Electronic Supplementary Material (ESI) for Nanoscale.

Elucidating the Surface Compositions of Pd@Pt_{nL} Core-Shell Nanocrystals through Catalytic Reactions and Spectroscopy Probes

Peng Zhai,[a†] Yifeng Shi,[b†] Qiuxiang Wang,[c] Younan Xia,[*b,c,d] Kunlun Ding[*a]

[a]Department of Chemical Engineering, Louisiana State University, Baton Rouge, Louisiana 70803, USA. E-mail: kunlunding@lsu.edu (for catalytic measurements and spectra characterization)

[b]School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, Georgia 30332, USA. E-mail: younan.xia@bme.gatech.edu (for material synthesis and electron microscope characterization)

[c]The Wallace H. Coulter Department of Biomedical Engineering, Georgia Institute of Technology and Emory University, Atlanta, Georgia 30332, USA

[d]School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, Georgia 30332, USA

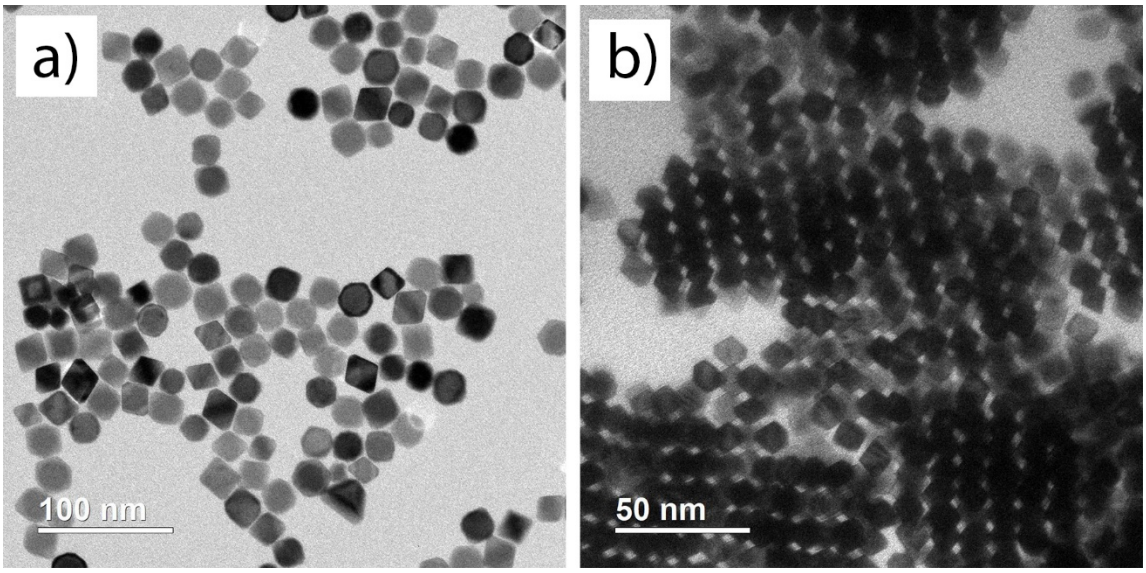

Figure S1. TEM images of (a) Pd octahedral and (b) Pt octahedral nanocrystals used as reference samples in this study.

