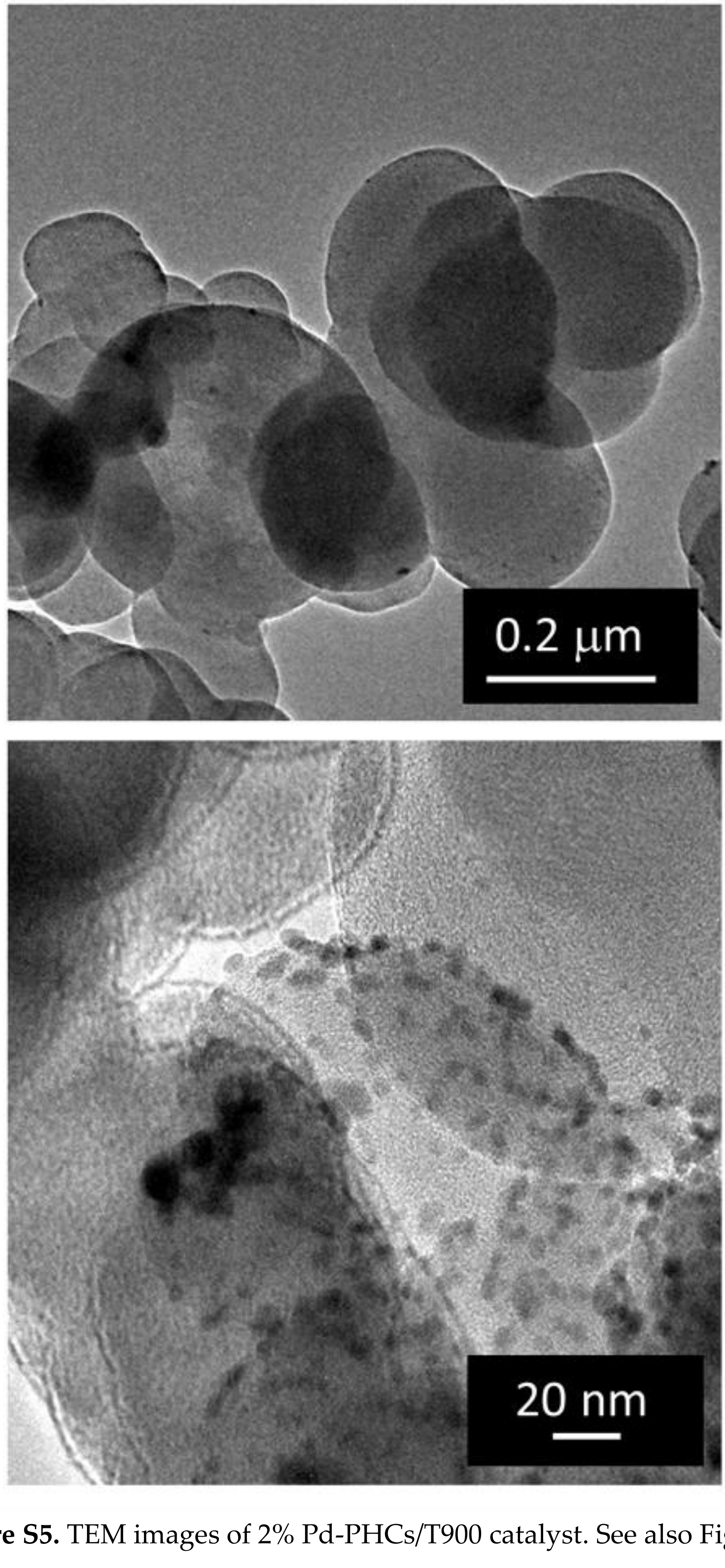


Figure S5. TEM images of 2% Pd-PHCs/T900 catalyst. See also Fig. 1d.

