

Supporting Information:

Bimetallic platinum rhenium catalyst for efficient low temperature dehydrogenation of perhydro benzyltoluene

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Supporting Table

Table S1 Sequential drying program of set pressures for the rotary evaporation of solvents at 50 °C during preparation of the catalysts.

Sequence	Starting pressure / mbar	Final pressure / mbar	Time range / min
1	140	100	10
2	100	80	20
3	80	40	120
4	40	20	30

Supporting Figures

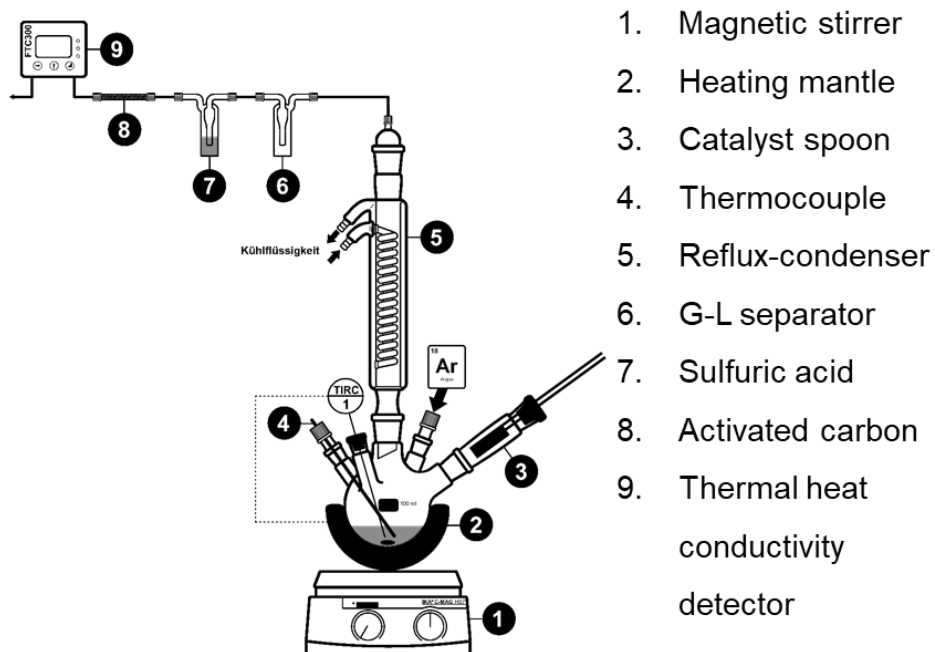


Figure S1: Schematic of the dehydrogenation set-up for semi-batch experiments in a 100 mL five-neck round-bottom flask.