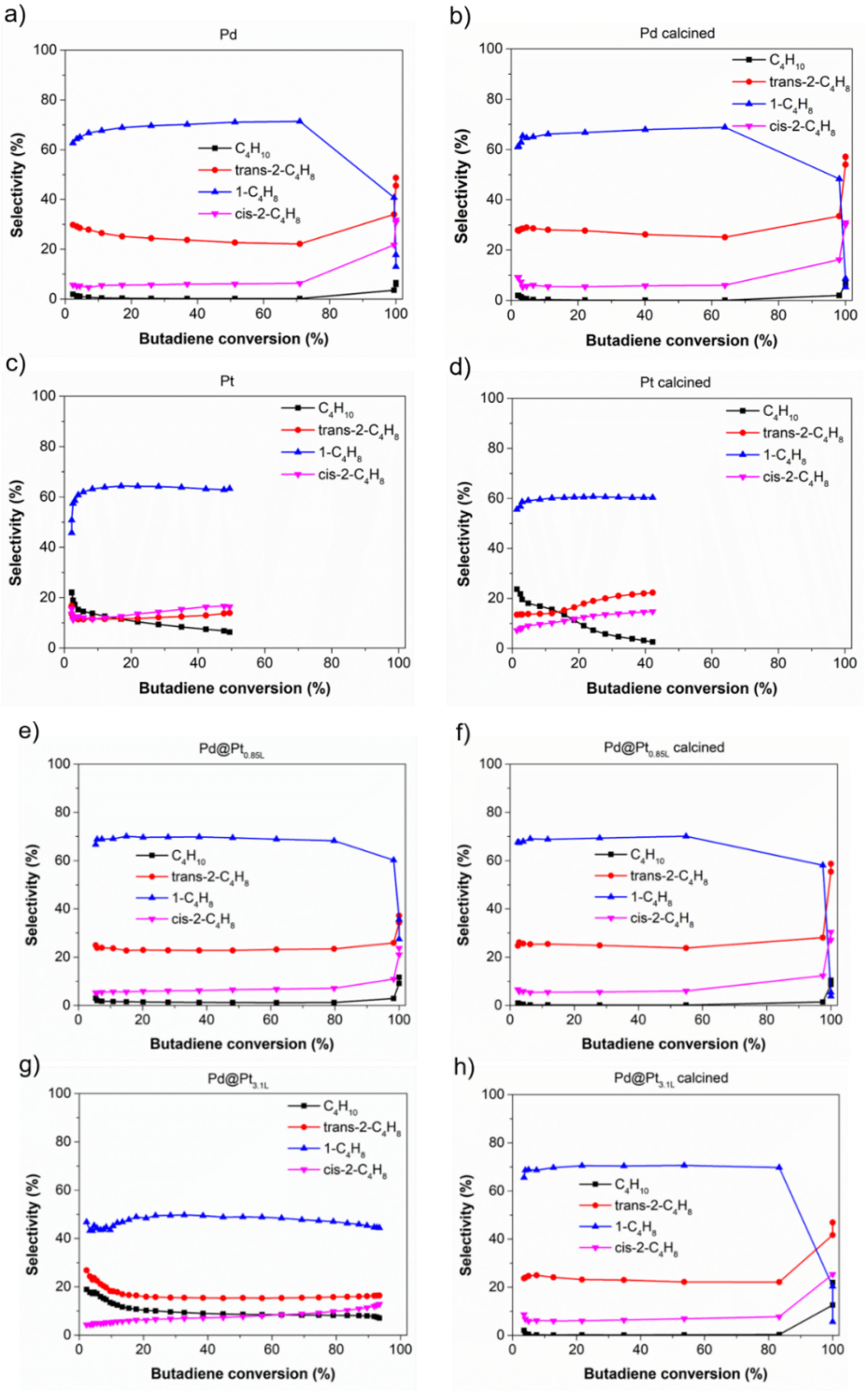

Figure S2. The selectivity of butadiene hydrogenation as a function of butadiene conversion on (a) non-calcined Pd, (b) calcined Pd, (c) non-calcined Pt, (d) calcined Pt, (e) non-calcined Pd@$Pt_{0.85L}$, (f) calcined Pd@$Pt_{0.85L}$, (g) non-calcined Pd@$Pt_{3.1L}$, and (h) calcined Pd@$Pt_{3.1L}$. All catalysts were reduced at 100 °C in 10% H_2/N_2 prior to catalytic tests.

