SUPPORTING INFORMATION

OX-1 METAL-ORGANIC FRAMEWORK NANOSHEETS AS ROBUST HOSTS FOR HIGHLY ACTIVE CATALYTIC PALLADIUM SPECIES

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Experimental Methods

Electron Microscopy

Scanning Electron Microscope (SEM) images were acquired on a Carl Zeiss Evo LS15 VP-Scanning Electron Microscope with a secondary electron detector, 15 kV accelerating voltage and 8 mm working distance. The crystals were sampled before the final centrifugation step of the synthesis and drop cast onto polished Al stubs. The samples were gold coated with a sputter coater in an Ar atmosphere.

Before transmission electron microscopy (TEM) observations the samples were deposited on the 3 mm carbon-coated copper grids (200 mesh) from suspension in isopropyl alcohol. Samples morphology was studied using Hitachi HT7700 transmission electron microscope. Images were acquired in bright-field TEM mode at 100 kV accelerating voltage.

X-Ray Diffraction

Powder X-ray diffraction (PXRD) patterns were collected using a benchtop Rigaku MiniFlex diffractometer with a 1D syntilation counter detector and a Cu Kα X-ray source. Samples were loaded into a 20×20×0.5 mm sample holder and weighed before measurement. The measurements were carried out with a step size of 0.02° at a speed of 1°min^{-1}. The patterns were then normalised by the mass of of the samples.

Inelastic Neutron Scattering

Inelastic neutron scattering (INS) measurements were conducted using the TOSCA spectrometer[1-2] at the ISIS Pulsed Neutron and Muon Source, Rutherford Appleton Laboratory (Chilton, UK). The high-resolution ($\Delta E/E \sim 1.25\%$) and broadband (0 – 4,000 cm^{-1}) spectra of each sample (~1 g) were collected at approximately 10 K.

TOSCA is an indirect geometry time-of-flight spectrometer where a pulsed, polychromatic beam of neutrons collide with the sample at a distance of ~17 m from the source. The scattered neutrons are then Bragg-reflected by a pyrolytic graphite analyser, and higher-order reflections beyond (002) are suppressed by a cooled ($T < 50$ K) beryllium (Be) filter, to selectively analyze neutrons of a consistent final energy. Therefore, neutrons with a final energy of approximately 32 cm^{-1} (~1 THz) are passed towards the ^{3}He detector bank. The detector array consists of a total of ten banks each having thirteen ^{3}He tubes with an effective length 250 mm. Five banks are located in the forward direction (scattering angle ~45°) and five in the backwards direction (~135°).

The use of a low (fixed) final energy translates into a direct relationship between energy transfer (E_T, cm^{-1}) and momentum transfer (Q, Å^{-1}) such that $E_T \approx 16Q^2$. Energy transfer and spectral intensity i.e. $S(Q, \omega)$ can then be obtained using the Mantid software.[3] A disc chopper is positioned to prevent frame overlap at a distance of 9.455 m from the moderator centre. The sample was wrapped in a 4×4 cm^2 aluminium foil sachet and placed in a 2 mm spaced stainless steel cell. To reduce the impact of the Debye–Waller factor on the observed spectral intensity the sample was cooled to approximately 10 K by a closed cycle refrigerator, and the spectra were recorded for 4-6 hours.

The neutron guide upgrade of the TOSCA spectrometer was completed in 2017, which has increased the neutron flux at the sample position by as much as 82 times.[4] This enables faster INS measurements and the use of a smaller sample mass.

Synchrotron Specular Reflection Infra-Red Spectroscopy

The specular reflection experiments were conducted at Beamline B22 MIRIAM in the Diamond Light Source synchrotron (Harwell Campus, Oxfordshire). High-resolution specular reflection measurements were carried out in a Bruker Vertex 80V FTIR interferometer, equipped with the Pike Technologies VeeMAX II variable angle specular reflectance accessory.