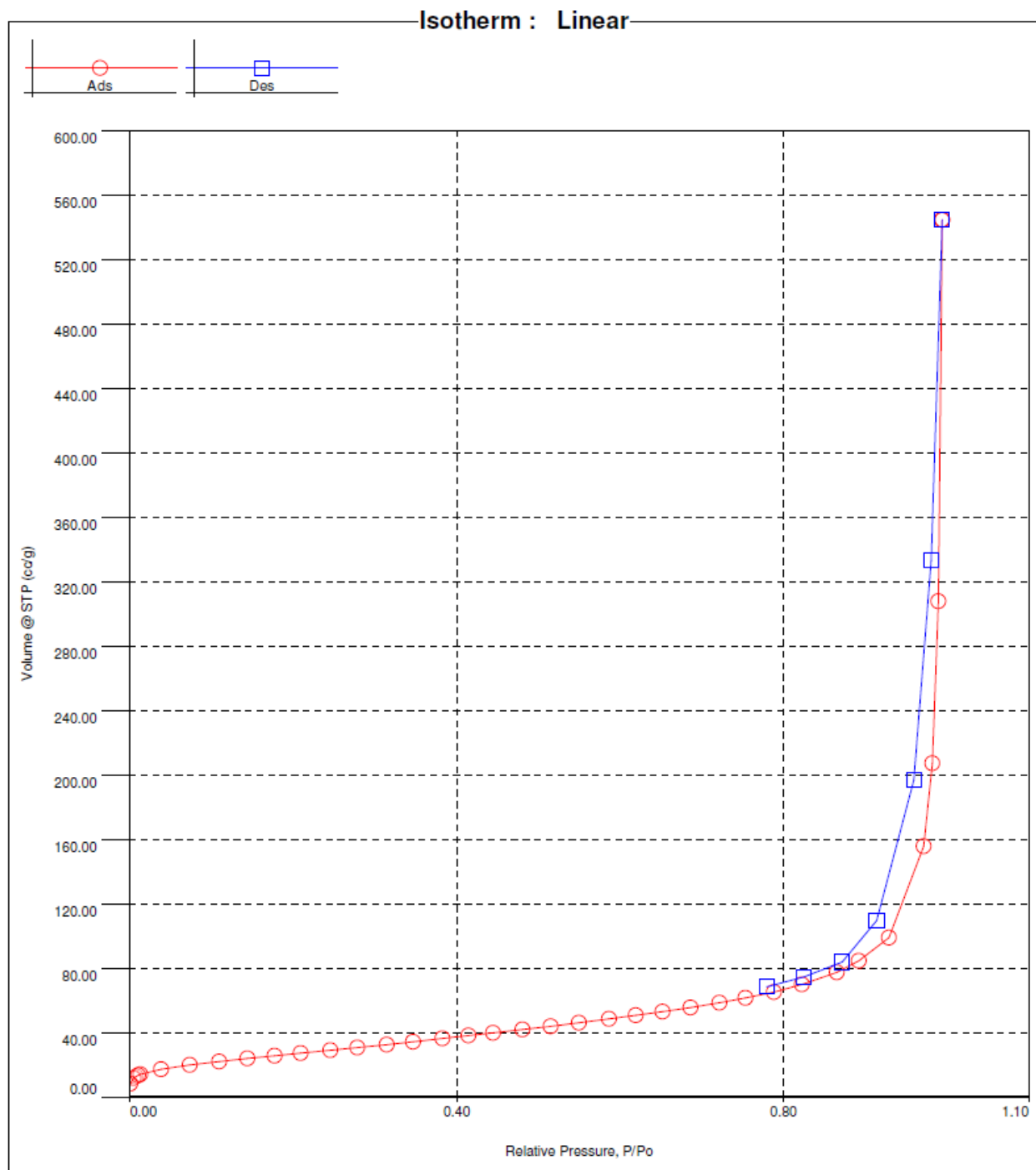


Figure S2: N₂ physisorption isotherms of the prepared alumina support material for BET and BJH analysis.

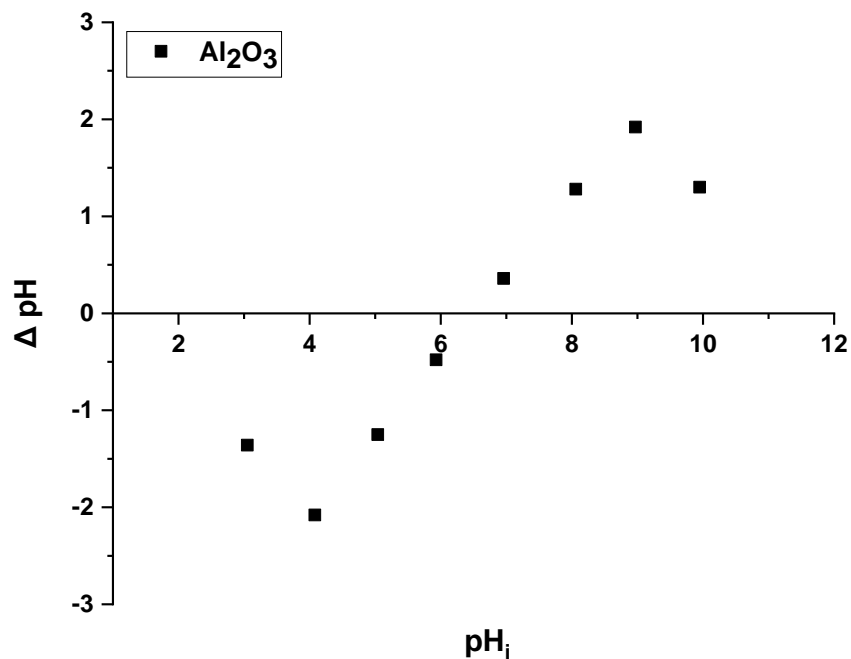


Figure S3: Point of zero charge for the prepared γ -Al₂O₃ support.