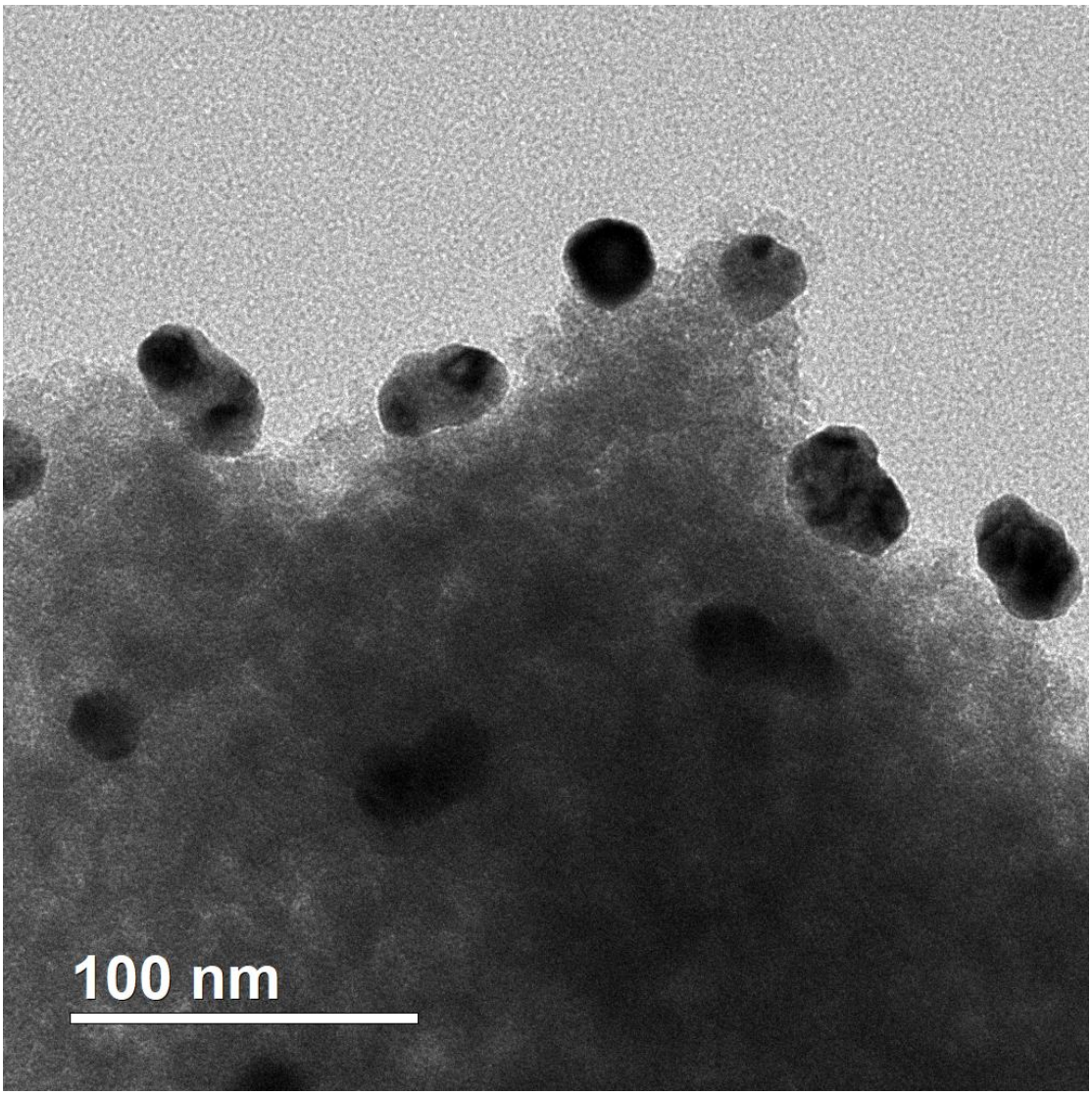

Figure S3. TEM image of the Pd octahedral nanocrystals (supported on SiO_2) after calcination under 10% O_2/N_2 at 400 °C for 30 min.