Synchrotron IR reflectivity spectra were collected on samples of pressed-powder pellets (diameter = 13 mm, thickness ~1 mm) prepared under uniaxial compression of 50 MPa pressure. XRD measurements were carried out to confirm the crystallinity of the pellets, shown in Figure 1 Specular reflection was obtained at an angle of 30° from the normal to the pellet's surface, where IR spectra were collected with a resolution of 2 cm^{-1} and 512 scans per spectral scan. Vacuum was pumped to better than 10^{-5} bar and maintained at room temperature (21°C). The synchrotron far-IR (FIR) measurements were performed for the spectral range 1000-0 cm^{-1} while the mid-IR (MIR) for the range 10000-0 cm^{-1}. The background spectra were collected by measuring the reflectance from a mirror once before the FIR measurements and once before the MIR measurements.

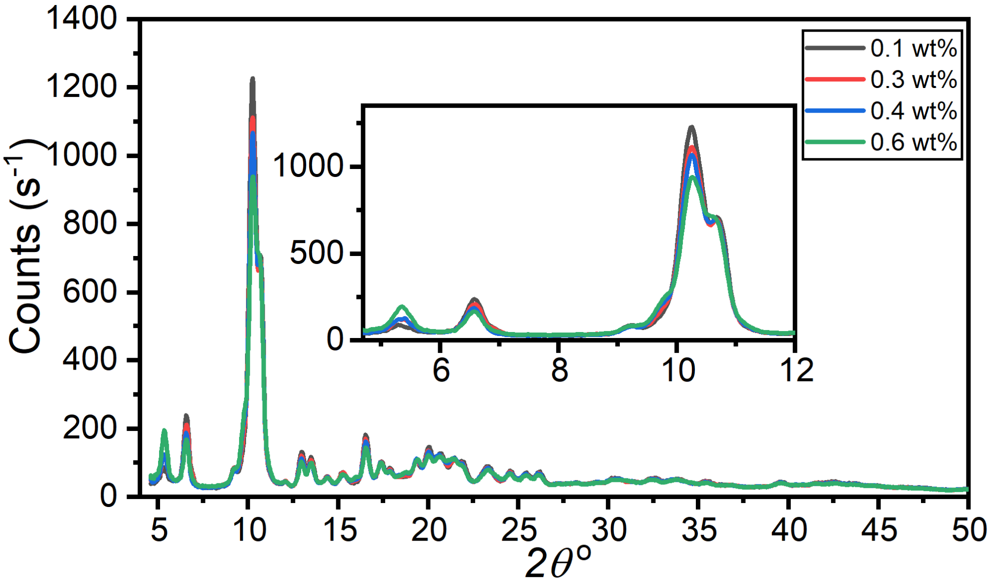

Figure 1. XRD patterns of Pd@OX-1 pellets pressed at 50 MPa showing retained structure of OX-1.

A custom MATLAB routine for a Kramers-Kronig transform was applied to the raw data, which is detailed in a previous publication.[5]