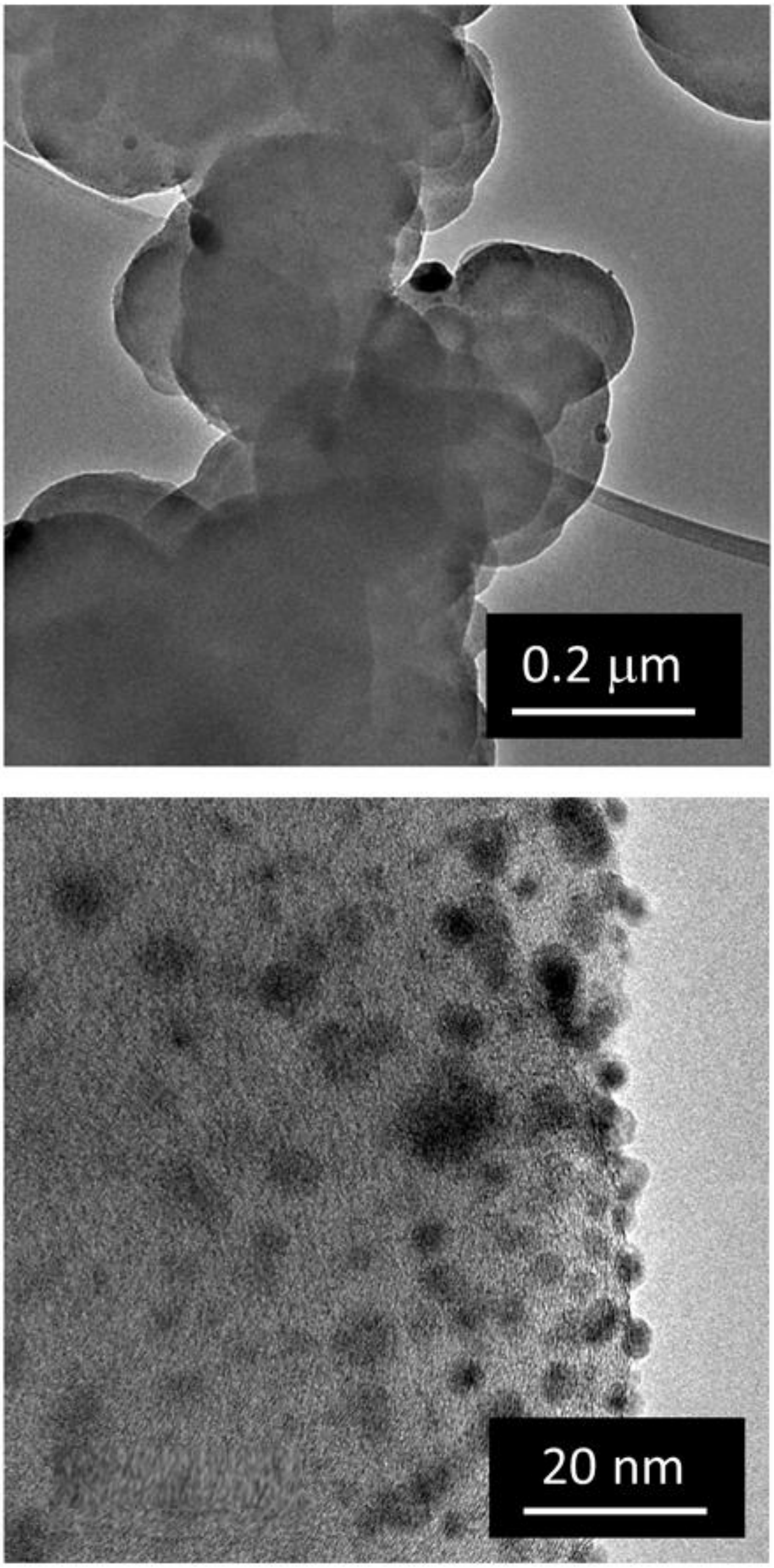


Figure S6. TEM images of 2% Pd-Ac/T900 catalyst. See also Fig. 1e.

