# Supplementary Materials

## Towards Rational Design of Core-Shell Catalytic Nanoreactor with high Performance Catalytic Hydrogenation of Levulinic acid

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**Characterization Techniques:**

Powder X-ray diffraction (PXRD) patterns of different samples were recorded with a Bruker D8 Advance X-ray diffractometer operated at a voltage of 40 kV and a current of 40 mA using Ni-filtered Cu Kα (λ=0.15406 nm) radiation. Ultra High Resolution Transmission electron microscopy (UHR-TEM) images were recorded in a JEOL JEM 2010 transmission electron microscope with operating voltage 200 kV equipped with a FEG. Field emission scanning electron microscopic images of samples were obtained using a JEOL JEM 6700 field emission scanning electron microscope (FE-SEM). Nitrogen sorption isotherms were obtained using a Quantachrome Autosorb 1C surface area analyzer at 77 K. Prior to the measurement, the samples were degassed at 423 K for approximately 4 h in high vacuum. Solid-state CP-MAS NMR studies were performed using a Bruker Avance III HD 400 MHz NMR spectrometer. X-ray photoelectron spectroscopy (XPS) was performed on an Omicron nanotech operated at 15 kV and 20 mA with a monochromatic Al Kα X-ray source. Chemical analysis was performed by using Optima 2100 DV (Perkin-Elmer) inductively coupled plasma atomic emission spectroscopy (ICP-AES). Pd surface area of $Pd@SiO_2$ and m-$SiO_2@Pd@SiO_2$ was quantified employing CO(g) chemisorption (Micromeritics ASAP 2020C). The samples were heated in $H_2$(g) at 350 °C for 2 h before performing CO chemisorption analysis at 35 °C. Based on the measured chemisorption, the Pd particle size was calculated.

