Pd-In intermetallic alloy nanoparticles: highly selective ethane dehydrogenation catalysts

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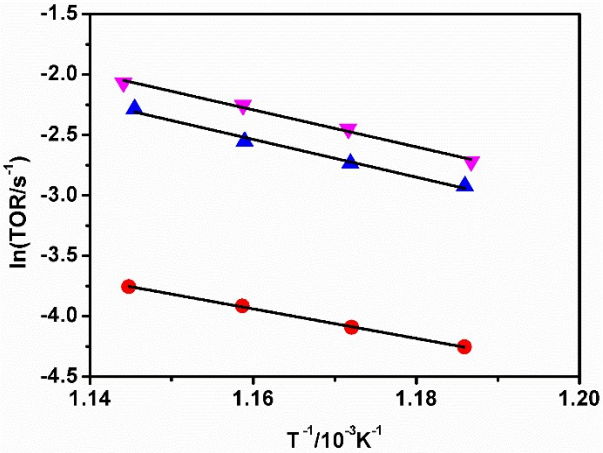
Electronic Supplementary Information

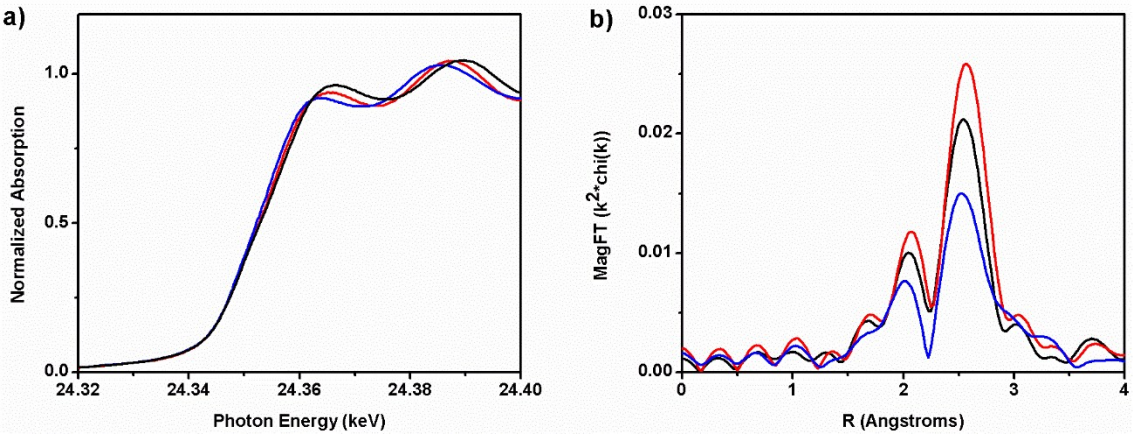
Contents

Arrhenius Plot

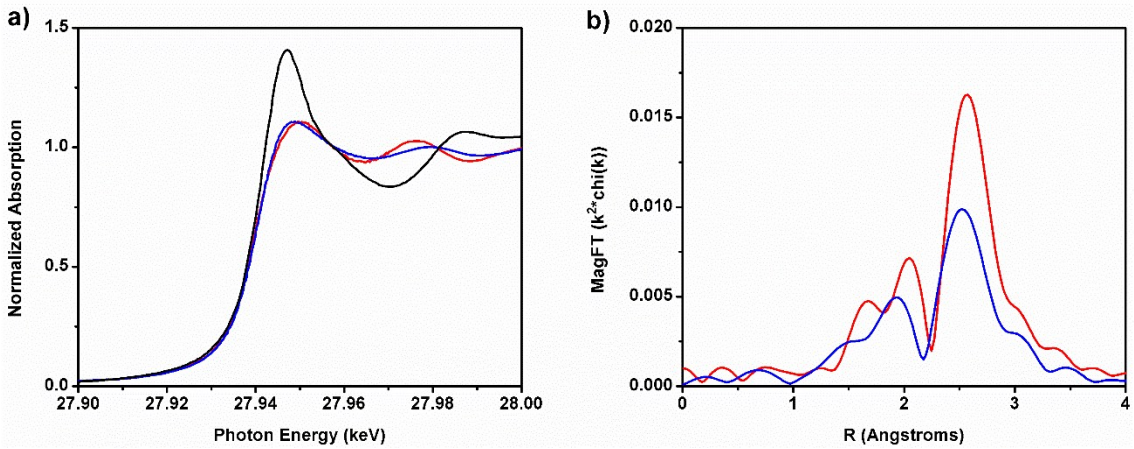


Supplementary fig. S1 Arrhenius plot for ethane dehydrogenation over Pd-In 0.2 (red), Pd-In 0.8 (blue) and Pd-In 2.0 (magenta) catalysts. Activation energy measurements were conducted between 570 and 600 ^{o}C under 5 % C_2H_6, 2 % H_2, 0.5 % C_2H_4, 43.2 % He, and balance N_2 at 1 atm with a total flow rate of 150 cm^3/min. The conversion in all tests are below 10 % and far from equilibrium as confirmed by approach to equilibrium index β. The TORs have been corrected with the approach to equilibrium index β.

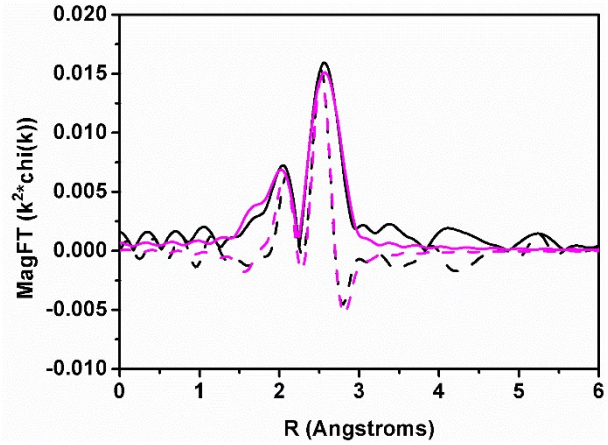