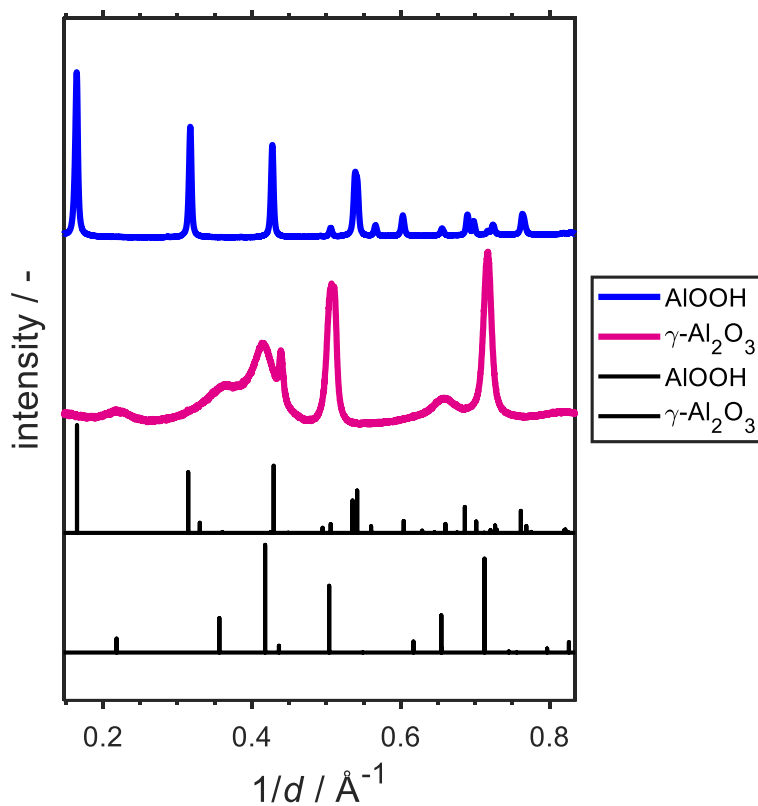


Figure S4: X-ray diffractograms of the as received boehmite precursor and of the calcined sample yielding alumina with references for AlOOH (COD-ID 9012247) and γ -Al₂O₃ (COD-ID 2015530).