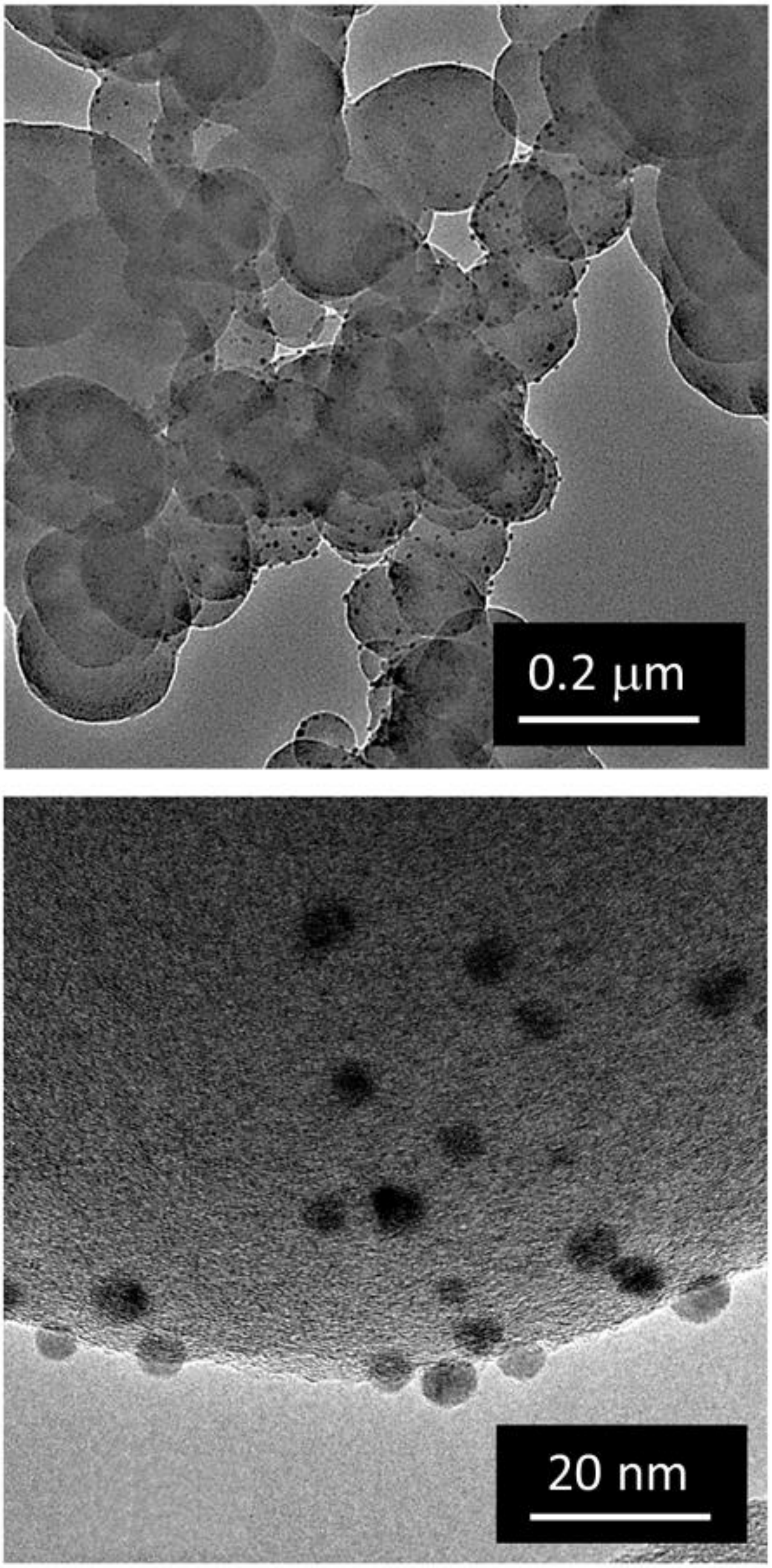


Figure S7. TEM images of 2% Pd-dba/T900 catalyst. See also Fig. 1f.