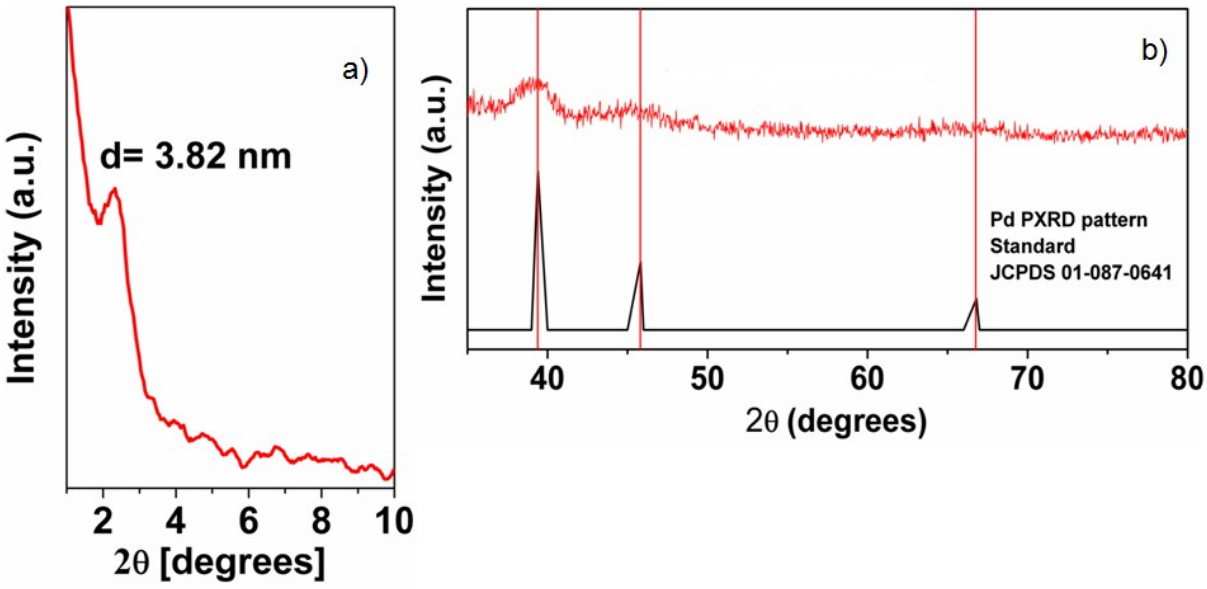


**Fig. S1.** Small angle powder XRD pattern of (panel a) & wide angle powder XRD pattern of (panel b)

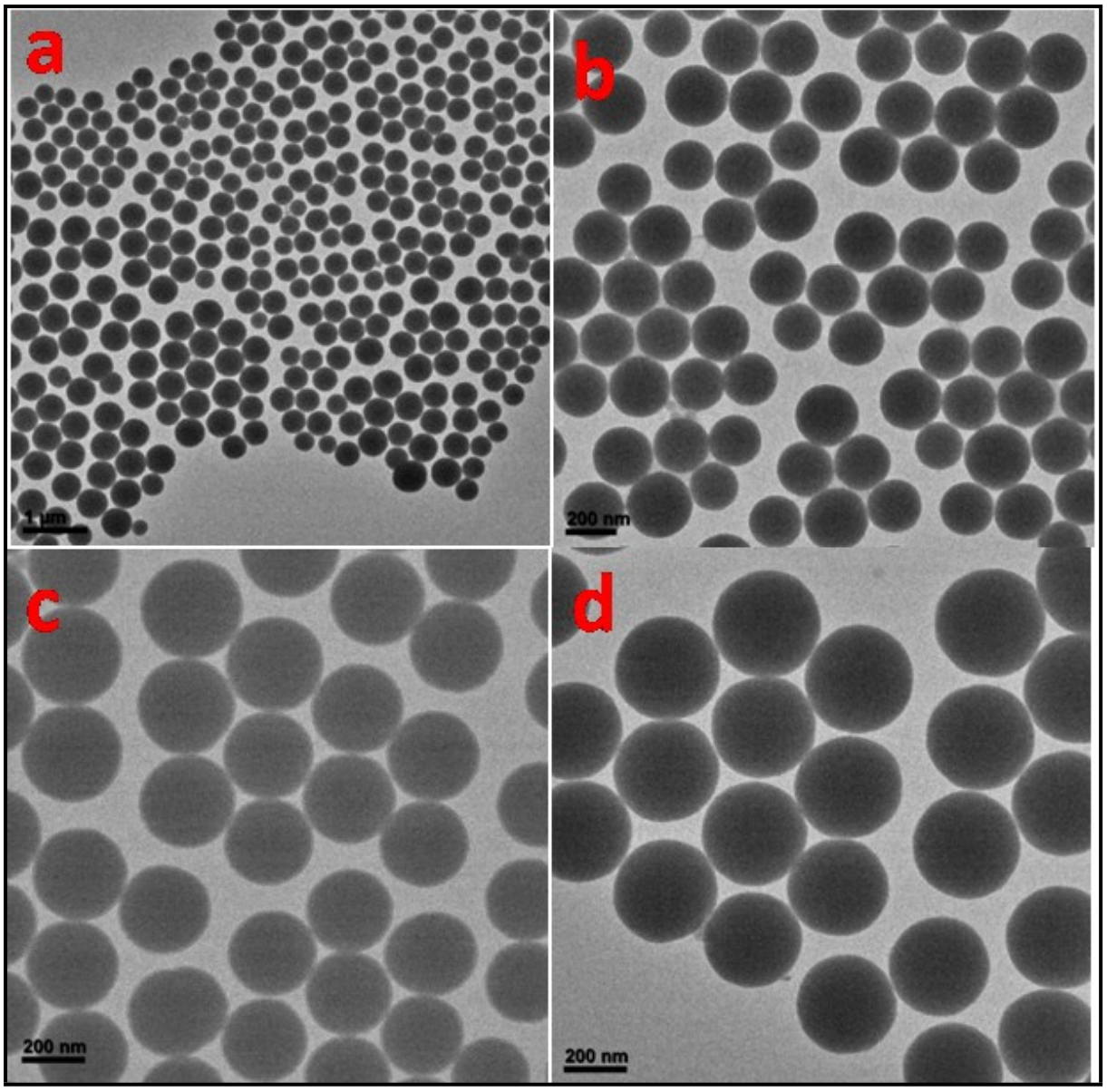


**Figure S2**. TEM images of $SiO_2$ nanospheres of different magnification

