

# Development of a 4,4'-biphenyl/phosphine-based COF for the heterogeneous Pd-catalysed telomerisation of 1,3-butadiene

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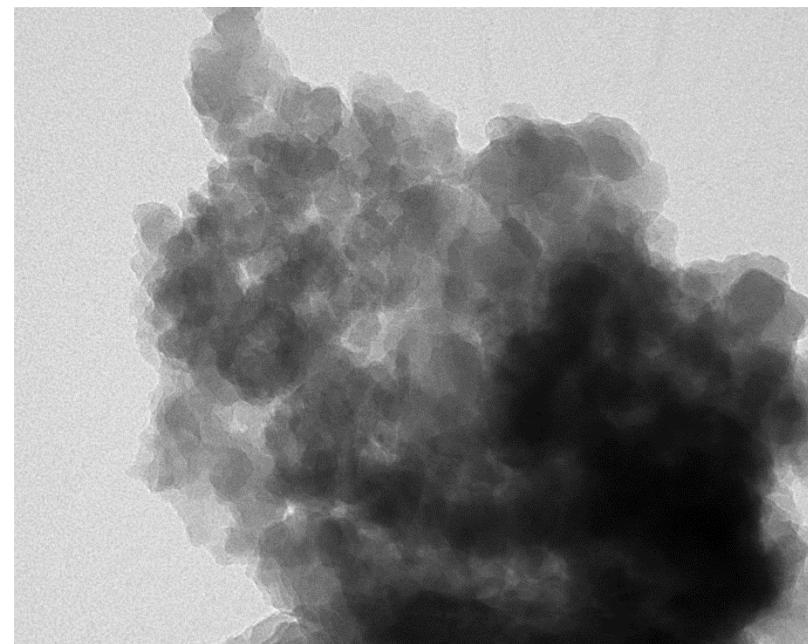
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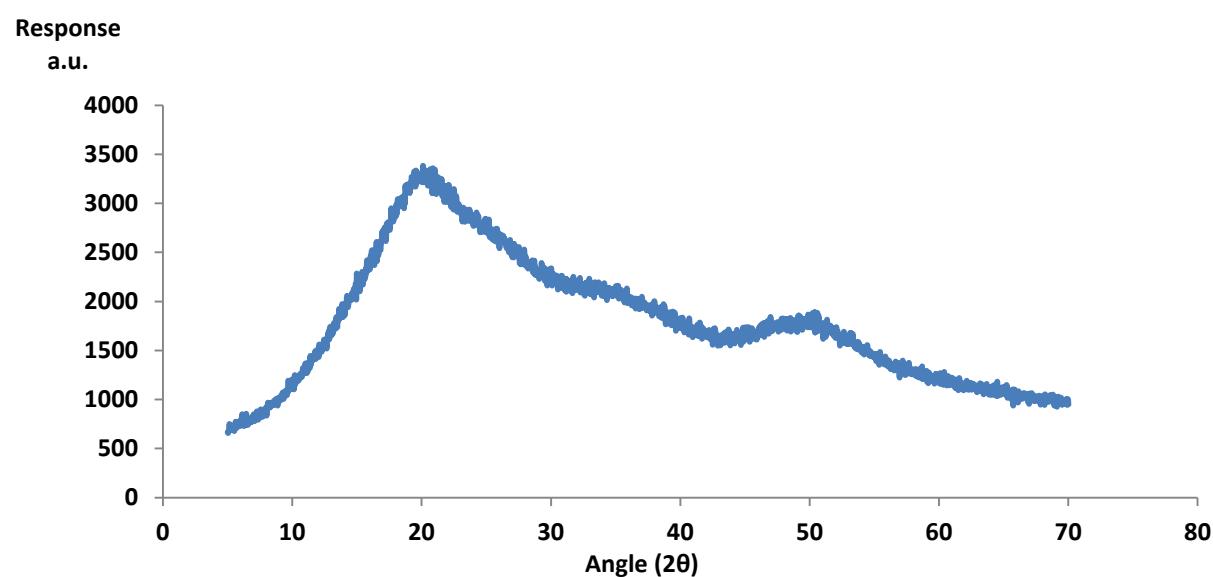
## ***Characterization of 1***