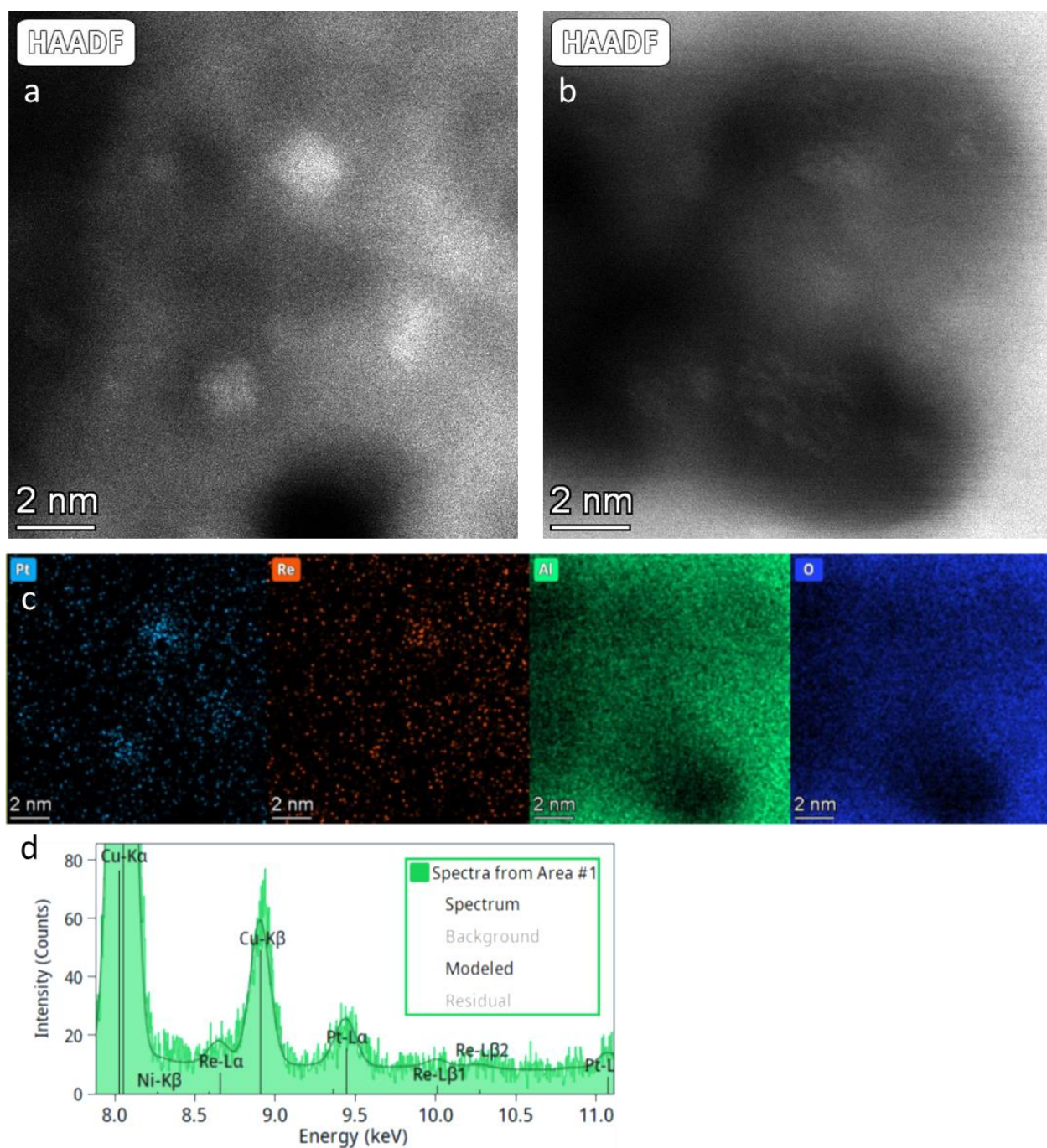


Figure S5: High-angle annular dark field scanning transmission electron micrographs (a) before and (b) after elemental mapping via energy-dispersive X-ray spectroscopy of catalyst Pt-Re 1:0.5 exhibiting sample damage of the Al₂O₃ support due to prolonged beam exposure. Note, that (c) elemental maps of Pt, Re, Al, and O and (d) the representative spectrum have to be considered with care due to identified sample damage even though the measured Al:O ratio of 2:2.97 is in good agreement with the expected ratio of 2:3.

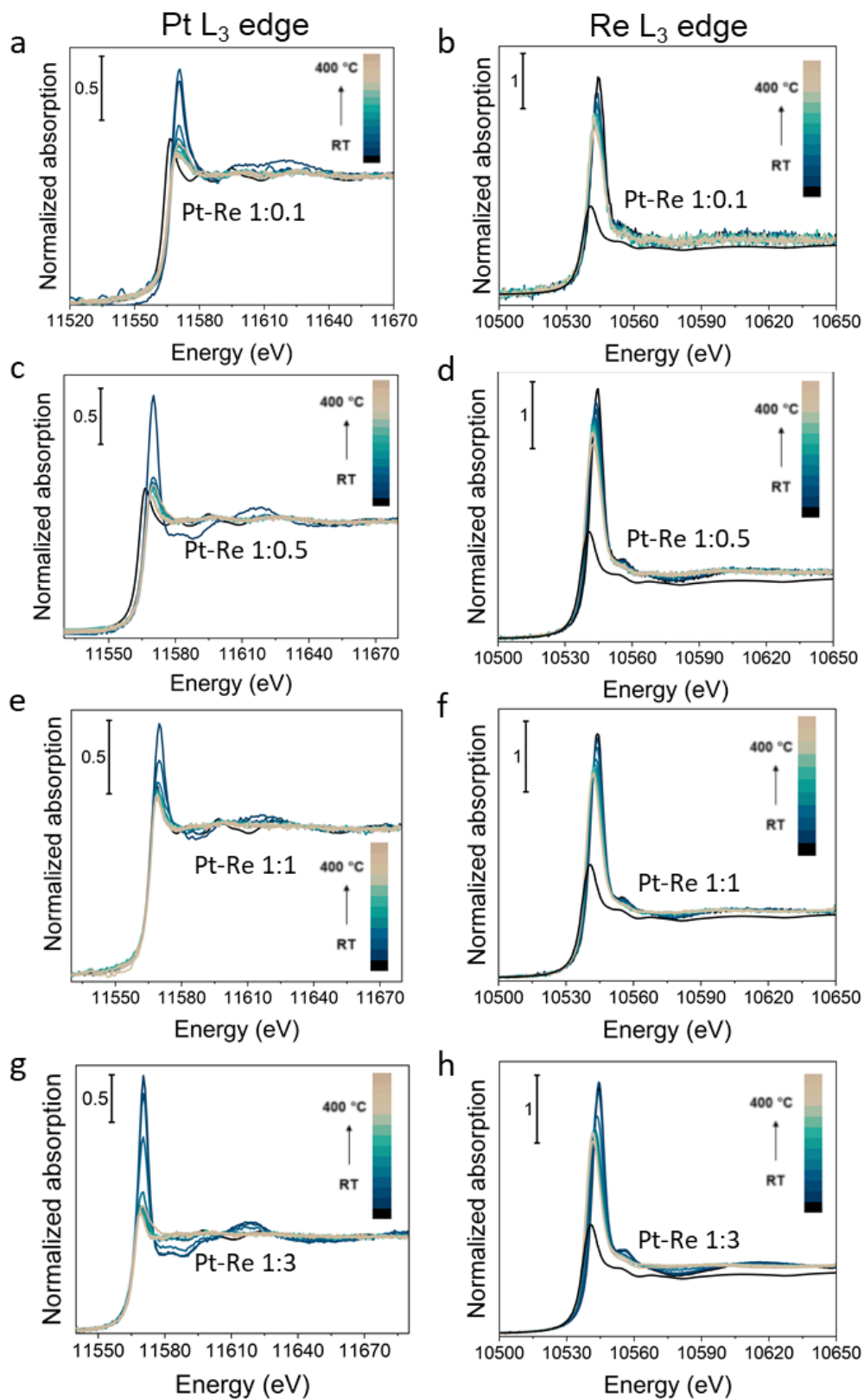


Figure S6: Comparison of *in situ* X-ray absorption near edge spectra at (a, c, e, g) the Pt and (b, d, f, h) Re L₃ edge during reduction of bimetallic Pt-Re catalysts at 400 °C with a heating rate of 10 °C min⁻¹ in 11% H₂/He. Pt and Re foil (black lines) are added as references.

