Supplementary Information

Impact of Impurities in Covalent Organic Frameworks on Catalytic Properties of Supported Isolated Pd Complexes

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Surface Area & Pore Size Distribution

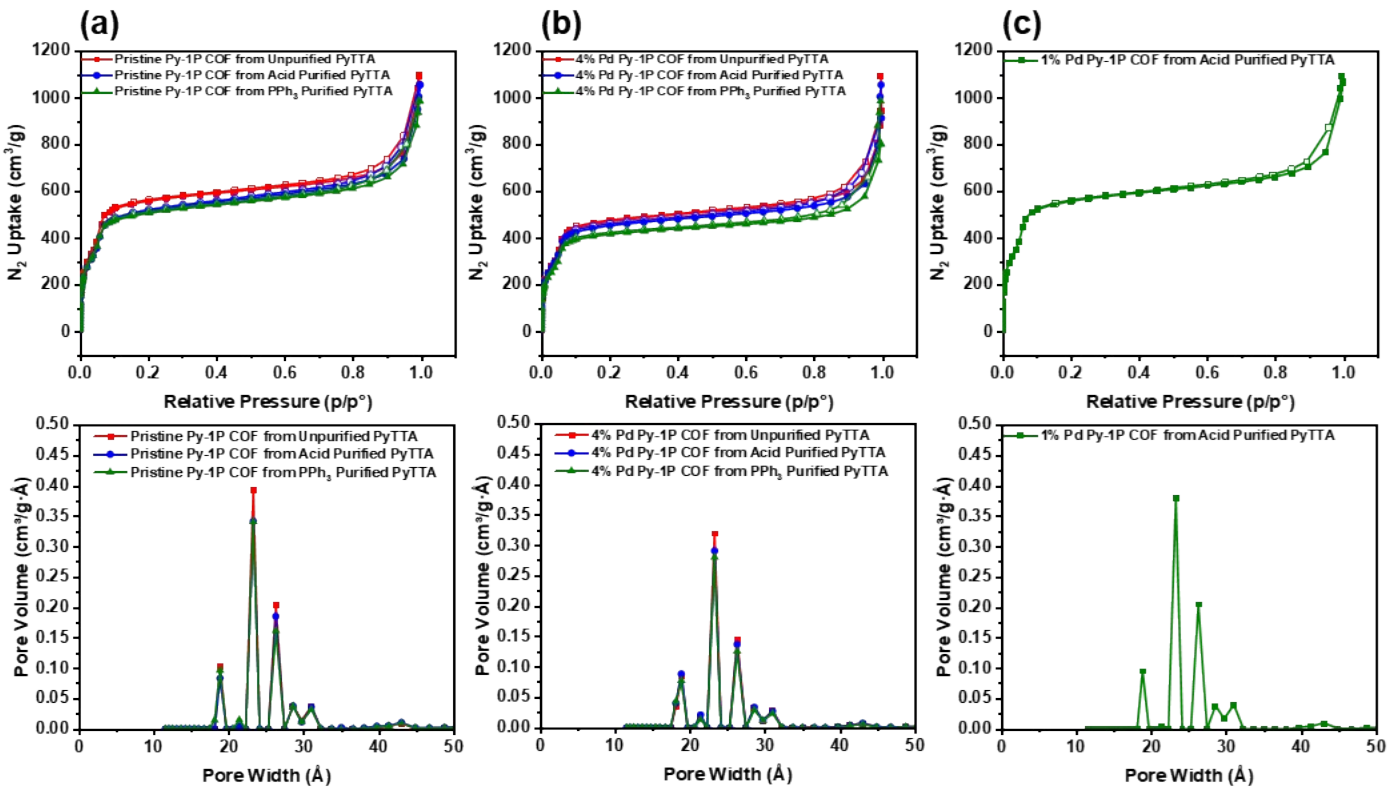

Figure S1: (Top) N_2 absorption isotherm and (bottom) pore size distribution of (a) pristine, (b) 4 wt. % Pd, and (c) 1 wt. % Pd Py-1P COF samples from PyTTA of various purifications.

Powder X-ray Diffraction (XRD)