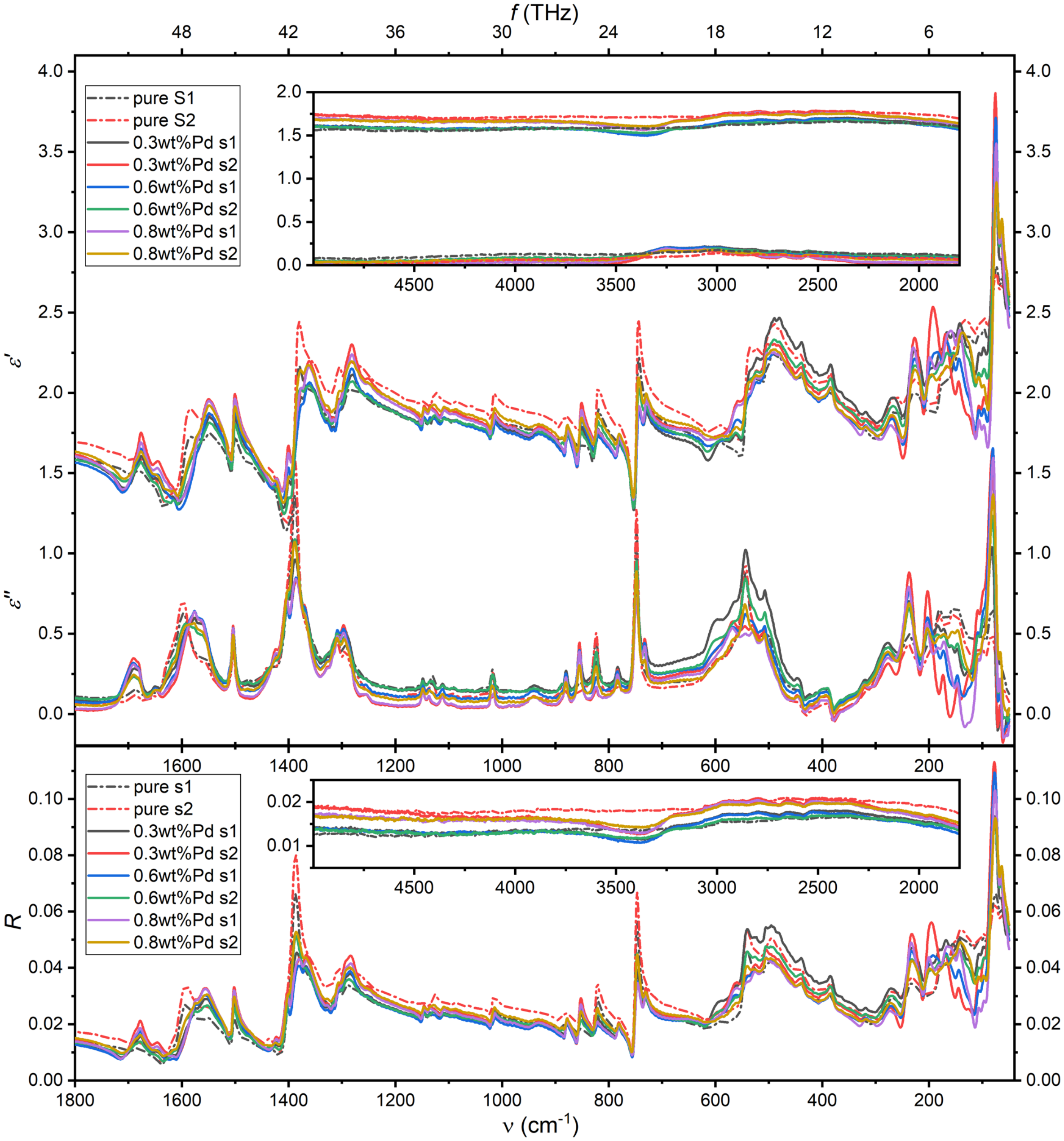

Figure 2. Specular reflection IR results: reflectivity spectra (R) and its Kramers-Kronig transformation[5] into the real (ε') and imaginary (ε'') parts of the dielectric function.

Catalytic Studies

General considerations The NMR measurements were performed using a Bruker DRX 500 spectrometer operating at 500.1 MHz for ^{1}H spectra; chemical shifts were measured relative to TMS as internal standard; all the measurements were performed at room temperature and processed using TopSpin 4.0 software package.

The GC measurements were performed with an Agilent 7890 GC system equipped with an Agilent 5977A mass-selective detector (electron ionization, 70 eV) or with a SCION 436-GC system with a flame ionization detector. Both systems were equipped with HP-5MS column (30 m × 0.25 mm × 0.25 μm film) using He as the carrier gas at a constant linear velocity of 30 $cm\times s^{-1}$. The following temperature program was used in all the GC-MS measurements: initial temperature: 60 °C, hold for 2 min, then 20 $°C\times min^{-1}$ to 300 °C and hold for 6 min. Data processing was conducted using Bruker Data Analysis 4.0 (GC-MS) or CompassCDS (GC-FID) software packages.

Suzuki reaction

General procedure for the Suzuki reaction. For all the reactions 0.2 wt.% Pd@OX-1 was used as a catalyst source. A screw-top reaction tube was charged with aryl halide (5×10^{-4} mol), Pd@OX-1 (from 1 to 100 mg; 1×10^{-8} to 1×10^{-6} mol in Pd), phenylboronic acid (73.2 mg, 6×10^{-4} mol), potassium carbonate (110.6 mg, 8×10^{-4} mol), and 1 mL of MeOH:H_2O (1:1) or *i*-PrOH:H_2O (1:1). The tube was equipped with magnetic stirring bar, then sealed tightly, and placed into a hot plate (from 100 °C to 150 °C) with continuous stirring. After specified time (from 1 h to 24 h) reaction mixture was cooled to room temperature and analyzed by GC-MS.