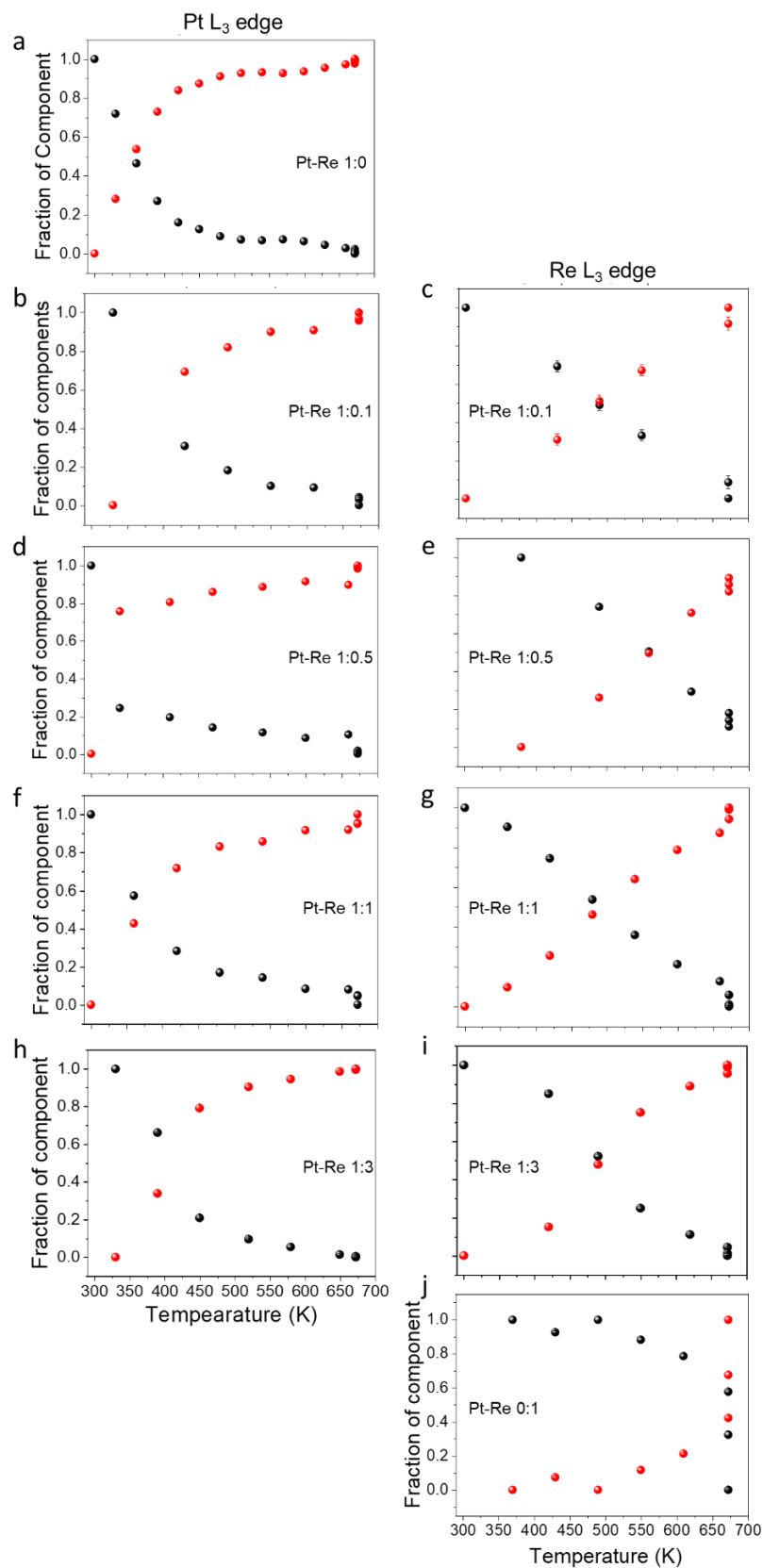


Figure S7: Linear combination analysis of X-ray absorption near edge structure spectra at the Pt (a, b, d, f, g) and Re L₃ edges (c, e, g, i, j) during TPR using the component of the first (black) and the last spectrum (red) recorded as internal reference.