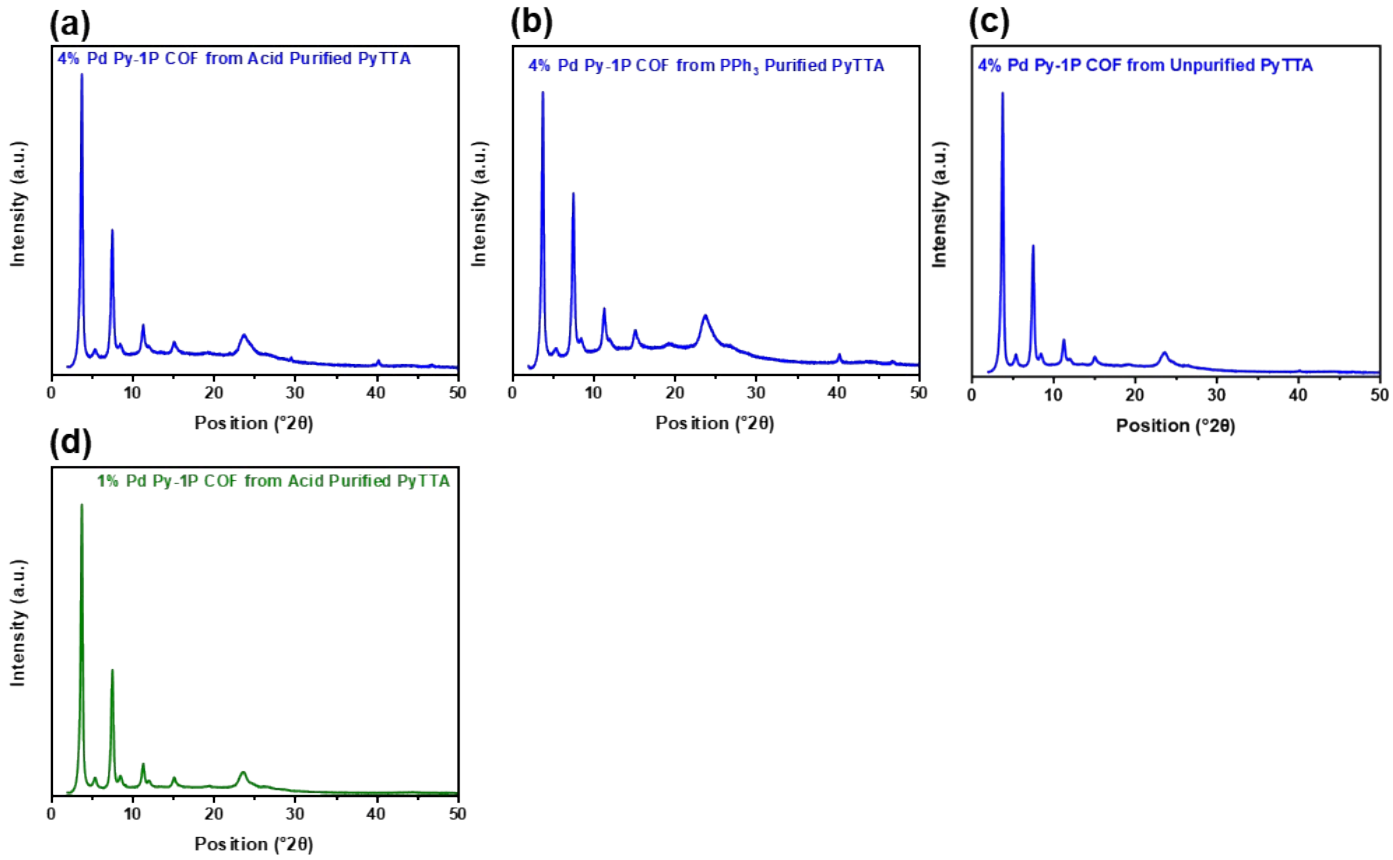

Figure S2: XRD spectra of (left) pristine, (middle) 4 wt. % Pd, and (right) 1 wt. % Pd Py-1P COF from (top) unpurified, (middle) acid purified, and (bottom) PPh_3 purified PyTTA.

X-ray Photoelectron Spectroscopy (XPS)

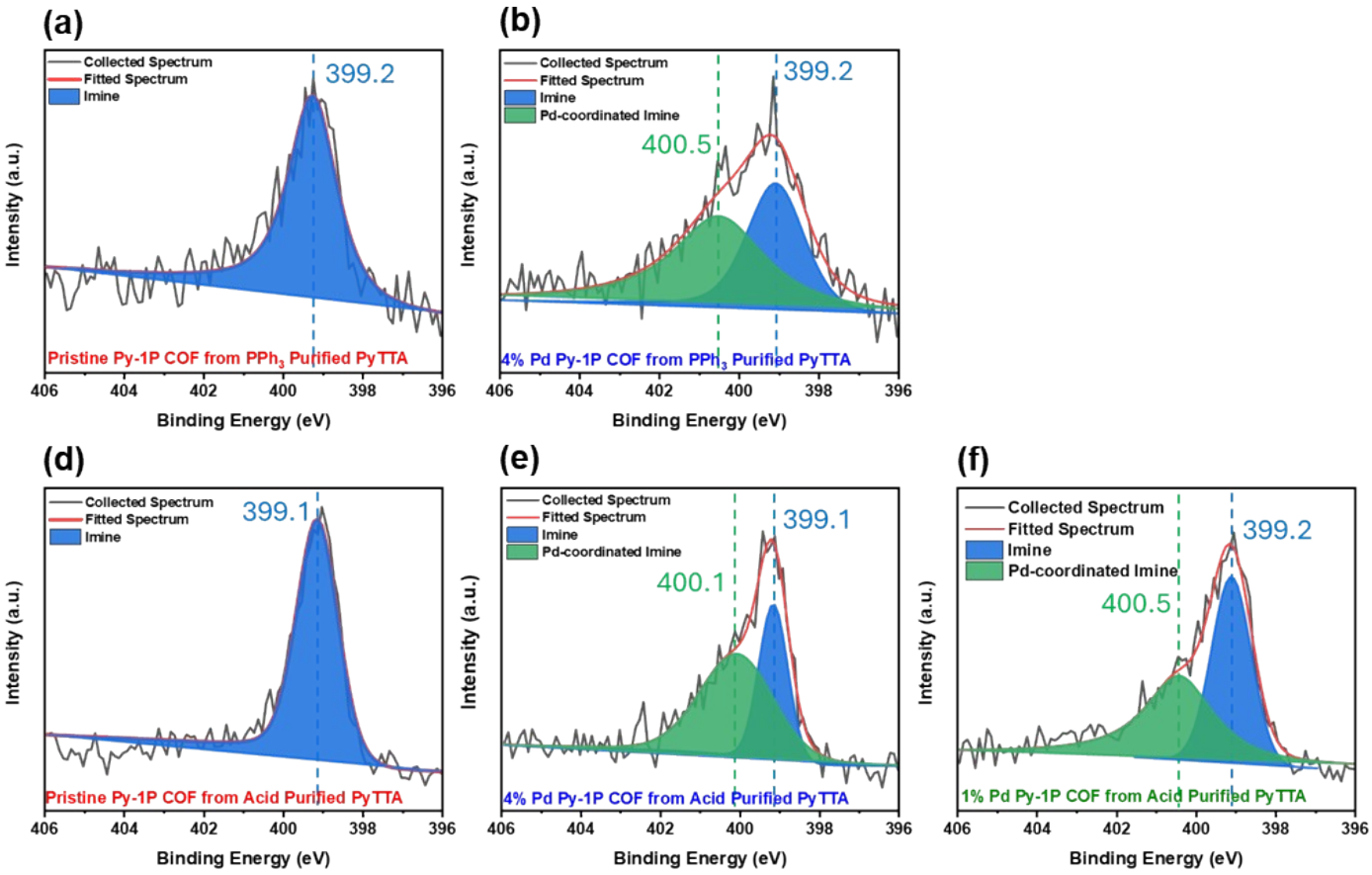

Figure S3: Nitrogen XPS spectra of (left) pristine, (middle) 4 wt. % Pd, and (right) 1 wt. % Pd Py-1P COF from (top) PPh_3 purified and (bottom) acid purified PyTTA.

