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Supporting Information

$[Pd(2\text{-}pymo)_2]_n/Al_2O_3$ as MOF Single Site Catalyst for the Selective Hydrogenation of Acetylene**

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Table S1. Definition of the symbols used in the SI.

Symbol	Definition	Unit
X	conversion	%
n	amount of substance	mol
n_0	amount of substance in the feed	mol
S	selectivity	%
$\dot{n}$	molar flow	mol · h^{-1}
σ	standard deviation	
m	catalyst mass	g
v	stoichiometric coefficient	

1. Detailed experimental data

Calculation of conversion $X_{acetylene}$ with internal standard propane:

$$X_{acetylene} = \frac{\dot{n}_{0,acetylene} - \dot{n}_{acetylene} \cdot \frac{\dot{n}_{0,propane}}{\dot{n}_{propane}}}{\dot{n}_{0,acetylene}}$$

Calculation of selectivity S_i based on the acetylene conversion and internal standard propane:

$$S_i = \frac{\dot{n}_i - \dot{n}_{0,i}}{\dot{n}_{0,acetylene} - \dot{n}_{acetylene} \cdot \frac{\dot{n}_{0,propane}}{\dot{n}_{propane}}} \cdot \frac{\nu_{acetylene}}{\nu_i}$$

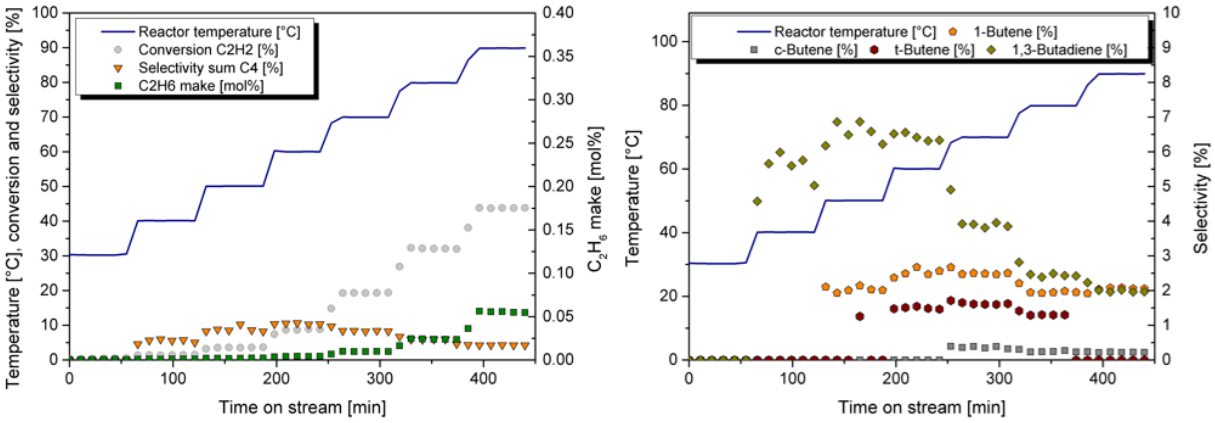

Figure S1. Left: Acetylene conversion, ethane make and sum of C_4 selectivity in regards to the reaction temperature of 250 mg $[Pd(2\text{-pymo})_2]_n$ as synthesized using feed #1 with a volume flow of 62.7 L · h^{-1} (Table 1 manuscript). Right: Detailed formation of 1-butene, c-butene, t-butene and 1,3-butdiene as function of the reaction temperature.

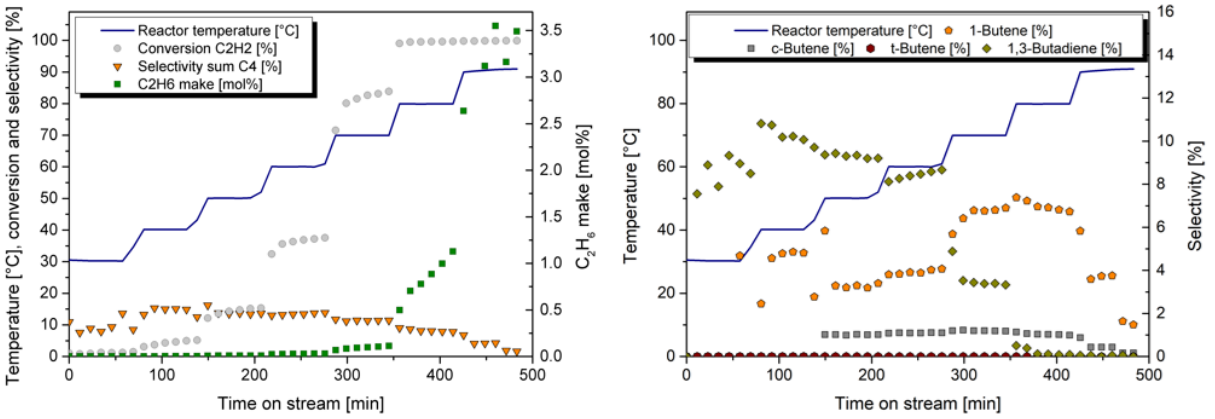

Figure S2. Left: Acetylene conversion, ethane make and sum of C_4 selectivity in regards to the reaction temperature of 11 pellets of prepared eggshell catalyst with a weight loading of 1.13 wt% $[Pd(2\text{-pymo})_2]_n$, tested under feed #1 with a volume flow of 12.9 L · h^{-1} (Table 1 manuscript). Right: Detailed formation of 1-butene, c-butene, t-butene and 1,3-butdiene as function of the reaction temperature.