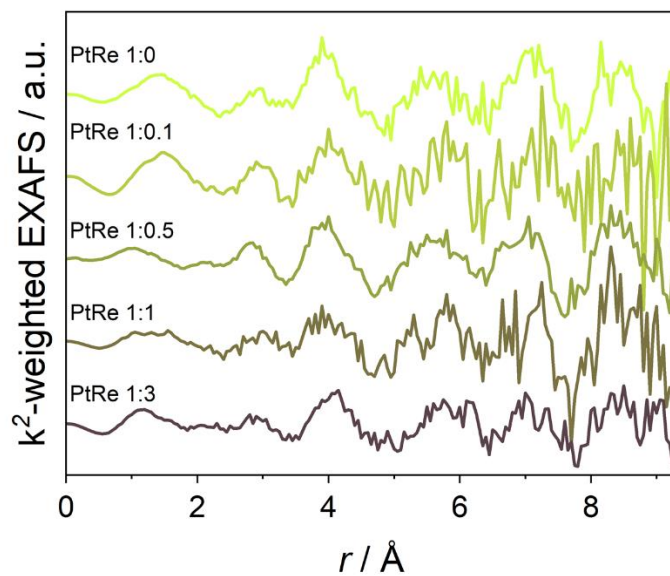


Figure S8: EXAFS spectra (Pt L₃ edge) of the bimetallic Pt-Re catalysts with various ratios after reduction at 400 °C for 30 min with 10 °C min⁻¹ in 11% H₂/He. Spectra were acquired after cool-down to room temperature in 11% H₂/He.