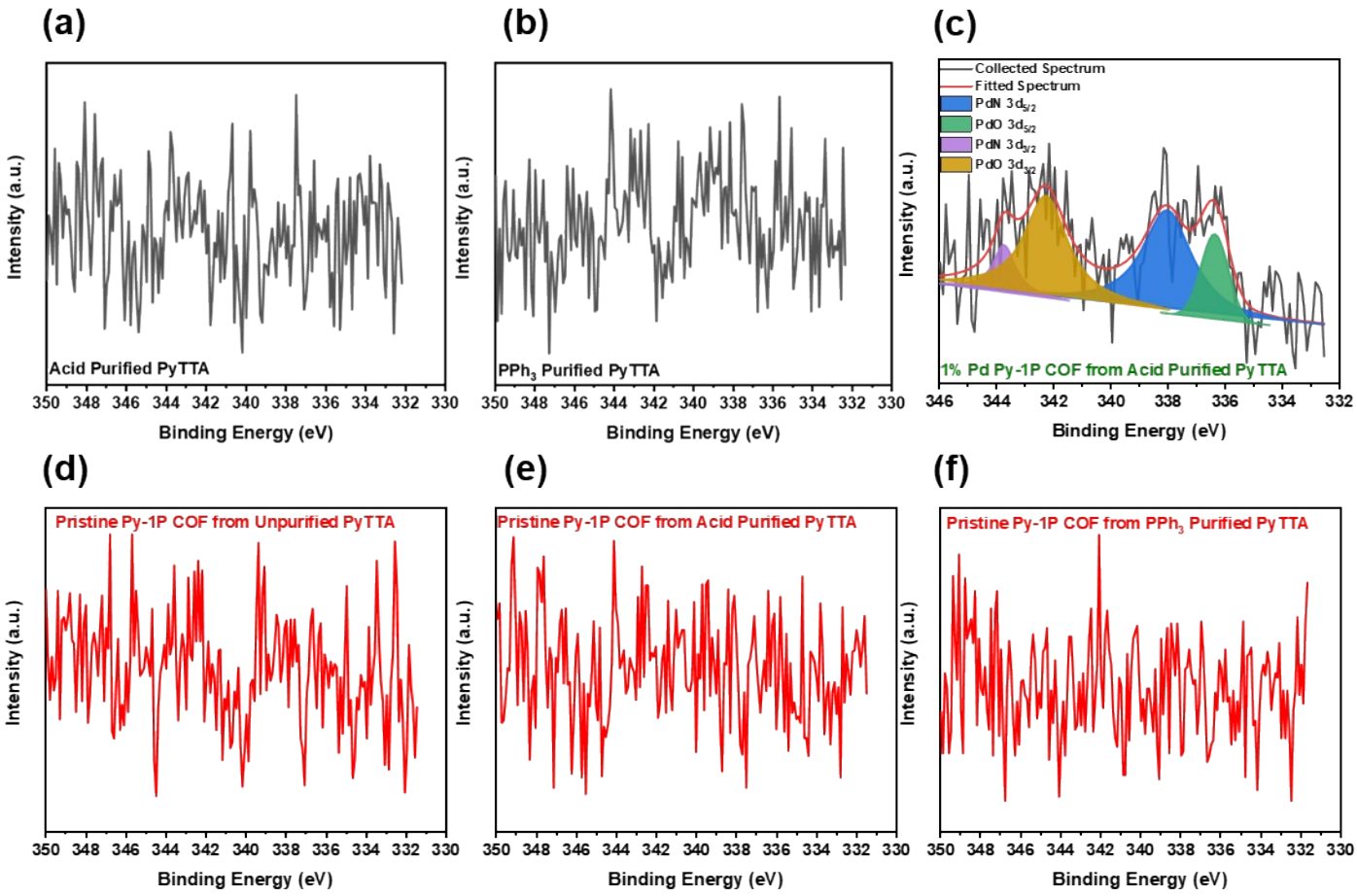

Figure S4: Palladium$_{3d}$ XPS spectra of (a) acid purified PyTTA, (b) PPh_3 purified PyTTA, (c) 1 wt. % Pd Py-1P COF from acid purified PyTTA , (d) pristine Py-1P COF from unpurified PyTTA, (e) pristine Py-1P COF from acid purified PyTTA and (f) pristine Py-1P COF from PPh_3 purified PyTTA.

Scanning Electron Microscopy (SEM)

The samples were adhered to a stage using a carbon-based tape, coated in gold at 10 mA and 10 Pa for 120 s prior to image capturing, and collected on a Hitachi SU-70 Scanning Electron Microscope.