Variation of palladium loadings in the Suzuki reaction. A screw-top reaction tube was charged with iodobenzene (102.0 mg, 5×10^{-4} mol), Pd@OX-1 (from 1 to 100 mg; 1×10^{-8} (0.002 mol%) to 1×10^{-6} mol (0.2 mol%) in Pd), phenylboronic acid (73.2 mg, 6×10^{-4} mol), potassium carbonate (110.6 mg, 8×10^{-4} mol), and 1 mL of MeOH:H_2O (1:1). The tube was equipped with magnetic stirring bar, then sealed tightly, and placed into a hot plate (from 100 °C to 150 °C) with continuous stirring. After specified time (from 4 h to 24 h) reaction mixture was cooled to room temperature and analyzed by GC-MS.

Recycling of Pd@OX-1 in the Suzuki reaction. A screw-top reaction tube was charged with iodobenzene (102.0 mg, 5×10^{-4} mol), Pd@OX-1 (25 mg; 2.5×10^{-7} mol (0.05 mol%) of Pd), phenylboronic acid (73.2 mg, 6×10^{-4} mol), potassium carbonate (110.6 mg, 8×10^{-4} mol), and 1 mL of *i*-PrOH:H_2O (1:1). The tube was equipped with magnetic stirring bar, then sealed tightly, and placed into a hot plate at 100 °C with continuous stirring. After 1 h reaction mixture was cooled to room temperature and analyzed by GC-FID. Product was extracted with acetone (5 mL), material was washed with 5 mL of water, and washed with additional 5 mL of acetone. Dried material was used under exactly the same conditions.

Optimization for Ar-Br activation in the Suzuki reaction. A screw-top reaction tube was charged with 4-bromoanisole (93.5 mg, 5×10^{-4} mol), Pd@OX-1 (1 mg; 1×10^{-8} mol (0.002 mol%) of Pd), phenylboronic acid (73.2 mg, 6×10^{-4} mol), potassium carbonate (110.6 mg, 8×10^{-4} mol), and 1 mL of *i*-PrOH:H_2O (1:1). The tube was equipped with magnetic stirring bar, then sealed tightly, and placed into a hot plate at 150 °C with continuous stirring. After 24 h reaction mixture was cooled to room temperature and analyzed by GC-MS.

Substrate scope examination for Pd@OX-1 in the Suzuki reaction. A screw-top reaction tube was charged with aryl halide (5×10^{-4} mol), Pd@OX-1 (10 mg; 1.0×10^{-7} mol (0.02 mol%) of Pd), aryl boronic acid (6×10^{-4} mol), potassium carbonate (110.6 mg, 8×10^{-4} mol), and 1 mL of *i*-PrOH:H_2O (1:1). The tube was equipped with magnetic stirring bar, then sealed tightly, and placed into a hot plate at 100 °C with continuous stirring. After 1 h reaction mixture was cooled to room temperature and yield was analyzed by GC-MS. Then, 1 mL of diclorometna was added to extract the product and the product yield was analyzed by ^1H NMR in $CDCl_3$.

Catalyst isolation for XAS study for the Suzuki reaction. For all the reactions 0.2 wt.% Pd@OX-1 was used as a catalyst source. Four parallel reaction were conducted to receive enough amount of the material.

A screw-top reaction tube was charged with iodobenzene (102.0 mg, 5×10^{-4} mol), Pd@OX-1 (100 mg; 1×10^{-6} mol of Pd), phenylboronic acid (73.2 mg, 6×10^{-4} mol), potassium carbonate (110.6 mg, 8×10^{-4} mol), and 1 mL of *i*-PrOH:H_2O (1:1). The tube was equipped with magnetic stirring bar, then sealed tightly, and placed into a hot plate at 100 °C with continuous stirring. After 4 h reaction mixture was cooled to room temperature, yield was determined by GC-MS. Product was extracted with acetone (5 mL), material was washed with 5 mL of water, and washed with additional 5 mL of acetone. Dried material was subjected to the XAS study.

