Supplementary Information

Shape and ligand effect of palladium nanocrystals on furan hydrogenation

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Experimental details of characterization

Fig. S1. Shape statistics of the as-prepared Pd octahedra.

Fig. S2. Shape statistics of the Pd octahedra after catalytic test.

Fig. S3. Effect of hydrogen pressure on furan hydrogenation over Pd nanocube and octahedron.

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Experimental details of characterization

Transmission electron microscopy (TEM) images and high-resolution TEM (HRTEM) images were recorded on an FEI Tecnai G220 microscope operated at 300 kV. The specimen was prepared by ultrasonically dispersing the sample powder in ethanol, and drops of the suspension were deposited on a carbon-coated copper grid and dried in air.

X-ray powder diffraction (XRD) patterns were recorded on a Rigaku Rint D/MAX-2500/PC diffractometer using Cu Kα radiation operated at 40 kV and 40 mA.

Fourier transformation infrared spectra (FTIR) were recorded on a Nicolet 6700 spectrometer. 1 wt. % of solid sample was mixed with 99 wt. % of KBr powder, ground, and then pressed into a wafer. In some cases, the sample dispersed in ethanol was directly dropped onto a KBr wafer and dried.

X-ray photoelectron spectroscopy (XPS) data were collected by a Thermo Fisher Escalab 250Xi equipped with an Al Kα monochromatic X-ray source (1486.6 eV) under ultrahigh vacuum condition (<10-8 Torr). The adventitious carbon 1s peak was calibrated at 284.8 eV to compensate for any charging effects.

Nitrogen adsorption-desorption isotherms were recorded at 77 K on a Quantachrome Autosorb-1-MP gas sorption analyzer. Before the measurements, the samples were degassed at 60 ℃ for 6 h. The specific surface areas of the samples were calculated by multipoint BET model.

Temperature-programmed oxidation (TPO) and CO pulse chemisorption was carried out on a Hiden Catlab equipped with a QGA mass spectrometer. The sample (20 mg) was pretreated by 40 ml/min Ar at 110 ℃ for 2 h and cooled down to 40 ℃ before analysis. For TPO, the sample was then heated from 40 to 500 ℃ at a rate of 5 ℃/min and kept at 500 ℃ for 30 min in a 40 ml/min of 20 vol% O_2/Ar flow. Upon chemisorption test, 5 vol% CO/Ar in a loop of 100 μL was periodically introduced until adsorption saturation.

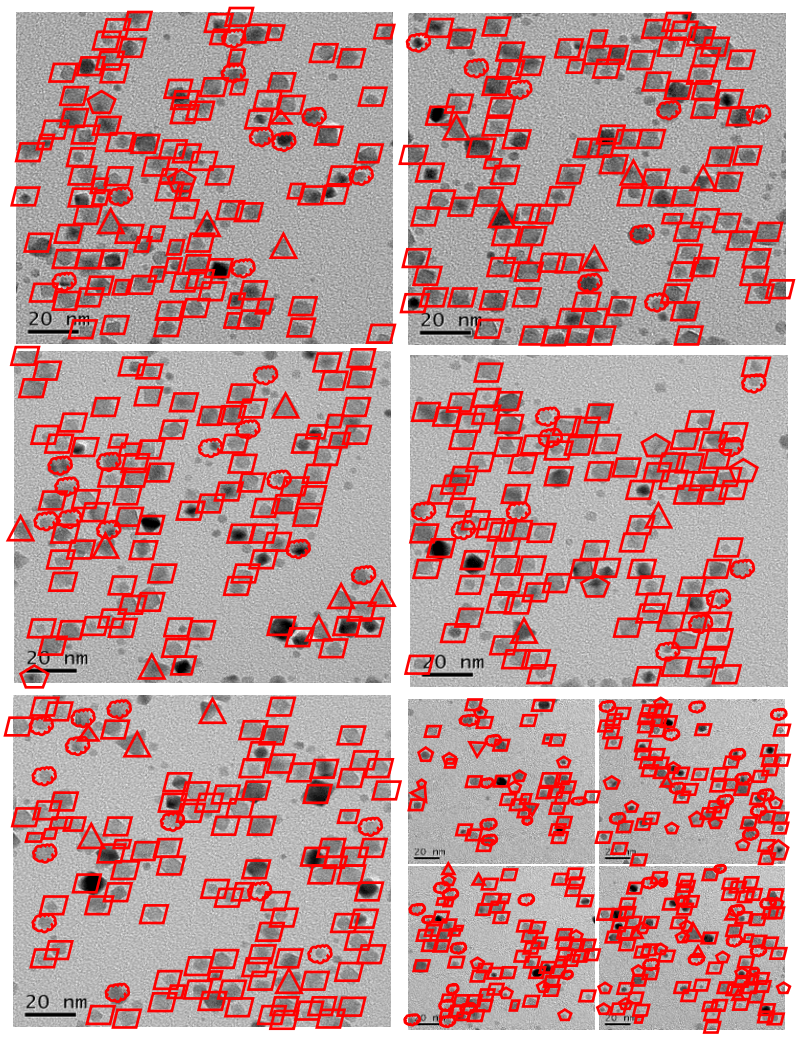

Fig. S1. Shape statistics of the as-prepared Pd octahedra.

