Supporting Information for "Liquid phase hydrogenation of phenylacetylene over Pd and PdZn catalysts in toluene: Effects of alloying and CO₂ pressurization" by H. Yoshida, T. Zama, S. Fujita, J. Panpranot, and M. Arai



1. XRD of Pd/ZnO samples prepared by impregnation and coprecipitation

Fig. S1 XRD patterns of Pd/ZnO (a) and alloyed PdZn/ZnO (b) catalysts prepared by impregnation or coprecipitation followed by reduction at either ambient temperature or 500 °C. The sizes of Pd and PdZn crystallites were determined from the Pd (111) (2Θ =40.1°) and PdZn (111) (2Θ =41.2°) line broadening, respectively, through the Scherrer equation and are given in Table 1 of the main text.

2. Determination of exposed Pd sites of Pd/ZnO samples

From XRD: The sizes of Pd and PdZn crystallites were determined by XRD line broadening with the Scherrer equation. Hemispherical shape was assumed for supported Pd and PdZn particles. It was assumed that, for the Pd particles, 12.08 Pd atoms existed in 1 nm²; for the alloyed PdZn particles, the surface composition of Pd/Zn was 1/1 and the number of exposed Pd atoms was calculated assuming an 12.08/2 atoms in 1 nm².

From CO chemisorption: The number of exposed Pt sites on Pd samples (prepared through the reduction at ambient temperature) was determined from the amount of CO chemisorbed with a stoichiometry of CO/Pd = 1/2. No CO chemisorption was observed for PdZn alloy samples.

3. Reaction results at longer reaction time



Fig. S2 Conversion – time and selectivity to styrene – time profiles for Pd (\circ , \Box) and alloyed PdZn catalysts (\bullet , \blacksquare) prepared by coprecipitation and reduction at ambient temperature and at 500 °C, respectively.





Fig. S3 ATR-FTIR spectra for liquid phenylacetylene (PA) pressurized by 0.6 MPa H_2 and/or CO₂ at pressures given. (a) 2100 - 2150 cm⁻¹ (C-C triple bond); (b) 3200 - 3400 cm⁻¹ (terminal CH bond).



Fig. S4 ATR-FTIR spectra for liquid styrene (ST) pressurized by 0.6 MPa H_2 and/or CO₂ at pressures given. (a) $1610 - 1660 \text{ cm}^{-1}$ (C-C double bond); (b) $3000 - 3150 \text{ cm}^{-1}$ (terminal CH bond).