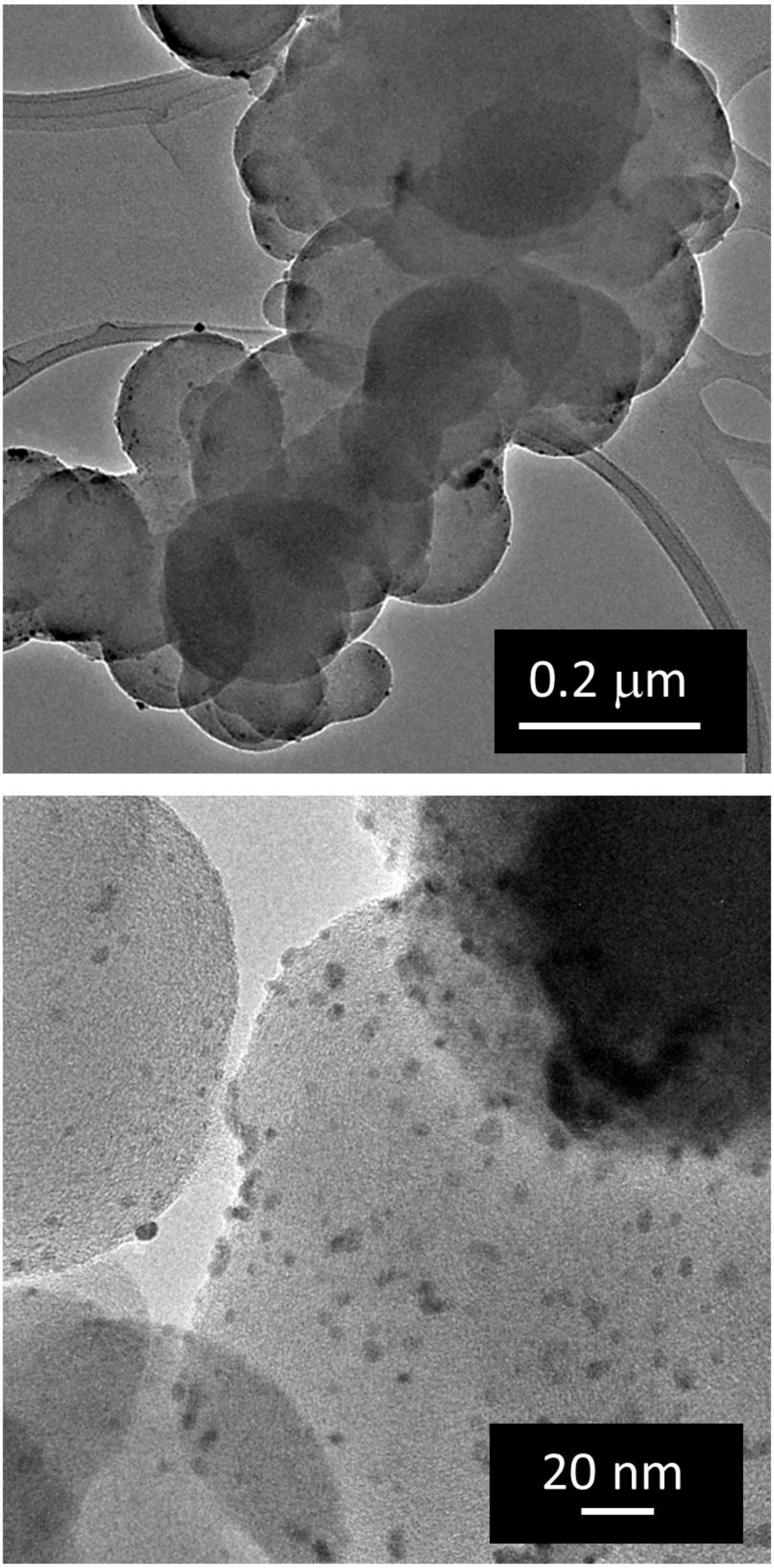
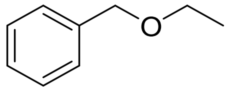


Figure S8. TEM images of the spent 2% Pd-PHCs/T900 catalyst after five cycles of the NVE hydrogenation.