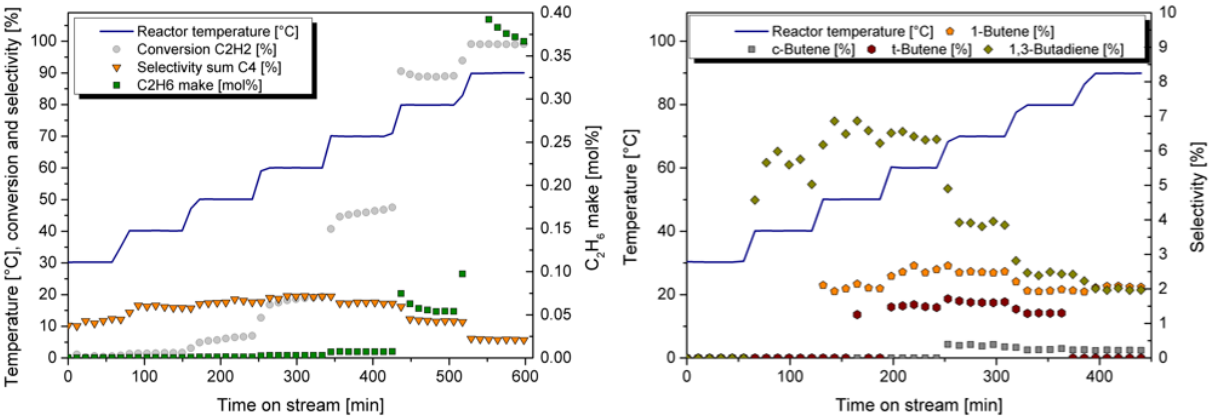

Figure S3. Left: Acetylene conversion, ethane make and sum of C_4 selectivity in regards to the reaction temperature of 22 pellets of the prepared egg-shell catalyst with a weight loading of 1.48 wt% $[Pd(2\text{-pymo})_2]_n$, tested under feed #2 with a volume flow of 62.7 L · h^{-1} (Table 1 manuscript). Right: Detailed formation of 1-butene, c-butene, t-butene and 1,3-butdiene as function of the reaction temperature.

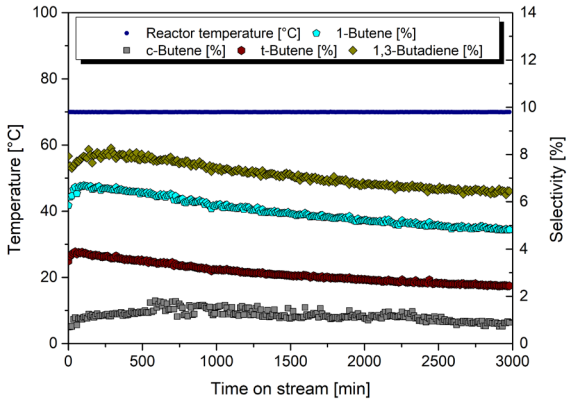

Figure S4. Detailed C4 formation of 22 pellets of prepared $[Pd(2\text{-pymo})_2]_n/Al_2O_3$ catalyst with a weight loading of 1.48 wt% $[Pd(2\text{-pymo})_2]_n$, tested for 50 h at 70 °C under 62.7 L · h^{-1} of feed #2 (Table 1).