XAS



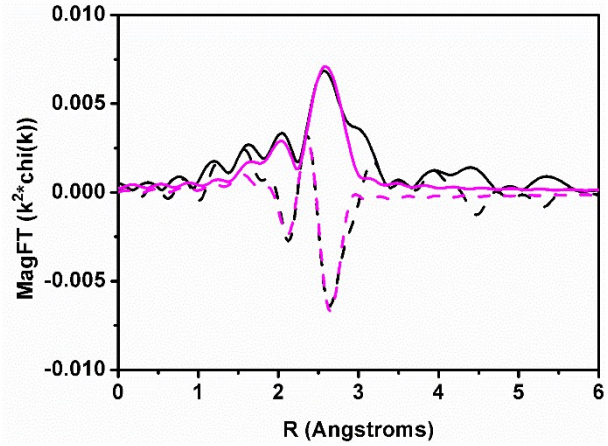
Supplementary fig. S2 a) XANES and b) magnitude of the Fourier Transform of the EXAFS at Pd edge of Pd (black), Pd-In 0.2 (red) and Pd-In 0.8 (blue) catalysts. The catalysts were reduced at 600 °C in a 4 % H_2/He mixture at 50 cm^3/min. After reduction, the samples were purged with He at 100 cm^3/min and cooled to room temperature before the XAS spectra were obtained.



Supplementary fig. S3 a) XANES at the In edge of Pd-In 0.2 (red) and Pd-In 0.8 (blue) catalysts compared with Indium oxide (black) and b) magnitude of the Fourier Transform of the EXAFS at the In edge of Pd-In 0.2 (red) and Pd-In 0.8 (blue) catalysts. The catalysts were reduced at 600 °C in a 4 % H_2/He mixture at 50 cm^3/min. After reduction, the samples were purged with He at 100 cm^3/min and cooled to room temperature before the XAS spectra were obtained.