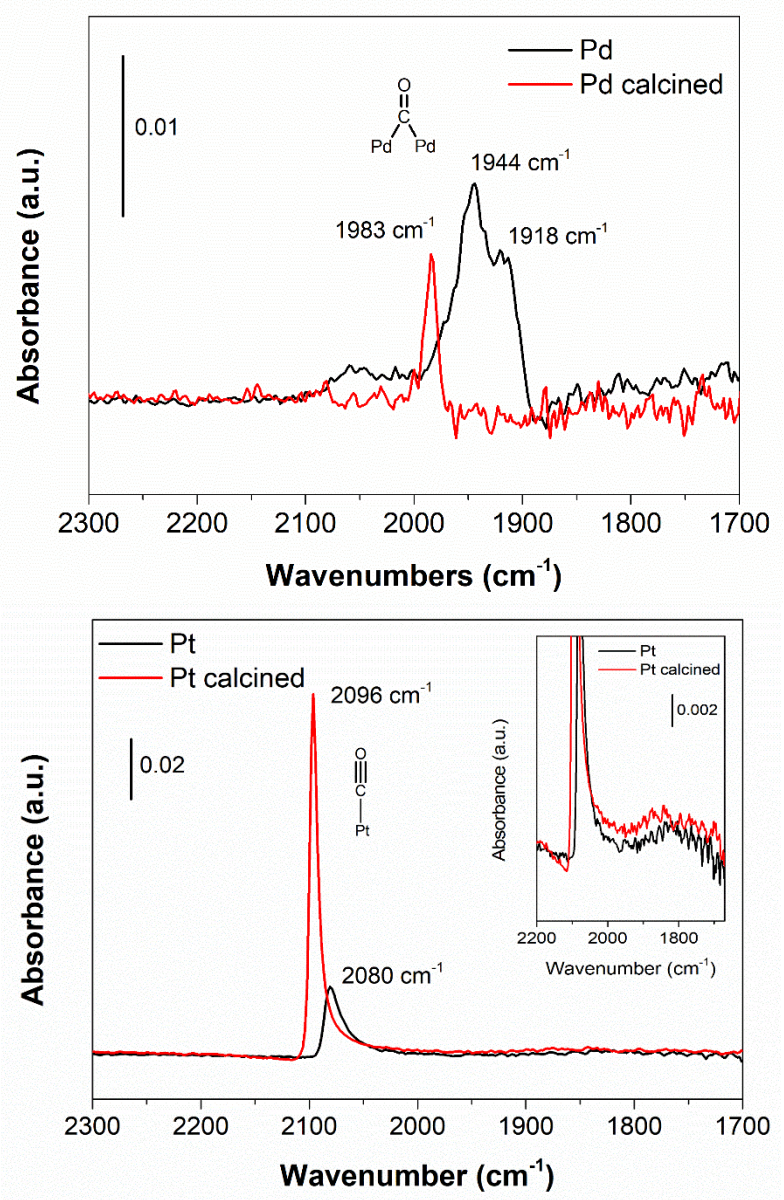

Figure S4. IR spectra of the CO adsorbed on Pd and Pt samples at room temperature. These catalysts were reduced at 100 °C in 10% H_2/N_2 prior to CO adsorption.