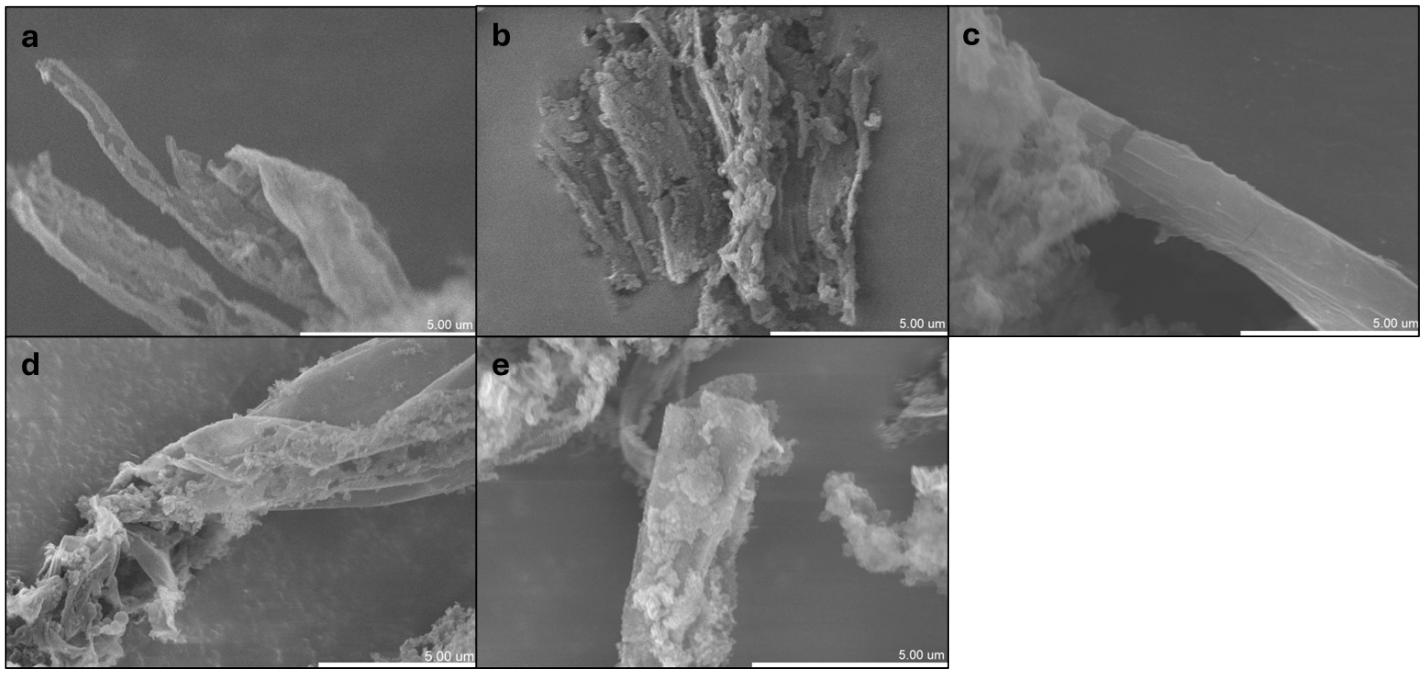

Figure S5: SEM images of (a) pristine Py-1P COF from acid purified PyTTA, (b) pristine Py-1P COF from PPh_3 purified PyTTA, (c) pristine Py-1P COF from unpurified PyTTA, (d) 1 wt. % Pd Py-1P COF from acid purified PyTTA, and (e) 4 wt. % Pd Py-1P COF from PPh_3 purified PyTTA.

Energy-Dispersive X-ray (EDX) Elemental Mapping

The samples were adhered to a stage using a carbon-based tape, coated in gold at 10 mA and 10 Pa for 120 s prior to image capturing, and collected on a Hitachi SU-70 Scanning Electron Microscope.