### ***TEM image***



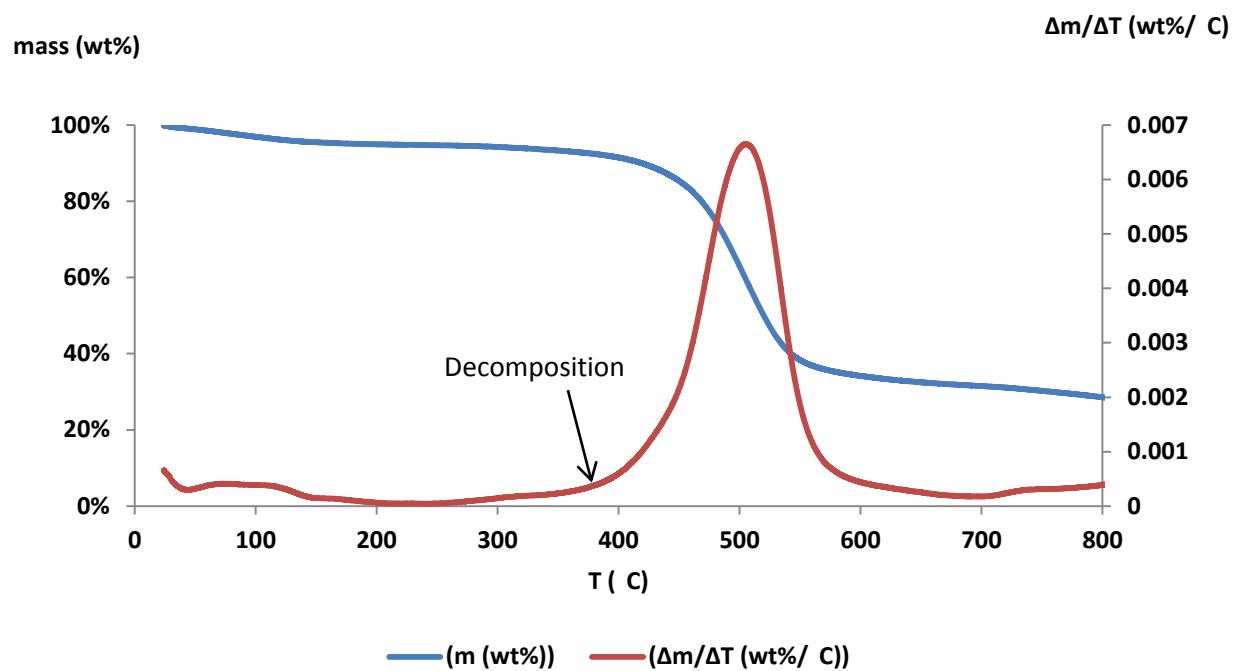
**Figure S1** Bright field TEM image of 1

### ***XRD Pattern***



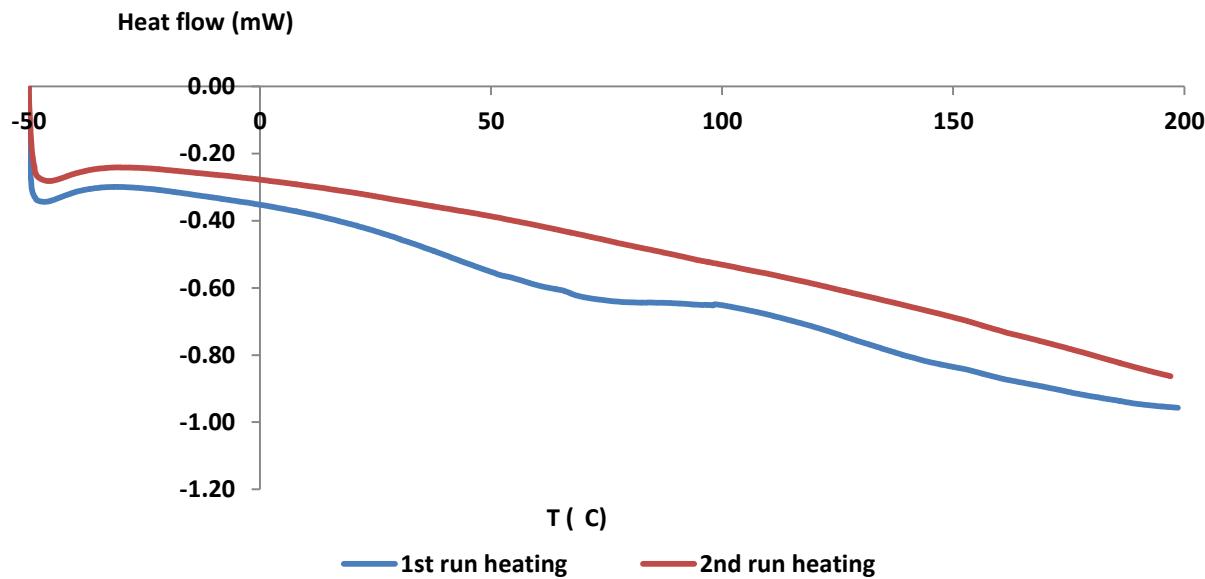
**Figure S2.** Powder XRD Pattern of 1.