Table S1. Pd@OX-1 performance on the Suzuki reaction

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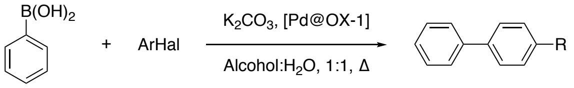
<tr><td colspan="6">
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<tr><td>ArHal</td><td>[Pd], mol%</td><td>Solvent</td><td>Temperature, °C</td><td>Time, h</td><td>Yield, %</td></tr>
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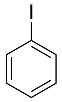
<tr><td rowspan="3">
</td><td>0.2</td><td rowspan="3">MeOH:H_2O</td><td>100</td><td>4</td><td>> 99</td></tr>
<tr><td>0.02</td><td>100</td><td>24</td><td>99</td></tr>
<tr><td>0.002</td><td>150</td><td>24</td><td>> 99</td></tr>
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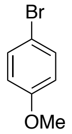
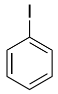
<tr><td rowspan="5">
</td><td rowspan="5">0.002</td><td rowspan="5">*i*-PrOH:H_2O</td><td>100</td><td>3</td><td>55</td></tr>
<tr><td>120</td><td>3</td><td>74</td></tr>
<tr><td>140</td><td>3</td><td>82</td></tr>
<tr><td>150</td><td>1</td><td>91</td></tr>
<tr><td>150</td><td>4</td><td>97</td></tr>
<tr><td colspan="6">Recycling possibility</td></tr>
<tr><td rowspan="5">
</td><td>0.05 (Cycle 1)</td><td rowspan="5">*i*-PrOH:H_2O</td><td rowspan="5">100</td><td>2</td><td>98</td></tr>
<tr><td>0.05 (Cycle 2)</td><td>2</td><td>98</td></tr>
<tr><td>0.05 (Cycle 3)</td><td>2</td><td>99</td></tr>
<tr><td>0.05 (Cycle 4)</td><td>2</td><td>99</td></tr>
<tr><td>0.05 (Cycle 5)</td><td>2</td><td>95</td></tr>
</table>

Heck reaction

General procedure for the Heck reaction. For all the reactions 0.2 wt.% Pd@OX-1 was used as a catalyst source. A screw-top reaction tube was charged with aryl halide (5×10^{-4} mol), Pd@OX-1 (from 1 to 100 mg; 1×10^{-8} to 1×10^{-6} mol of Pd), butyl acrylate (76.9 mg, 6×10^{-4} mol), triethylamine (81.0 mg, 8×10^{-4} mol), and 1 mL of DMF. The tube was equipped with magnetic stirring bar, then sealed tightly, and placed into a hot plate (from 100 °C to 150 °C) with continuous stirring. After specified time (from 1 h to 24 h) reaction mixture was cooled to room temperature and analyzed by GC-MS.

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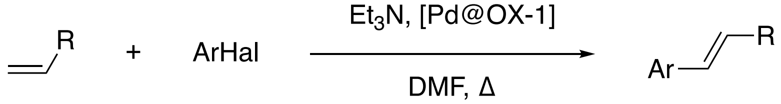
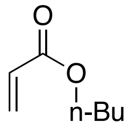
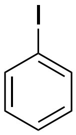
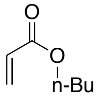
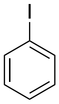
Ar-Br activation in the Heck reaction. A screw-top reaction tube was charged with 4-bromoanisole (93.5 mg, 5×10^{-4} mol), Pd@OX-1 (25 mg; 2.5×10^{-7} mol (0.05 mol%) of Pd), butyl acrylate (76.9 mg, 6×10^{-4} mol), triethylamine (81.0 mg, 8×10^{-4} mol), and 1 mL of DMF. The tube was equipped with magnetic stirring bar, then sealed tightly, and placed into a hot plate at 150 °C with continuous stirring. After 24 h reaction mixture was cooled to room temperature and analyzed by GC-MS.

Substrate scope examination for Pd@OX-1 in the Heck reaction. A screw-top reaction tube was charged with aryl iodide (5×10^{-4} mol), Pd@OX-1 (10 mg; 1.0 10^{-7} mol (0.02 mol%) of Pd), acrylate (6×10^{-4} mol), triethylamine (81.0 mg, 8×10^{-4} mol), and 1 mL of DMF. The tube was equipped with magnetic stirring bar, then sealed tightly, and placed into a hot plate at 100 °C with continuous stirring. After 4 h reaction mixture was cooled to room temperature and yield was analyzed by GC-MS. Then, the product yield was analyzed by ^{1}H NMR in $CDCl_3$.