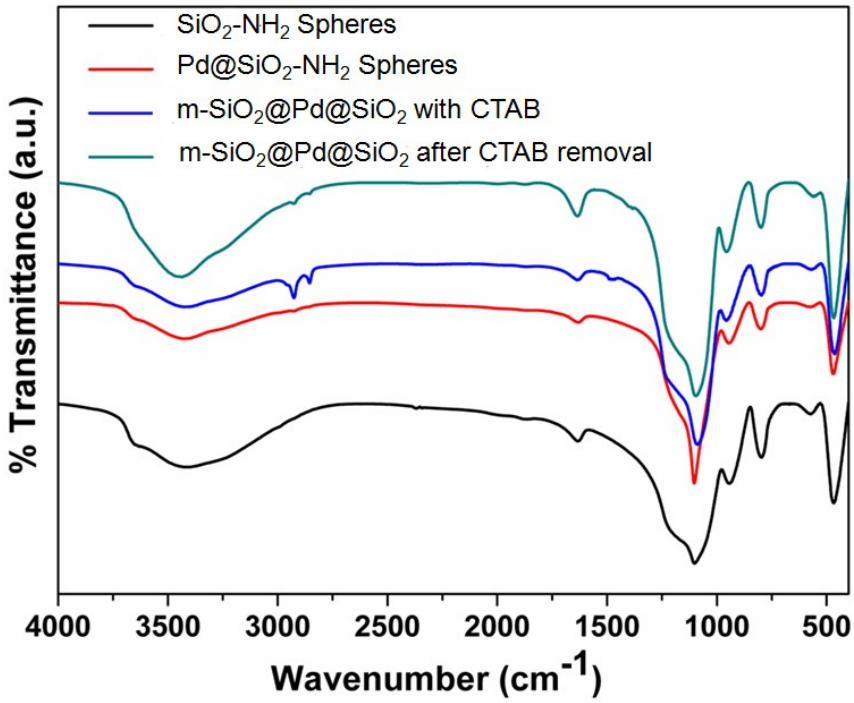


**Figure S3**. FT-IR images of all silica samples at different steps

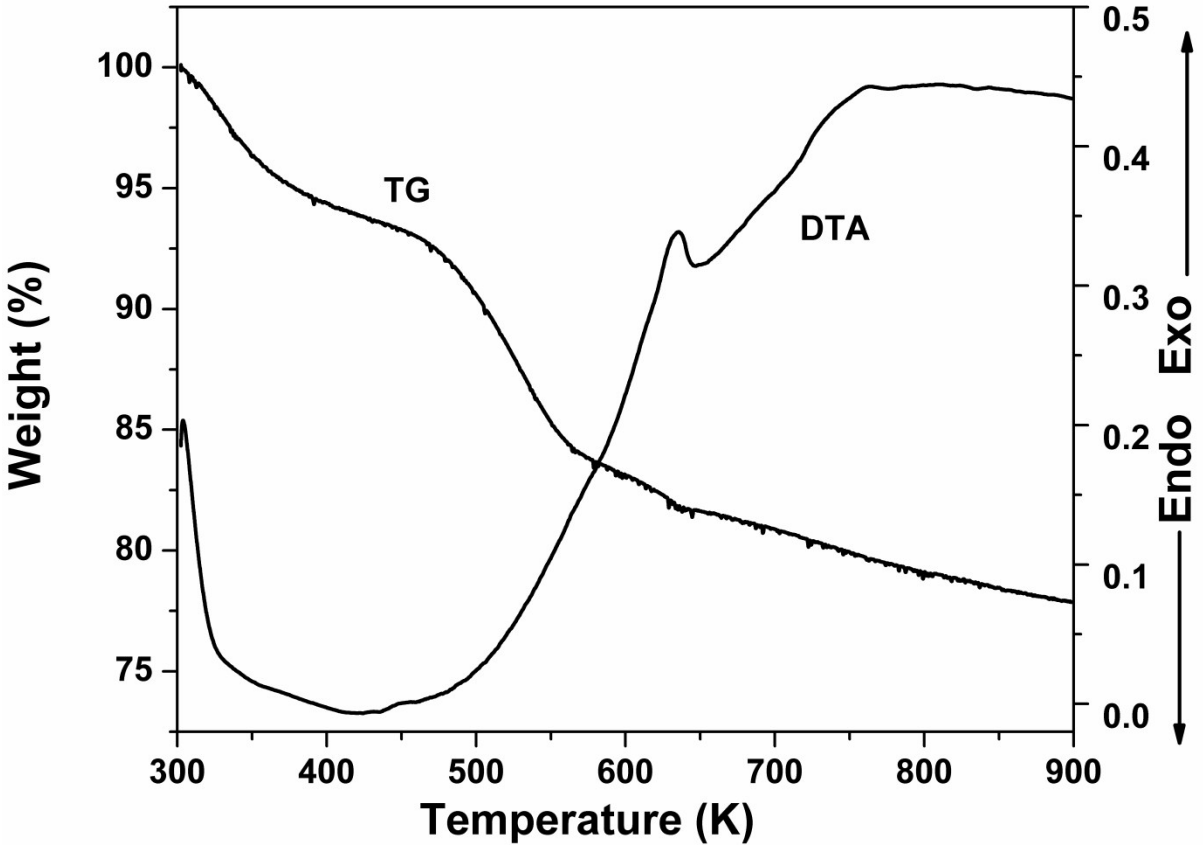


**Figure S4**. TG-DTA profile of Pd@$SiO_2$

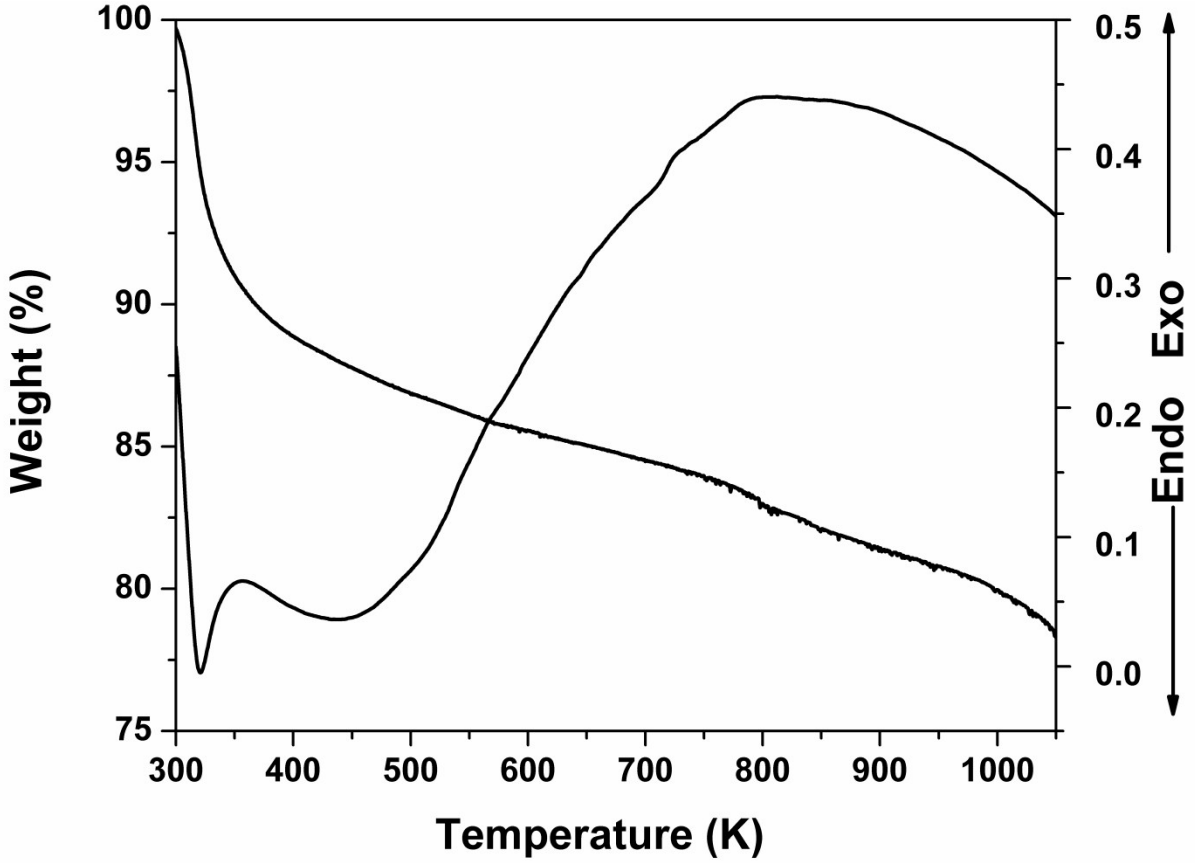