### Thermogravimetric analysis



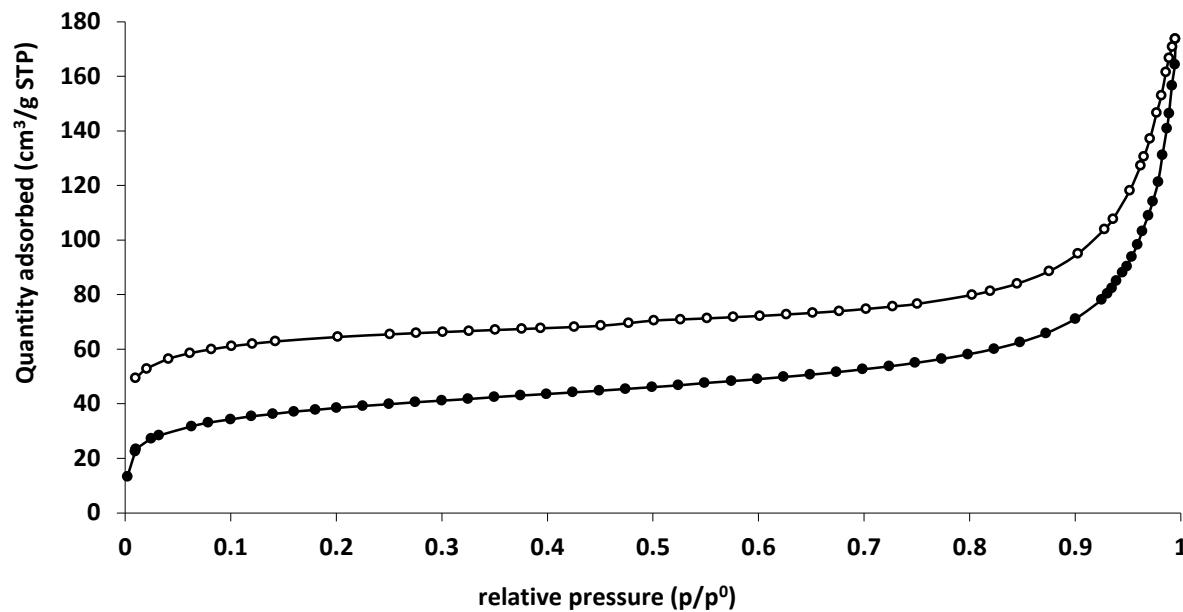
**Figure S3** TGA analysis of **1** showing significant weight loss due to decomposition after 380°C.