Catalyst isolation for XAS study for the Heck reaction. For all the reactions 0.2 wt.% Pd@OX-1 was used as a catalyst source. Four parallel reaction were conducted to receive enough amount of the material. A screw-top reaction tube was charged with iodobenzene (102.0 mg, 5×10^{-4} mol), Pd@OX-1 (100 mg; 1×10^{-6} mol of Pd), butyl acrylate (76.9 mg, 6×10^{-4} mol), triethylamine (81.0 mg, 8×10^{-4} mol), and 1 mL of DMF. The tube was equipped with magnetic stirring bar, then sealed tightly, and placed into a hot plate at 100 °C with continuous stirring. After 4 h reaction mixture was cooled to room temperature, yield was determined by GC-MS. Product was extracted with DMF (5 mL), material was washed with 5 mL of DMF, followed by 5 mL of acetone. Dried material was subjected to the XAS study.

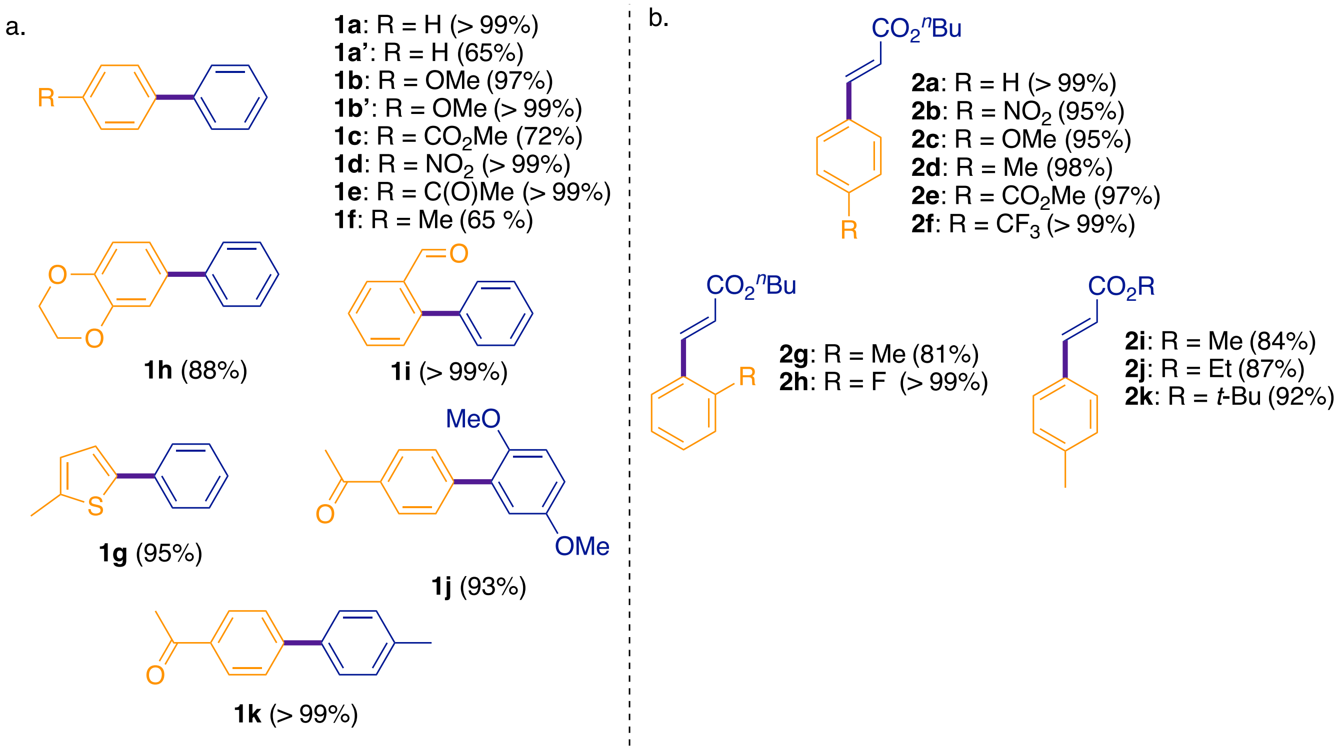
Table S2. Pd@OX-1 performance on the Heck reaction