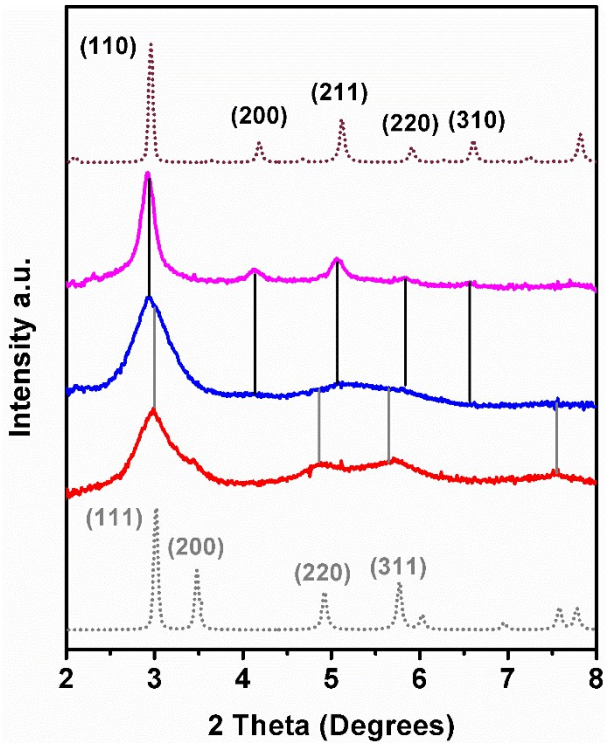


Supplementary figure S4. Fitting results of the R-space EXAFS spectrum at Pd edge of pre-reduced Pd-In 2.0 as an example for Pd-In catalysts. The solid black line represents the FT magnitude, the dashed black line the imaginary part of the FT while the magenta solid and dashed lines are the fits of the magnitude and the imaginary part respectively. (3.0 $Å^{-1}$ < k < 12.0 $Å^{-1}$, 1.6 Å < R < 2.9 Å).

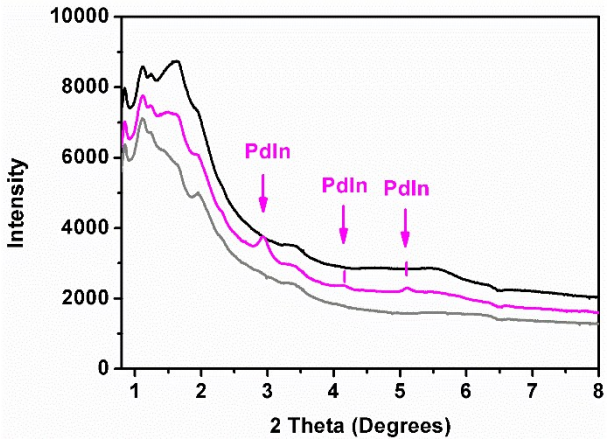


Supplementary figure S5. Fitting results of the R-space EXAFS spectrum at In edge of pre-reduced Pd-In 2.0 as an example for Pd-In catalysts. The solid black line represents the FT magnitude, the dashed black line the imaginary part of the FT while the magenta solid and dashed lines are the fits of the magnitude and the imaginary part respectively. (3.0 $Å^{-1}$ < k < 12.0 $Å^{-1}$, 1.8 Å < R < 2.8 Å).

XRD



Supplementary fig. S6 Background subtracted *in situ* XRD pattern of Pd-In-0.2 (red), Pd-In-0.8 (blue), and Pd-In-2.0 catalyst (magenta, 1/2 the original peak intensity) compared with the simulated XRD pattern (with major peaks indexed) of bulk FCC Pd (grey, dotted), and bulk PdIn intermetallic compound phase (black, dotted) at 600 °C after the catalysts were reduced under 50 cm^3/min 3 % H_2/Ar flow at 600 °C for 20 min. The grey vertical line marks the diffraction features in the samples from FCC Pd phase, while the black vertical line marks those from PdIn IMC phase. Except for peak displacement caused by thermal induced lattice expansion, the patterns show the same features as those taken at RT, indicating unchanged crystal structure of the catalysts in the two different temperature.



Supplementary fig. S7 XRD pattern raw data of Pd-In 2.0/SiO_2 catalysts (magenta) compared with empty cell (grey) and the cell loaded with only SiO_2 (black). The data was recorded *in situ* at RT in 3 % H_2/Ar flow after the samples were reduced under 50 cm^3/min 3 % H_2/Ar flow at 600 °C for 20 min. The data of Pd-In 2.0/SiO_2 and SiO_2 are slightly shifted up in vertical axis for better visualization.