### Differential scanning calorimetry



**Figure S4.** DSC results of **1**.

### *N<sub>2</sub>-physisorption*



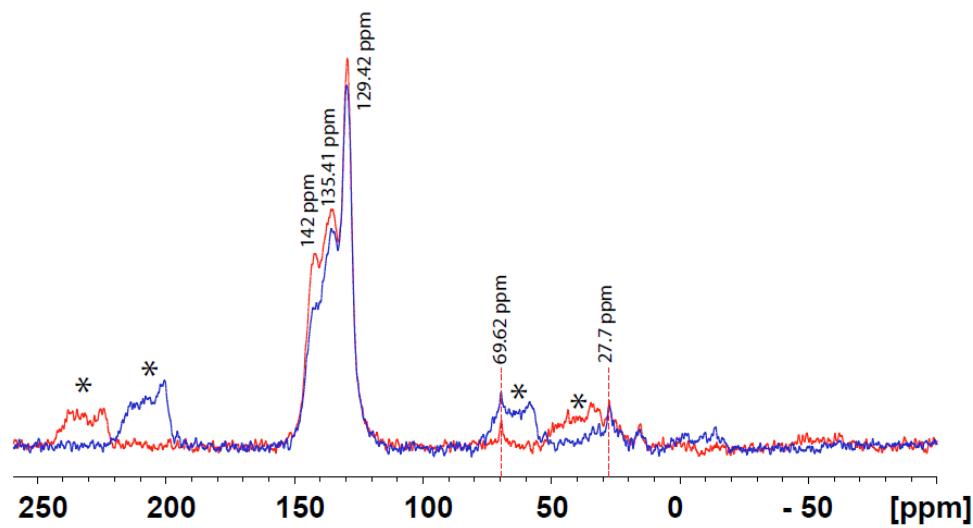
**Figure S5.** N<sub>2</sub>-physisorption graph of **1**. (● = adsorption, ○ = desorption).

### *<sup>13</sup>C MAS-solid-state NMR spectra*

<sup>1</sup>H-<sup>13</sup>C cross-polarization (125.721 MHz) on Poly PPh<sub>3</sub> (Phenyl caps)

MAS: 10kHz & 12kHz, T: RT, Relaxation delay: 5s

500MHz



**Figure S6.** (<sup>1</sup>H-<sup>13</sup>C) CP (cross polarization) spectra of **1** employing a CP contact time of 1 ms. Spectra were recorded with MAS rates of 10kHz (blue) and 12kHz (red) and are overlaid to identify spinning side bands (\*).

## Characterization of 0.52Pd@1

### Thermogravimetric analysis

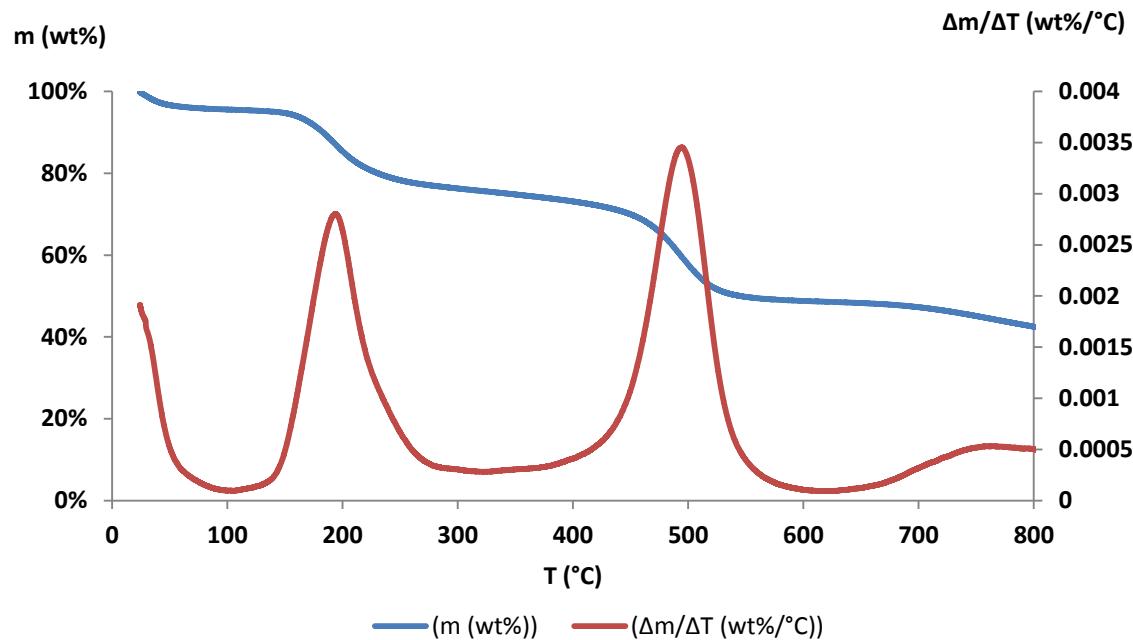


Figure S7 TGA analysis of 0.52Pd@1.