Identification of the hydrogenation products.

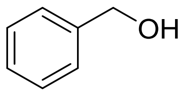
Benzyl ethyl ether (BEE).



^{1}H NMR (400 MHz, MeOH), δ_H/ppm: 6.95-6.85 (m, 5H), 4.09 (s, 2H), 3.15 (q, *J* = 7.0 Hz, 2H), 0.82 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, MeOH), δ_C/ppm: 138.6, 128.4, 127.9, 127.7, 72.7, 65.8, 14.4. MS (EI, 70 eV), *m*/*z* (I_{rel}/%): 136 (7) M$^+$, 135 (11), 107 (17), 105 (5), 92 (84), 91 (100), 89 (5), 79 (34), 77 (19), 65 (16), 51 (9).

The spectral data obtained are in agreement with those previously reported [1-3].

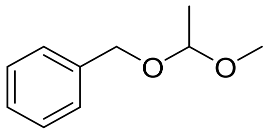
Benzyl alcohol (BAL).



^{1}H NMR (400 MHz, MeOH), δ_H/ppm: 6.82-6.96 (m, 5H), 4.20 (s, 2H). ^{13}C NMR (101 MHz, MeOH), δ_C/ppm: 141.7, 128.3, 127.3, 127.0, 64.4. MS (EI, 70 eV), *m*/*z* (I_{rel}/%): 108 (84) M$^+$, 107 (59), 106 (7), 105 (10), 92 (23), 91 (42), 90 (9), 89 (10), 80 (10), 79 (100), 78 (14), 77 (70), 65 (11), 63 (8), 53 (7), 52 (8), 51 (24), 50 (11).

The spectral data obtained are in agreement with those previously reported [3, 4].

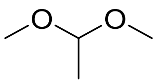
1-Benzyloxy-1-methoxyethane.



^{13}C NMR (101 MHz, MeOH), δ_C/ppm: 128.4, 127.6, 100.7, 67.8, 52.0, 18.7. MS (EI, 70 eV), *m*/*z* (I_{rel}/%): 134 (29), 108 (12), 107 (14), 106 (6), 105 (12), 92 (21), 91 (100), 89 (6), 79 (17), 78 (5), 77 (19), 65 (15), 63 (5), 59 (36), 51 (12), 44 (20), 43 (7), 40 (65).

The ^{13}C NMR data are in agreement with those previously reported [5].

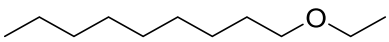
1,1-Dimethoxyethane (DME).



^{1}H NMR (400 MHz, MeOH), δ_H/ppm: 4.14 (q, *J* = 5.3 Hz, 1H), 2.90 (s, 6H), 0.84 (d, *J* = 6.3 Hz, 3H). ^{13}C NMR (101 MHz, MeOH), δ_C/ppm: 101.8, 52.1, 18.2. MS (EI, 70 eV), *m*/*z* (I_{rel}/%): 90 (0.1) M$^+$, 75 (47), 59 (100), 57 (7), 47 (10), 43 (23), 41 (6).

The spectral data obtained are in agreement with those previously reported [3, 4].

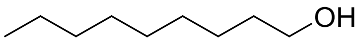
Nonyl ethyl ether (NEE).