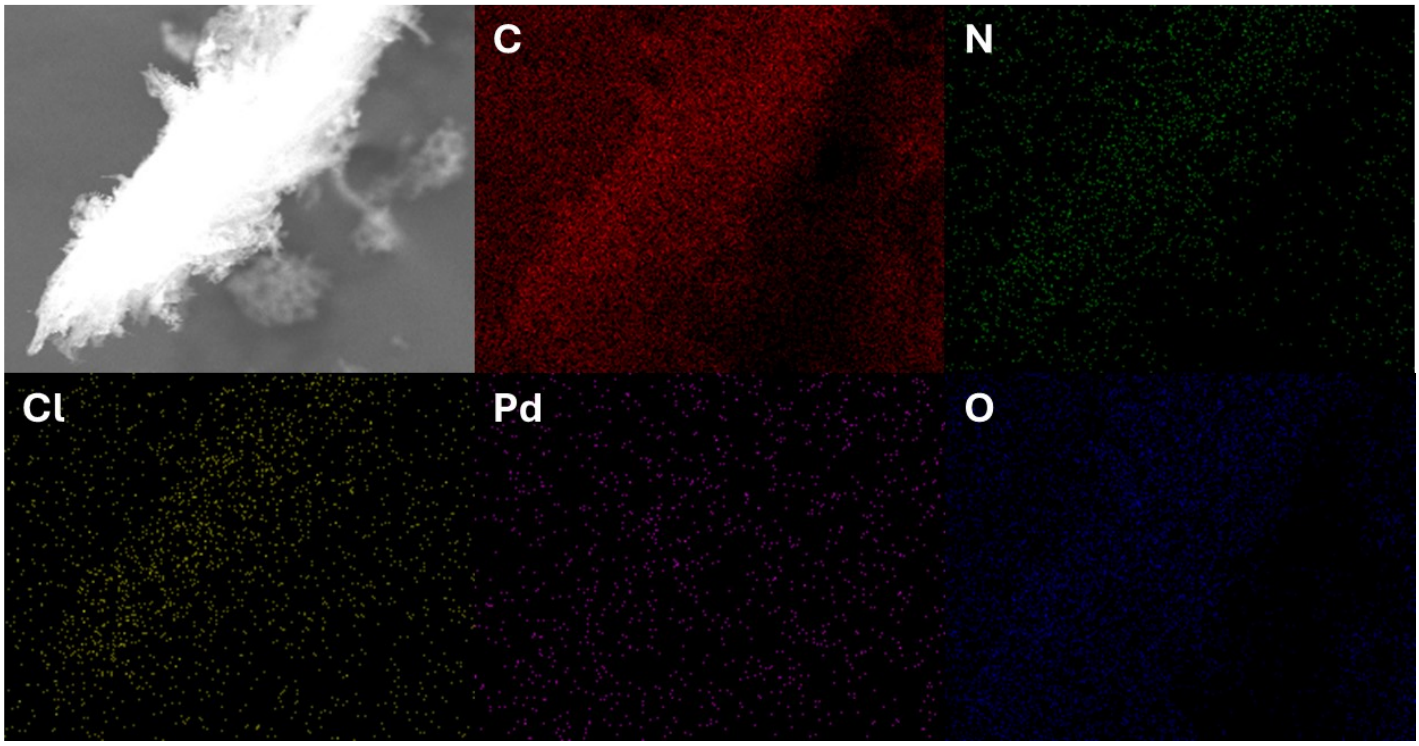

Figure S6: Elemental mapping of pristine Py-1P COF from acid purified PyTTA.

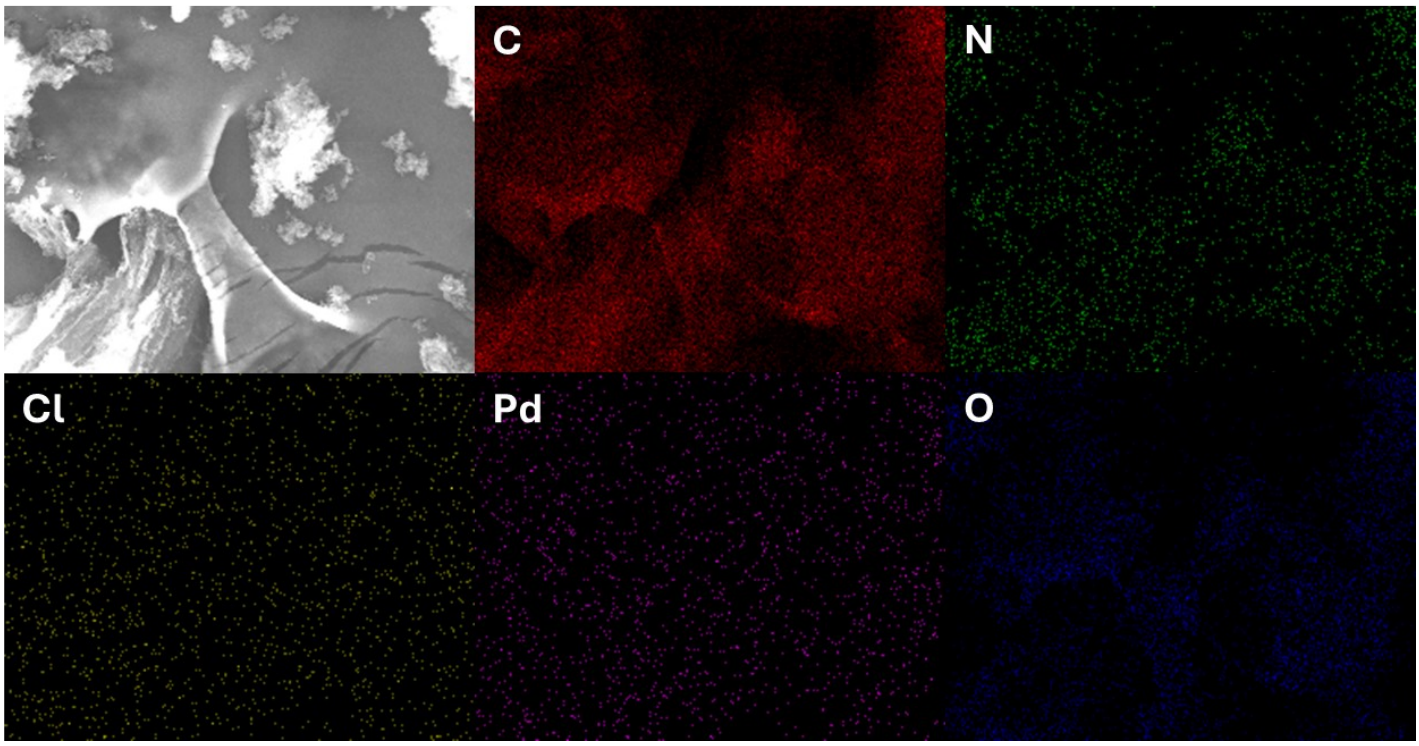

Figure S7: Elemental mapping of pristine Py-1P COF from PPh_3 purified PyTTA.