**Figure S5**. TG-DTA profile of m-$SiO_2$@Pd@$SiO_2$

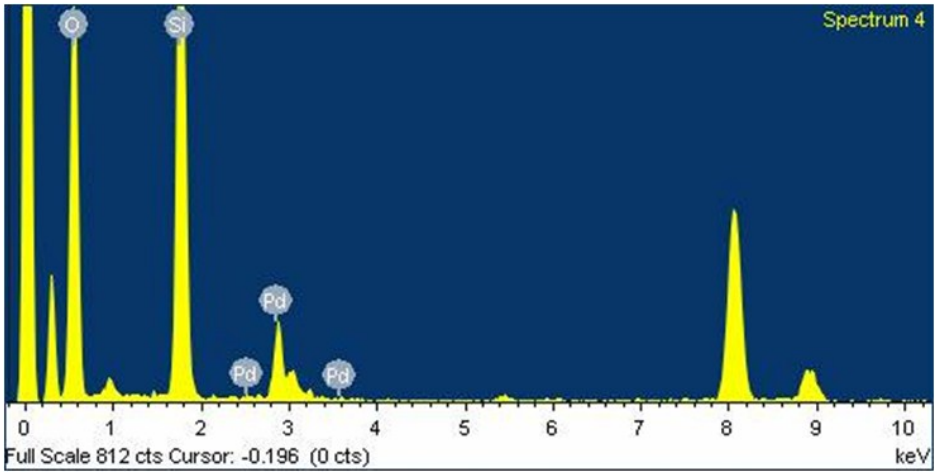


**Figure S6**. Energy dispersive X-ray spectrum profile of Pd@$SiO_2$

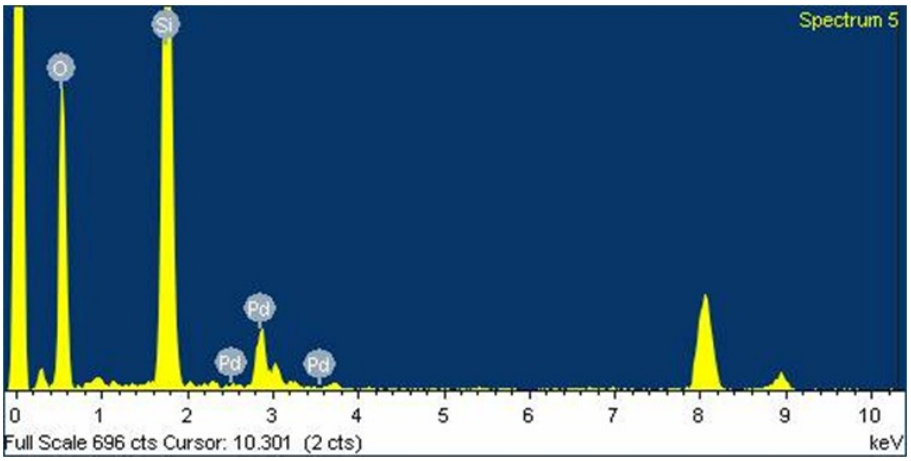


**Figure S7**. Energy dispersive X-ray spectrum profile of m-$SiO_2$@Pd@$SiO_2$

**Table S1**: Pd nanoparticle size derived from CO Chemisorption and TEM measurements

| **Catalyst** | **Particle size from CO chemisorption [nm]** | **Particle size from TEM [nm]** |
|---|---|---|
| m-$SiO_2$@Pd@$SiO_2$ | 7.2 | 5.4 |
| Pd@$SiO_2$ | 5.9 | 6.2 |