^{1}H NMR (400 MHz, MeOH), δ_H/ppm: 3.22 (q, *J* = 7.0 Hz, 2H), 3.16 (t, *J* = 6.7 Hz, 2H), 1.29 (quin, *J* = 7.0 Hz, 2H), 1.03 (m, 12H); 0.91 (t, *J* = 7.0 Hz, 3H), 0.63 (t, *J* = 6.7 Hz, 3H). ^{13}C NMR (101 MHz, MeOH), δ_C/ppm: 70.8, 66.1, 32.0, 29.8, 29.7, 29.6, 29.4, 26.2, 22.7, 14.5, 13.5. MS (EI, 70 eV), *m/z* (I_{rel}/%): 126 (18), 98 (27), 97 (23), 85 (9), 84 (18), 83 (28), 82 (13), 71 (15), 70 (40), 69 (33), 68 (17), 59 (100), 57 (23), 56 (42), 55 (33), 47 (19), 43 (32), 42 (13), 41 (42), 39 (8).

The MS data are in agreement with those previously reported [6].

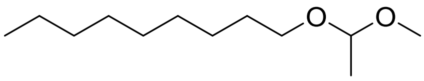
Nonyl alcohol (NAL).



^{1}H NMR (400 MHz, MeOH), δ_H/ppm: 1.19 (quin, *J* = 6.9 Hz, 2H), 0.97 (m, 12H), 0.57 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, MeOH), δ_C/ppm: 62.2, 32.7, 32.1, 29.7, 29.6, 29.4, 25.9, 22.7, 13.4. MS (EI, 70 eV), *m/z* (I_{rel}/%): 98 (30), 97 (33), 84 (26), 83 (41), 82 (16), 71 (14), 70 (79), 69 (68), 68 (26), 67 (12), 57 (37), 56 (100), 55 (93), 54 (9), 53 (6), 44 (8), 43 (69), 42 (36), 41 (80), 40 (12), 39 (19).

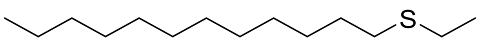
The spectral data obtained are in agreement with those previously reported [3, 4].

1-Nonyloxy-1-methoxyethane.



^{13}C NMR (101 MHz, MeOH), δ_C/ppm: 101.1, 66.0, 52.0, 29.9, 29.6, 26.3, 18.7. MS (EI, 70 eV), *m/z* (I_{rel}/%): 187 (5), 171 (4), 85 (14), 71 (24), 70 (7), 69 (8), 61 (8), 59 (100), 57 (23), 56 (11), 55 (15), 43 (33), 42 (7), 41 (20).

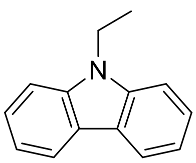
Dodecyl ethyl sulfide (DES).



^{1}H NMR (400 MHz, MeOH), δ_H/ppm: 2.37 (t, *J* = 6.9 Hz, 2H), 2.18 (q, *J* = 7.0 Hz, 2H), 1.24 (quin, *J* = 7.2 Hz, 2H), 1.12-0.85 (m, 18H), 0.90 (t, *J* = 7.4 Hz, 3H), 0.58 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, MeOH), δ_C/ppm: 32.1, 31.5, 29.7, 29.7, 29.7, 29.5, 29.4, 28.9, 28.8, 25.6, 22.7, 14.2, 13.4. MS (EI, 70 eV), *m/z* (I_{rel}/%): 230 (26) M^+, 201 (100), 97 (11), 83 (14), 75 (25), 69 (18), 62 (14), 55 (22), 43 (16), 41 (19).

The MS data are in agreement with those previously reported [3].

9-Ethylcarbazole (9-EC).



^{1}H NMR (400 MHz, C_6H_6), δ_H/ppm: 8.05 (d, *J* = 7.6 Hz, 2H), 3.71 (q, *J* = 7.1 Hz, 2H), 0.91 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, C_6H_6), δ_C/ppm: 139.8, 125.3, 123.0, 120.3, 118.6, 108.1, 36.7, 12.9. MS (EI, 70 eV), *m/z* (I_{rel}/%): 195 (49) M^+, 181 (15), 180 (100), 167 (8), 166 (10), 152 (17), 140 (8), 139 (6).

The spectral data obtained are in agreement with those previously reported [3, 4].

References

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