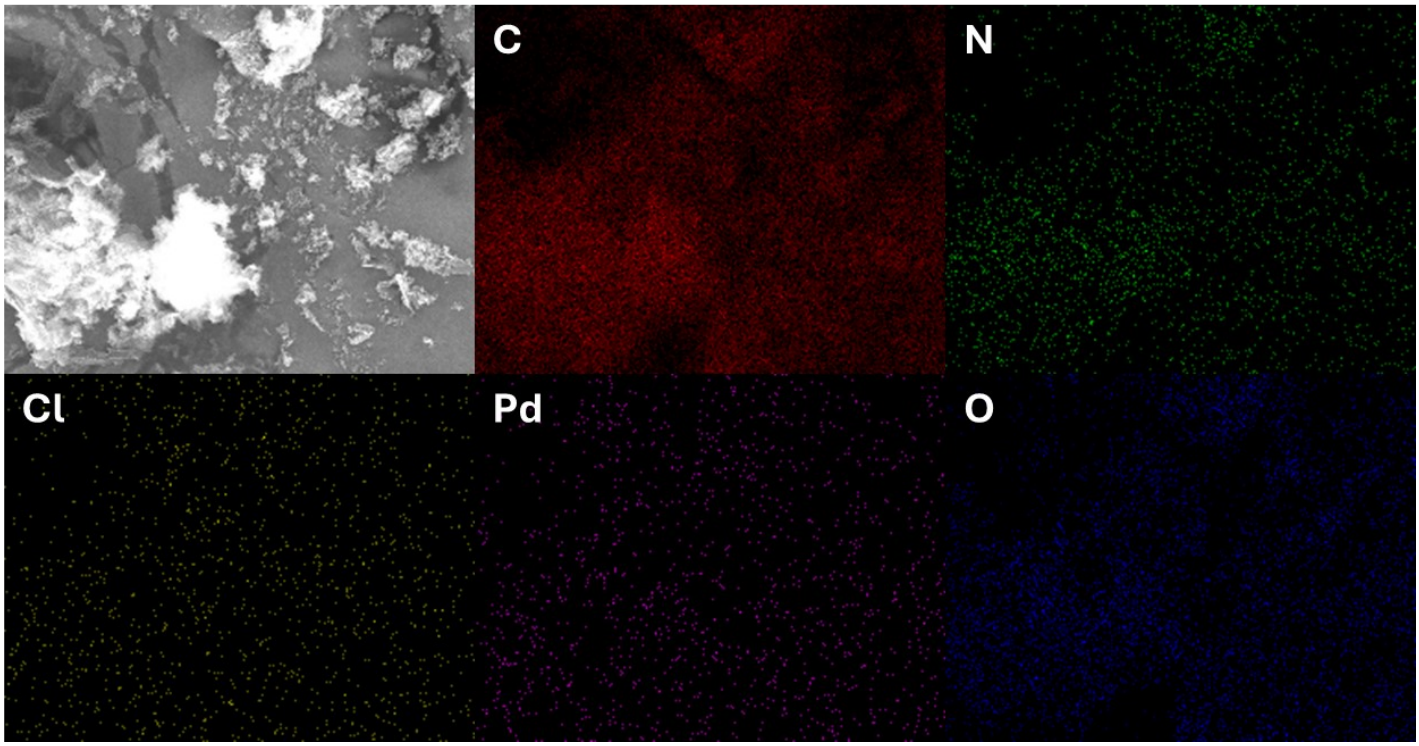

Figure S8: Elemental mapping of pristine Py-1P COF from unpurified PyTTA.

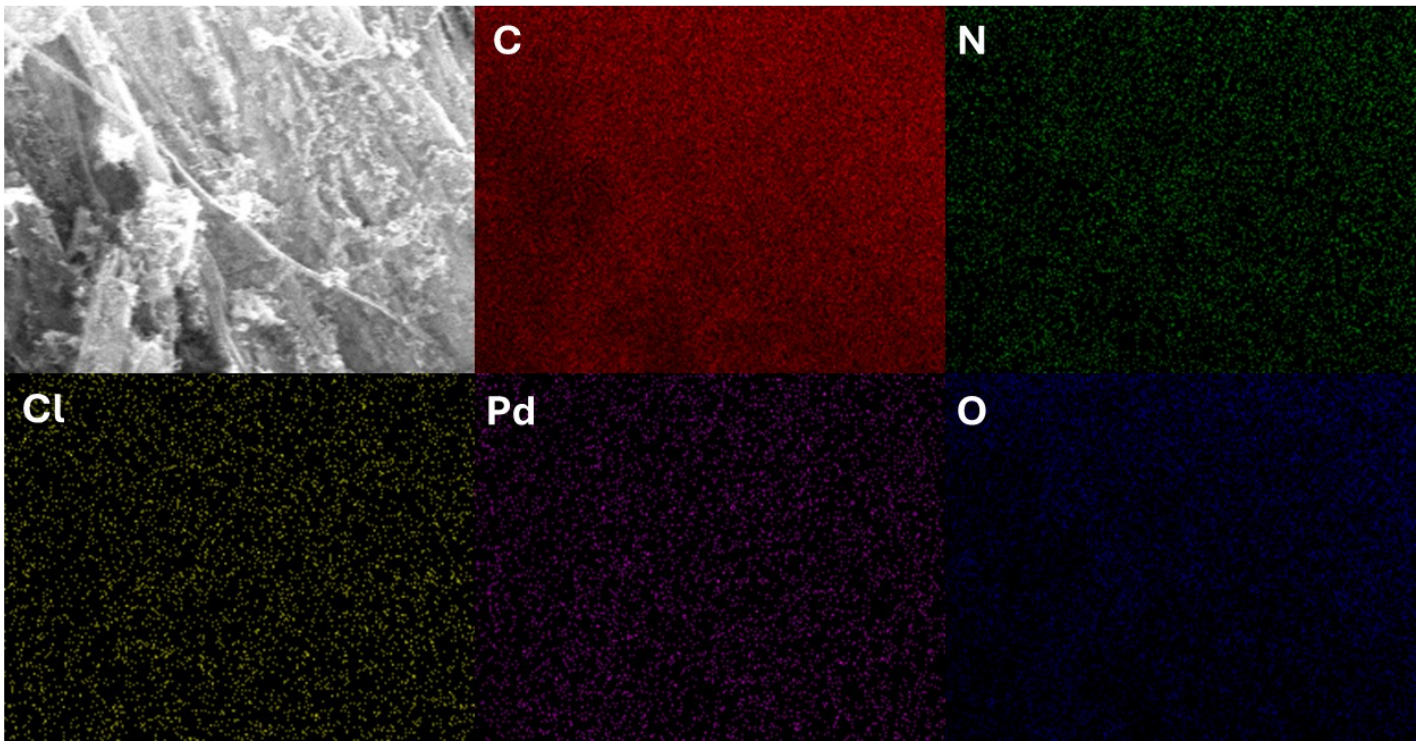

Figure S9: Elemental mapping of 1 wt. % Pd Py-1P COF from acid purified PyTTA.