Olefin	ArHal	[Pd], mol%	Solvent	Temperature, °C	Time, h	Yield, %
Activity of Various loadings						
		0.2	DMF	100	4	> 99
		0.02	DMF	100	4	10
		0.02	DMF	100	24	98
		0.002	DMF	150	24	> 99
Recycling possibility						
		0.2 (Cycle 1)	DMF	100	4	> 99
		0.2 (Cycle 2)	DMF	100	4	97
		0.2 (Cycle 3)	DMF	100	4	91
		0.2 (Cycle 4)	DMF	100	4	86
		0.2 (Cycle 5)	DMF	100	4	88

Reactions scope

Scheme S1. Pd@OX-1 catalysed Suzuki and Heck reactions [a,b,c]



[a] Yields determined by ^{1}H NMR; [b] Aryl iodide used as substrate: **1a-c**,**1g**,**2a-k**; [b] aryl bromide used as substrate: **1a'**,**b'**,**d-f**, **h-k**

X-ray Absorption Spectroscopy (XAS)

EXAFS spectra were acquired on B18, the Core XAS beamline at Diamond Light Source.[6] Data at the Zn K-edge were acquired in transmission mode with ionization chambers filled with Ar and pressure adjusted to absorb 10% and 70% of the beam before and after the sample, respectively. B18 Double Crystal Monochromator was equipped with Si(111) crystal pair, and Pt-coated mirrors for were inserted in the beam path to remove high energy harmonics.

For Pd K-edge, we used Si(311) crystals. Data were acquired in fluorescence mode using a 36-element monolithic Ge detector (Canberra) with XSPRESS2 acquisition electronics. For both experiments, the beam was partially defocused to obtain a beam footprint on the sample of approximately 1×1 mm^2.

Samples were pressed into 8 mm pellets at 0.5 ton applied weight using a standard Specac benchtop hydraulic press. For transmission Zn K-edge measurements 10 mg of MOF powder for mixed with 35 mg of cellulose binder. For fluorescence Pd K-edge measurements 50 mg of MOF powder was used without binder, while the PdonC sample required 120 mg of pure material. $Pd_2(dba)_3$ was measured in transmission through a pellet pressed from 45 mg of pure material.

The Demeter software package[7] was used to process the raw data and subsequently fit the Pd K edge EXAFS spectra for the Pd@OX-1 samples before and after the Heck and Suzuki reactions. Table S3 shows final fitting parameters for the three EXAFS fits at the Pd K edge reported in the main text.

Table S3: EXAFS fitting parameters for Pd@OX-1 as synthesised, after Heck and after Suzuki reactions. S_0^2 was fixed to a value of 0.88 obtained from the fit for the EXAFS spectrum of reference Pd foil measured simultaneously with the samples. Correlation between variables is less than 90% for all fits reported.

Pd@OX-1 as synthesised				
k-range	3-14.5	Independent points	14.3	R-factor
R-range	1.15-3.15	Number of variables	7	0.004
Path	N	ΔE_0 (eV) (E_0 = 24355)	R (Å)	σ^2 (Å^2)
Pd.1	4.3 ±0.3	-2.8 ±0.4	2.798 ±0.003	0.009 ±0.0004
C7.1	4.0 ±0.3	-2.8 ±0.4	2.037 ±0.004	0.005 ±0.0009
Pd@OX-1 after Heck				
k-range	2.5-14.2	Independent points	16.4	R-factor
R-range	1.15-3.4	Number of variables	7	0.034
Path	N	ΔE_0 (eV) (E_0 = 24355)	R (Å)	σ^2 (Å^2)
Pd.1	10.4 ±0.9	-3.5 ±0.6	2.774 ±0.008	0.014 ±0.001
C7.1	1.2 ±0.7	-3.5 ±0.6	2.003 ±0.025	0.005 ±0.005
Pd@OX-1 after Suzuki				
k-range	2.7-14.6	Independent points	16.4	R-factor
R-range	1.7-3.9	Number of variables	6	0.008
Path	N	ΔE_0 (eV) (E_0 = 24353)	R (Å)	σ^2 (Å^2)
Pd.1	10.6 ±0.6	-2.1 ±0.4	2.766 ±0.003	0.009 ±0.0004
Pd.2	5.3 ±0.3	-2.1 ±0.4	3.847 ±0.02	0.008 ±0.002

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