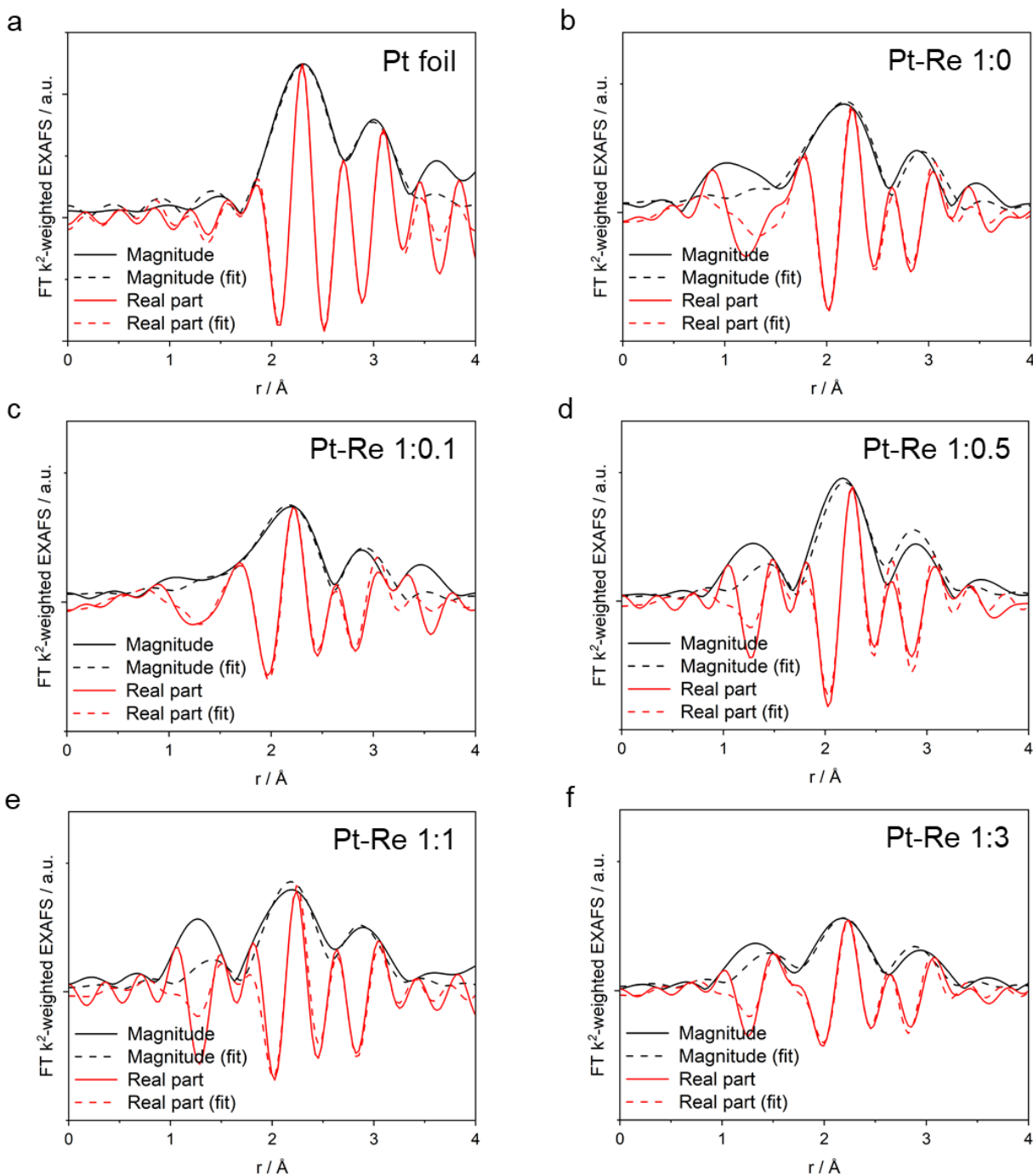


Figure S9: Fits of the Fourier-transformed EXAFS spectra (Pt L_3 edge) of (a) Pt foil and (b-f) the bimetallic Pt-Re catalysts with various ratios after reduction at 400 °C for 30 min with 10 °C min⁻¹ in 11% H₂/He. Spectra were acquired after cool-down to room temperature in 11% H₂/He.

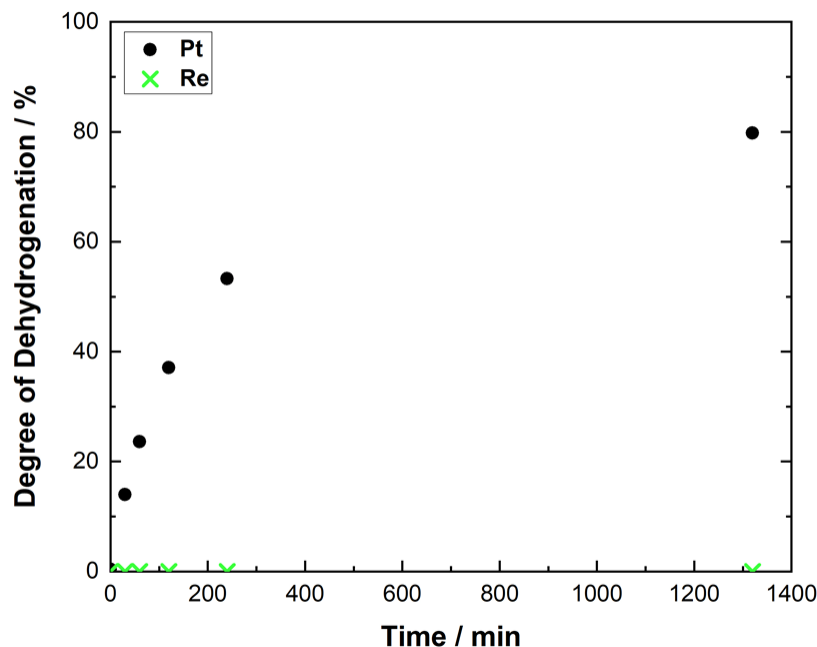


Figure S10: Degree of dehydrogenation during H₂ release from H12-BT using monometallic catalysts. Reaction conditions: 250 °C, 1 atm, 0.0001 mol_{Pt} mol⁻¹_{LOHC}, 31.01 g_{H12-BT}, 0.30 wt.% or Pt, 0.30 wt.% Re, 1320 min, 0 mL_{Ar} min⁻¹. Calculations according to Equation (5) in manuscript based on GC-FID analysis of liquid samples.