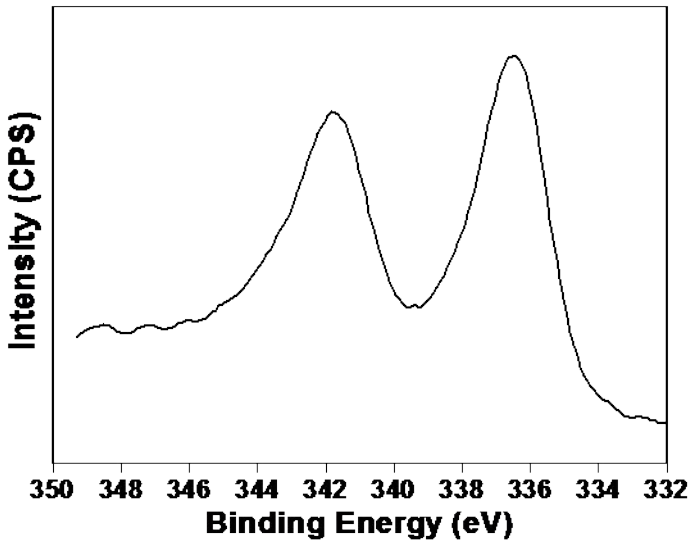


**Figure S8**. XPS spectrum of Pd-3d region for Pd@C catalyst.

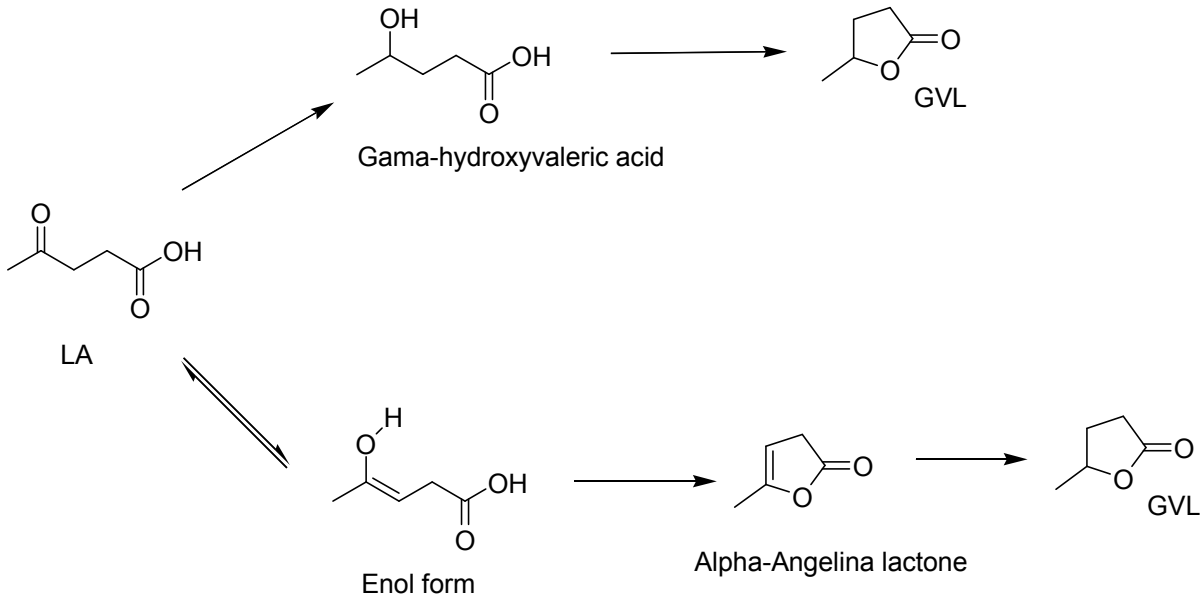


**Figure S9**. Mechanism for LA hydrogenation .