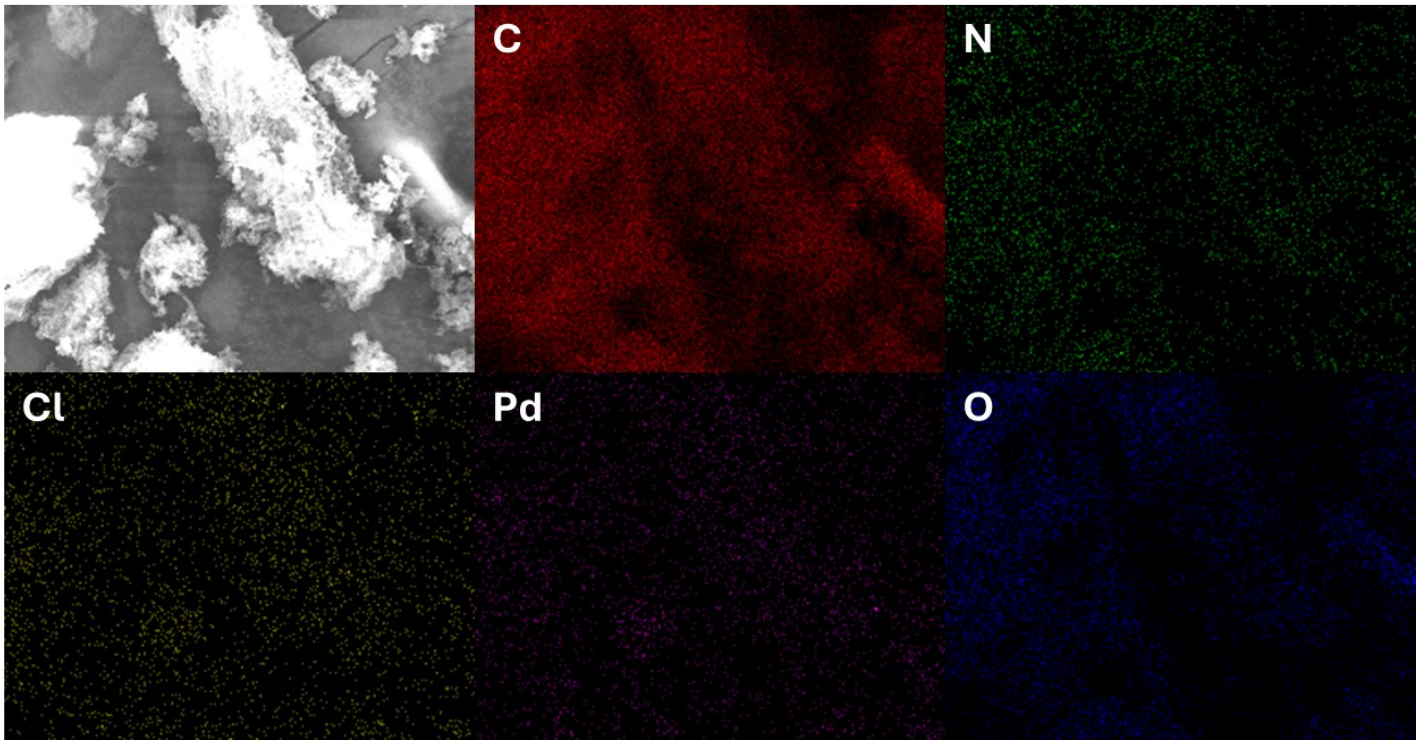

Figure S10: Elemental mapping of 4 wt. % Pd Py-1P COF from PPh_3 purified PyTTA.

Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS)