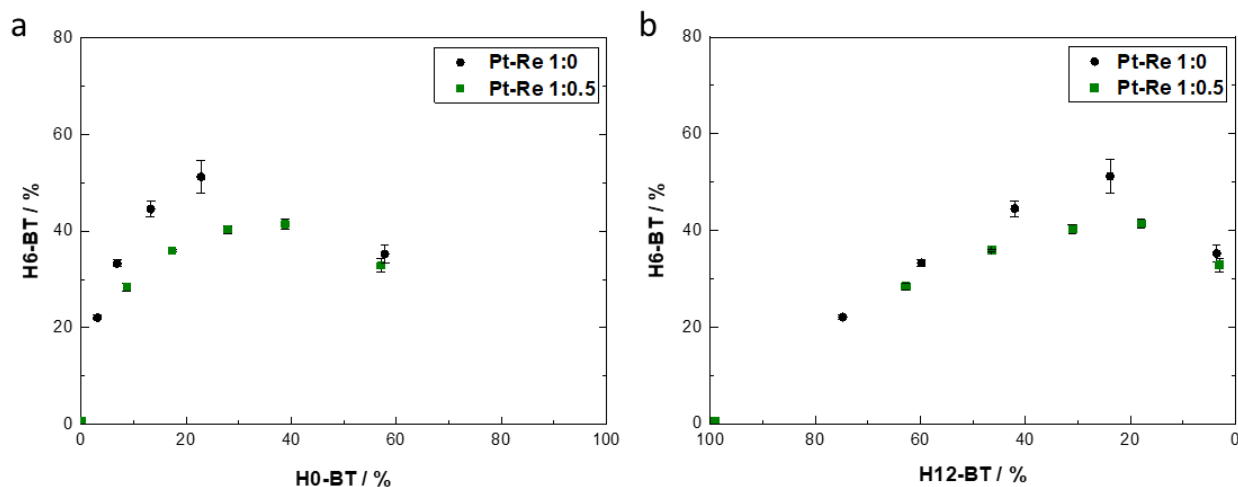


Figure S11: Relationship between the fraction of H6-BT and (a) the fraction of H0-BT or (b) formed H12-BT during H₂ release from H12-BT using monometallic Pt-Re 1:0 and bimetallic Pt-Re 1:0.5 catalysts. Reaction conditions: 250 °C, 1 atm, 0.0001 mol_{Pt} mol⁻¹_{LOHC}, 31.01 g_{H12-BT}, 0.30 wt.% Pt, 0 or 0.15 wt.% Re, 1320 min, 300 mL_{Ar} min⁻¹. Calculation based on GC-FID analyses of liquid samples.

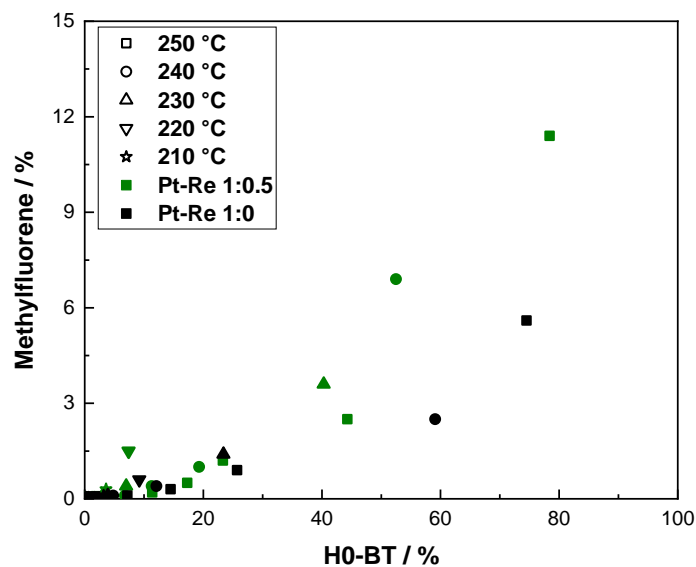


Figure S12: Formation of methylfluorene during H₂ release from H12-BT at various temperatures using monometallic Pt-Re 1:0 and bimetallic Pt-Re 1:0.5 catalysts. Reaction conditions: 210-250 °C, 1 atm, 0.0001 mol_{Pt} mol⁻¹_{LOHC}, 31.01 g_{H12-BT}, 0.30 wt.% Pt, 0 or 0.15 wt.% Re, 240 min, 300 mL_{Ar} min⁻¹. Calculation based on GC-FID analyses of liquid samples.

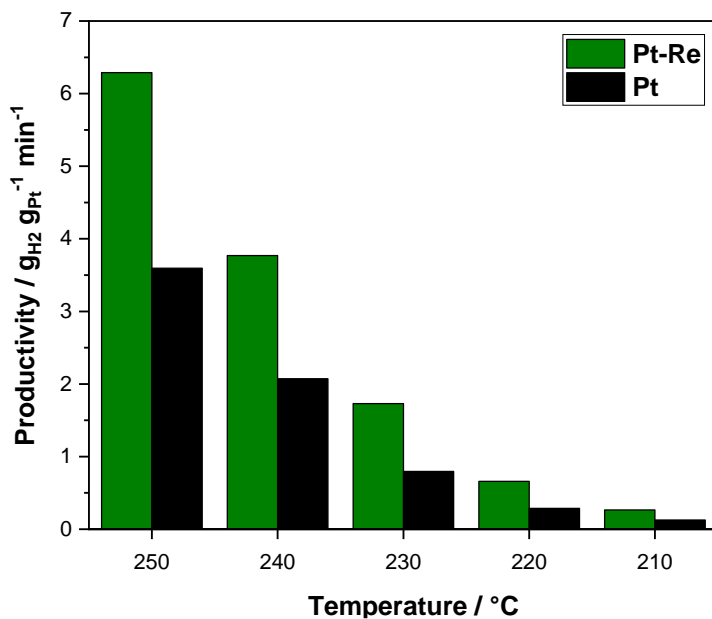


Figure S13: Productivity of Pt during H₂ release from H12-BT at various temperatures using monometallic Pt-Re 1:0 and bimetallic Pt-Re 1:0.5 catalysts. Reaction conditions: 210-250 °C, 1 atm, 0.0001 mol_{Pt} mol⁻¹_{LOHC}, 31.01 g_{H12-BT}, 0.30 wt.% Pt, 0 or 0.15 wt.% Re, 240 min, 300 mL_{Ar} min⁻¹. Calculation based on TCD measurements of H₂ release.