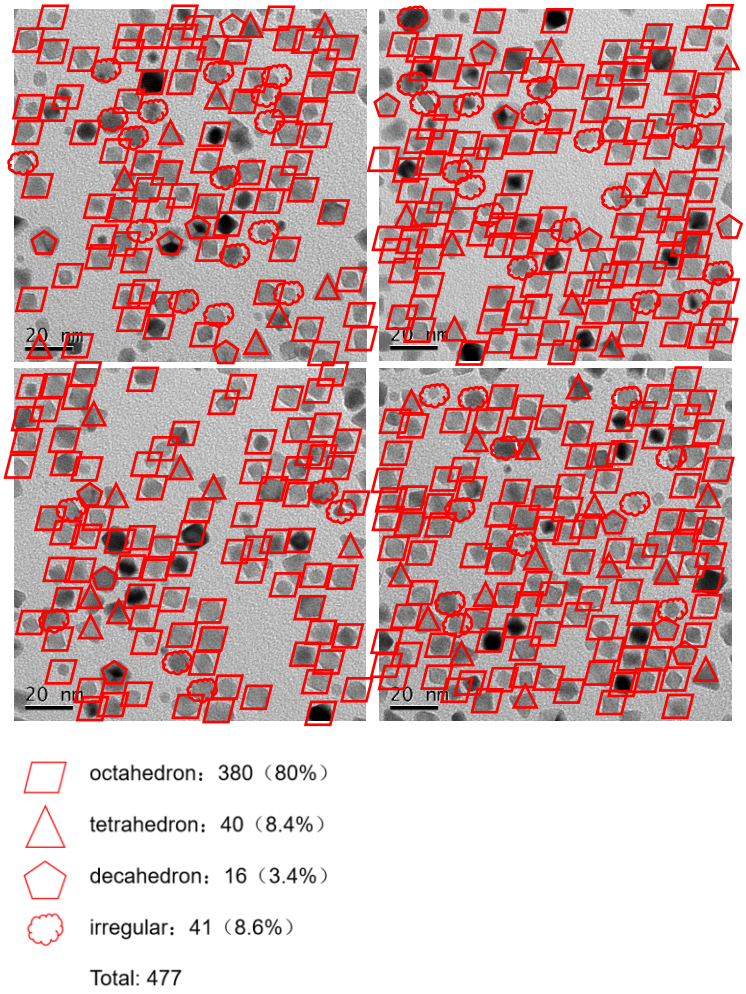

Fig. S2. Shape statistics of the Pd octahedra after catalytic test. It was found that after catalytic test, the octahedron was still predominant shape, and the proportion of octahedron had little change compared to that of as-prepared one. The proportion of tetrahedron increased after reaction probably due to the deformation and evolution of partial irregular and tiny particles. In general, the Pd octahedron is stable enough in furan hydrogenation.

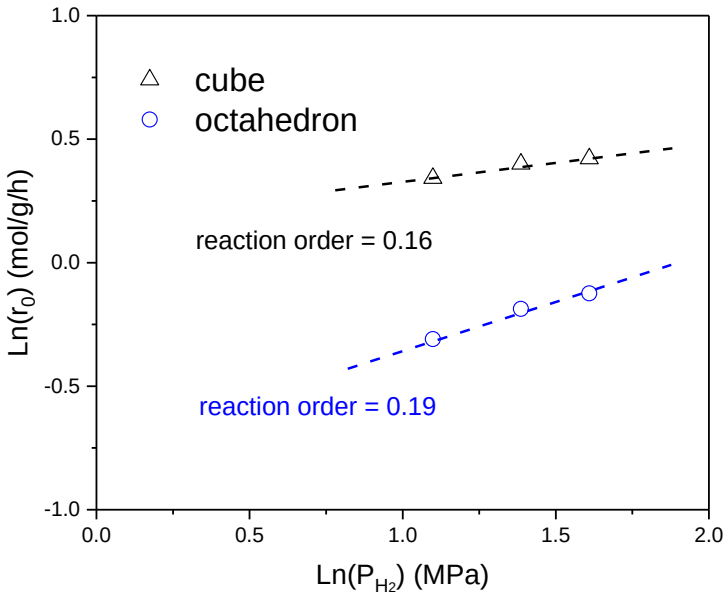

Fig. S3. Effect of hydrogen pressure on furan hydrogenation over Pd nanocube and octahedron. Reaction conditions: furan, 13.5 mmol; ethanol, 19 ml; n-tetradecane, 0.18 g; catalyst loading, 5 mg; agitating speed, 1000rpm; temperature, 25 ℃.