2. Additional analysis data

Electron microscopy

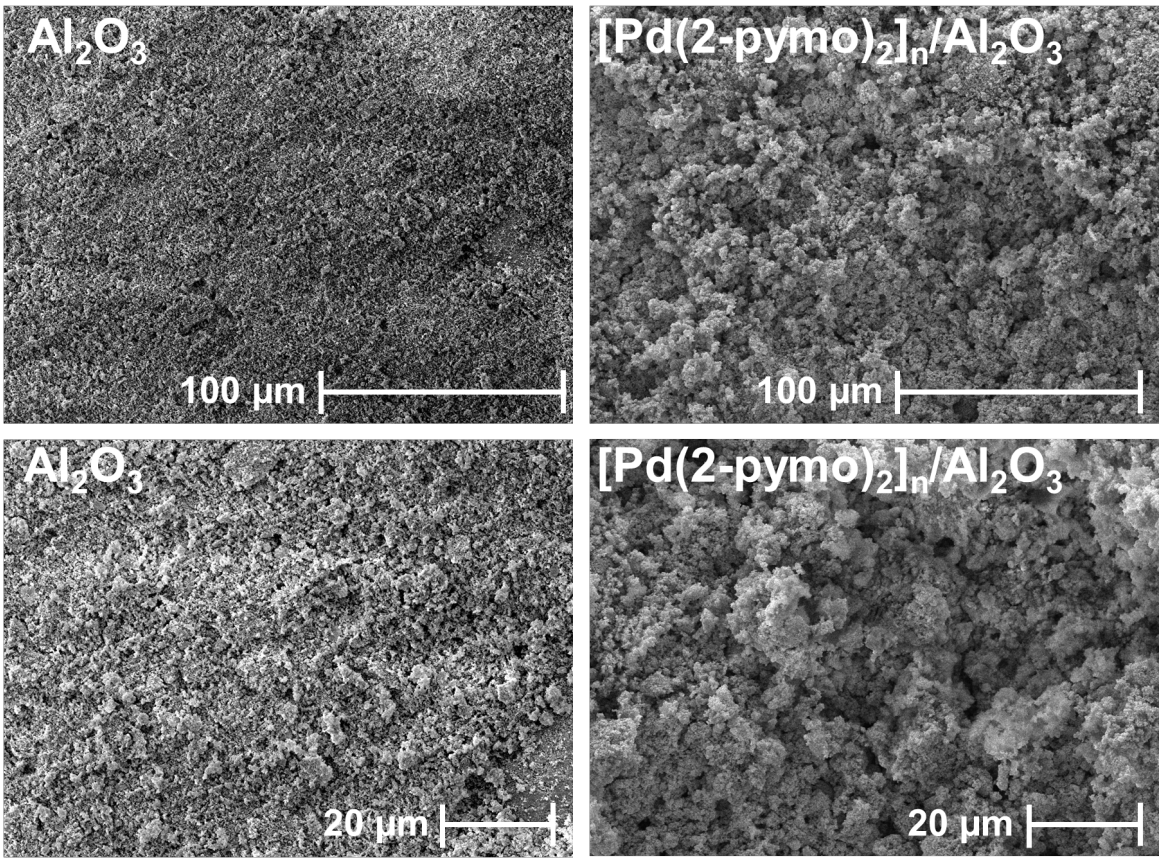

Figure S5. Electron microscopy of pure Al_2O_3 support (left) and $[Pd(2\text{-}pymo)_2]_n/Al_2O_3$ (right).

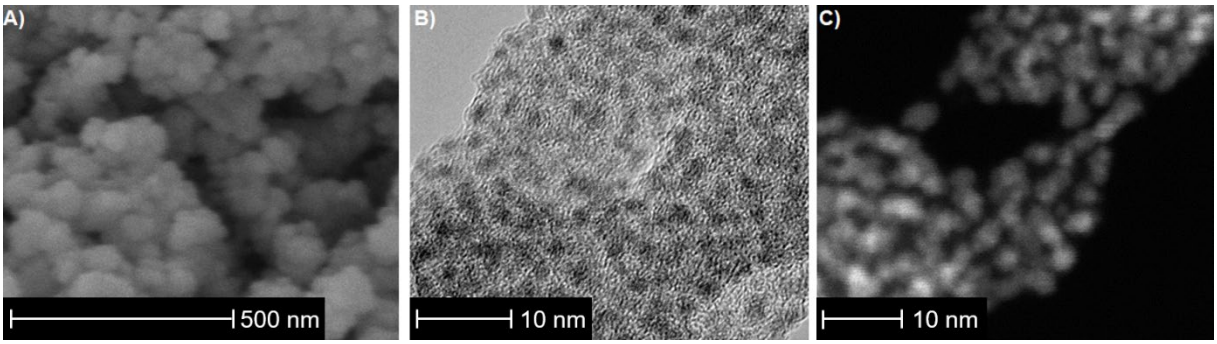

Figure S6. Electron microscopy of $[Pd(2\text{-}pymo)_2]_n$: A) Scanning Electron Microscopy (SEM), B) Scanning Transmission Electron Microscopy (STEM), C) STEM dark field (DF).

X-ray fluorescence spectroscopy

Table S2. Comparison of the XRF analysis of the $[Pd(2\text{-pymo})_2]_n$ as synthesized and after 8 h on stream.

Compound	Pristine	After 8 h on stream	Unit
$C_8H_6N_4O_2$	77.8	76.2	wt%
Pd	21.8	23.4	wt%
Cl	0.2	0.2	wt%
Ca	597	622	ppm
P	519	526	ppm
Si	246	299	ppm
Zr	26	28	ppm
Mn	15	14	ppm
Fe	10	20	ppm
Cu	3	3	ppm

Puls CO-chemisorption

Table S3. Results of CO-chemisorption measurements of 117 mg $[Pd(2\text{-pymo})_2]_n$ in powder form, measured with a TPDRO 1100 from ThermoFisher Scientific.

	Value	Unit
Relative CO consumption	217.5	$\mu mol \cdot g^{-1}$
Relative Pd content	2198.8	$\mu mol \cdot g^{-1}$
CO consumption / Pd content	**9.9**	**%**
Surface area CO chemisorption	44.4	$m^2 \cdot g^{-1}$
BET surface area N_2-physisorption	600.3	$m^2 \cdot g^{-1}$
Ratio surface are CO-chem./ N_2-physi.	**7.4**	**%**