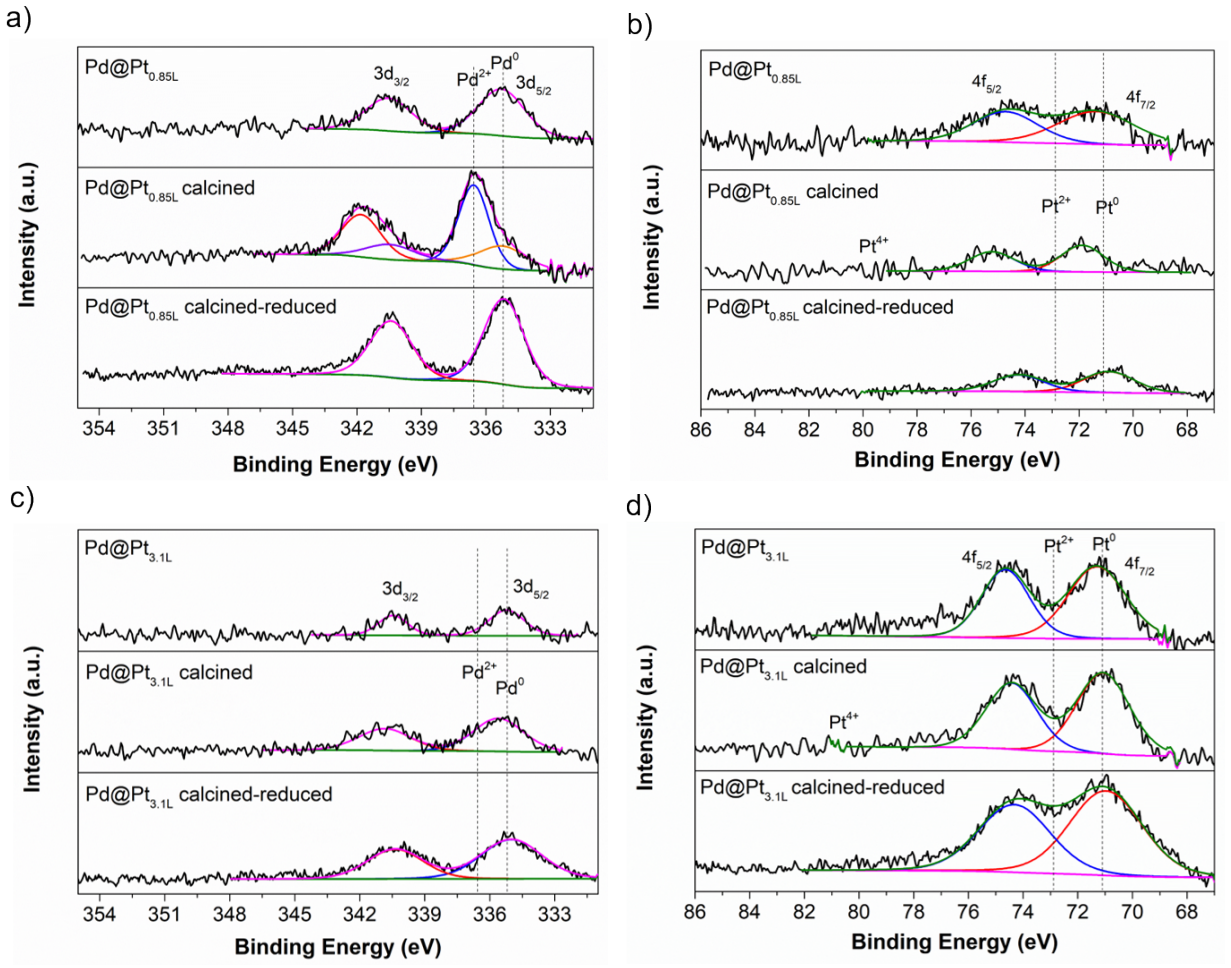

Figure S5. XPS spectra of two different Pd@Pt bimetallic catalysts after undergoing different treatments. (a) Pd 3d and (b) Pt 4f spectra of Pd@$Pt_{0.85L;}$ (c) Pd 3d and (d) Pt 4f spectra of Pd@$Pt_{3.1L}$.

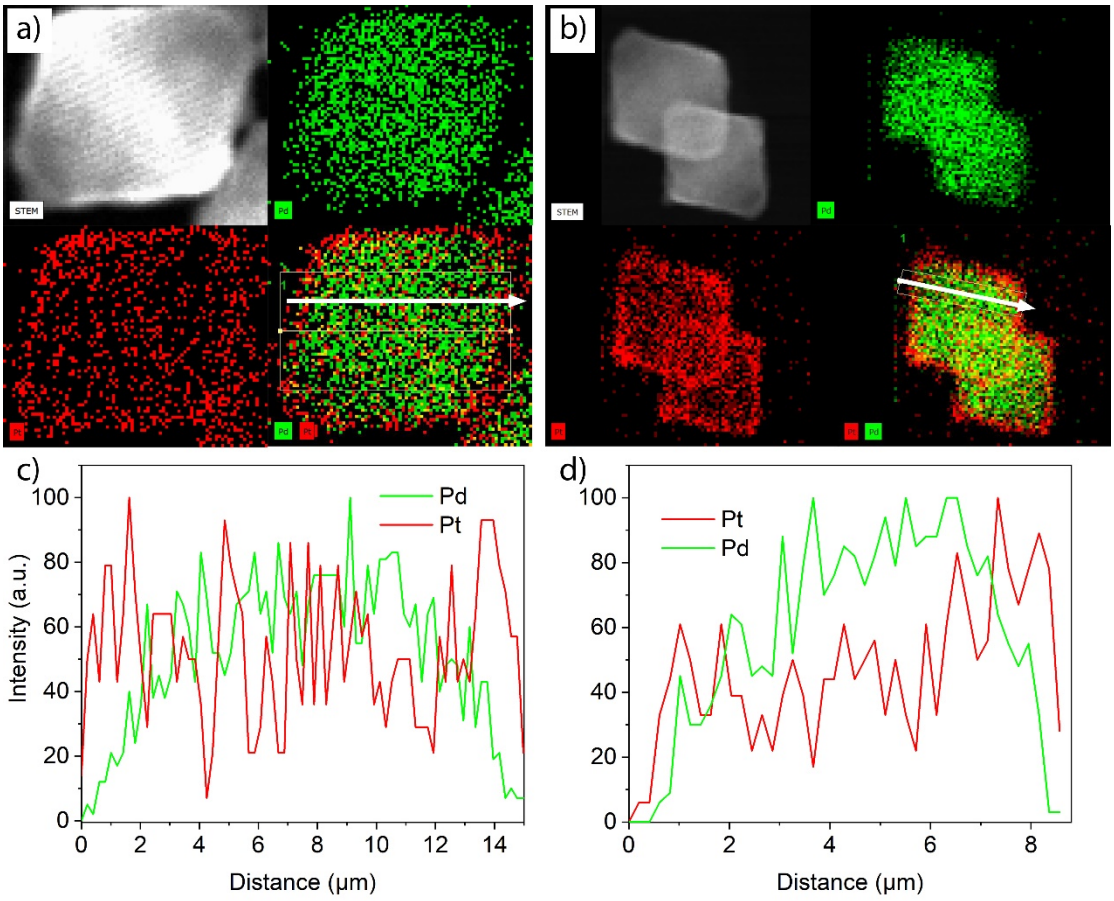

Figure S6. EDX mapping of (a) Pd@$Pt_{3.1L}$ before calcination and (b) after calcination. The corresponding line scan profiles are given in (c) and (d), respectively.