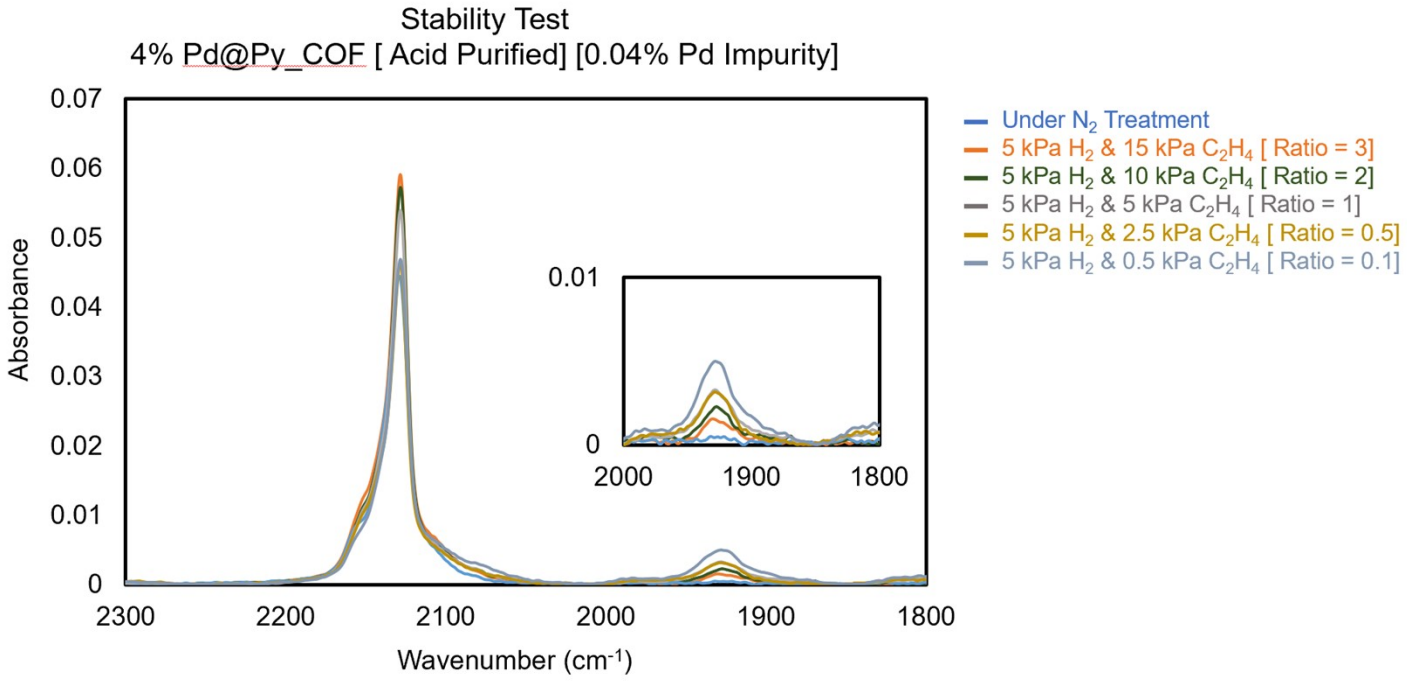

Figure S11: Stability test for 4 wt. % Pd Py-1P COF from acid purified PyTTA by varying hydrogen and ethylene partial pressure ratio.

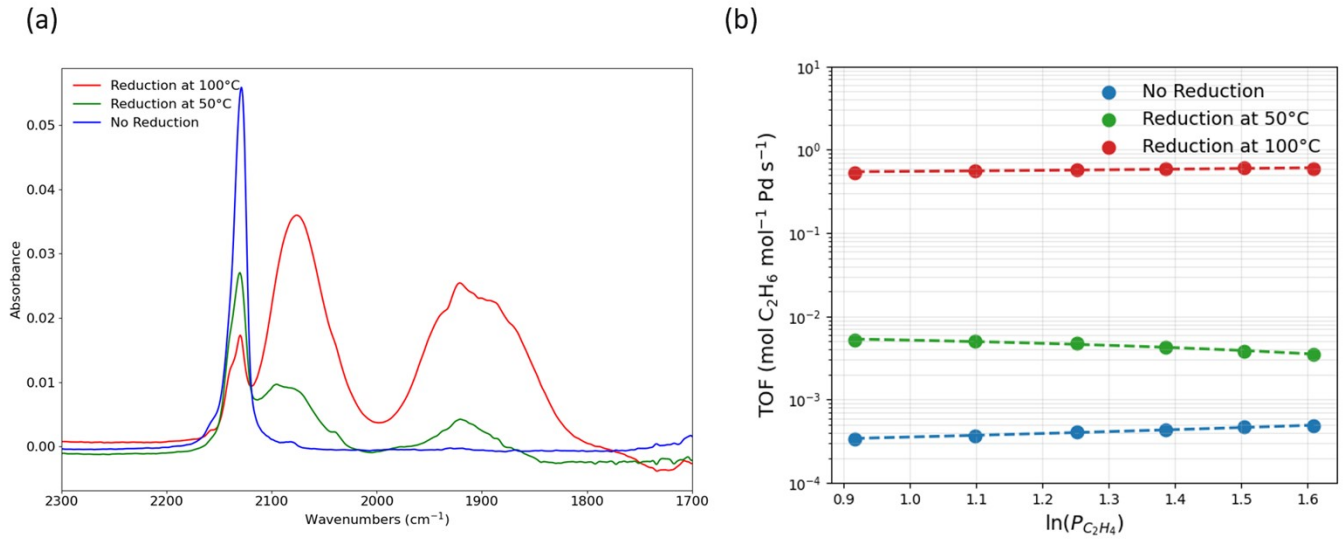

Figure S12: (a) CO-DRIFTS spectra of 1 wt% Pd@Py-COF [PPh_3 Purified] under reduction environment for two different temperatures (50 °C and 100 °C), (b) Corresponding TOF values for ethylene hydrogenation as a function of ethylene partial pressure after each pretreatment.

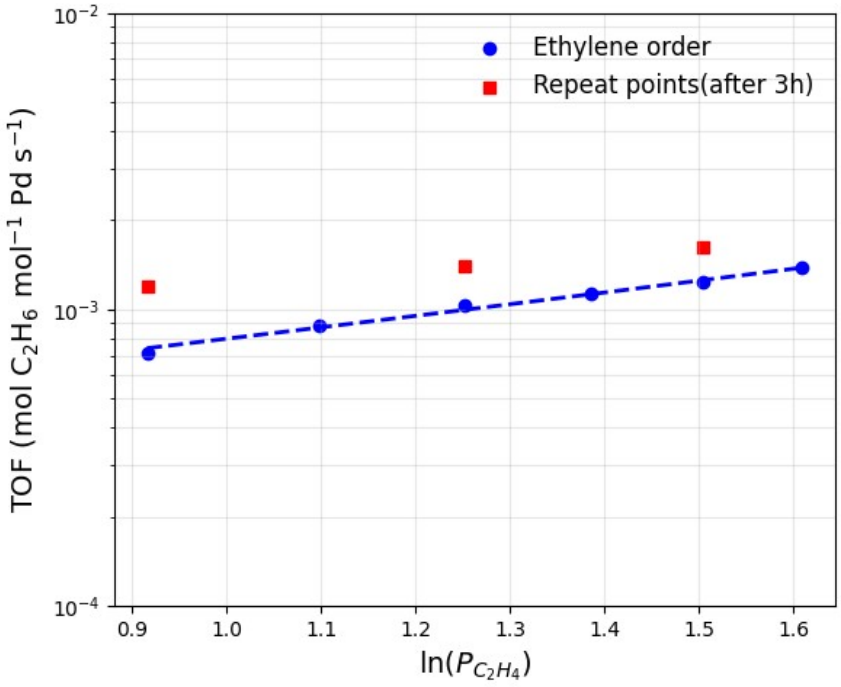

Figure S13: Stability test of the 1% $PdCl_2$@Py-1P COF. Dependence of TOF on C_2H_4 partial pressure was measured at a constant H_2 partial pressure of 5 kPa. The stability test was performed at the initial condition after ~3 h measurement.