### $N_2$ -physisorption

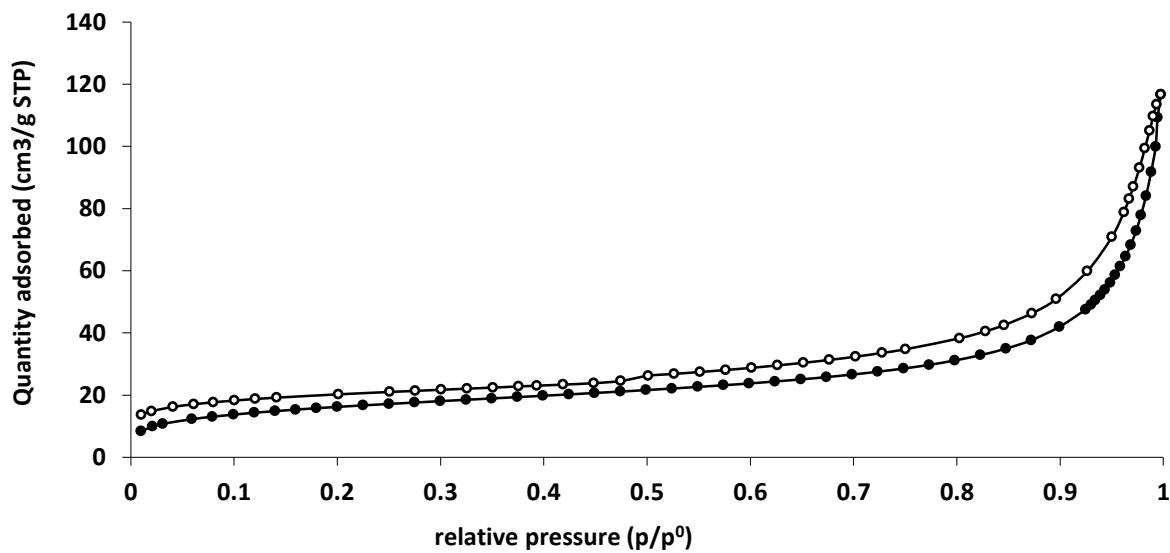
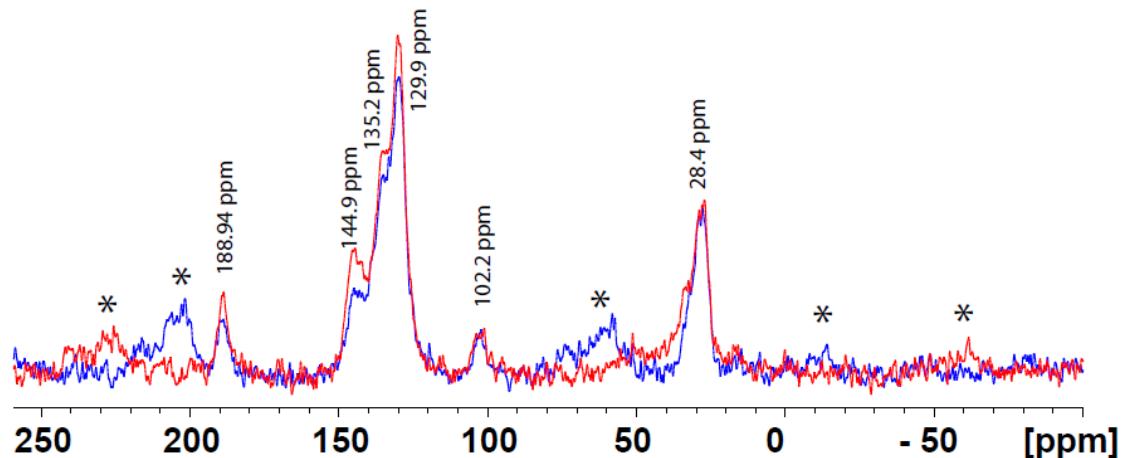


Figure S8  $N_2$ -physisorption graph of 0.52Pd@1. (● = adsorption, ○ = desorption).

### ***<sup>13</sup>C MAS-solid-state NMR spectra***

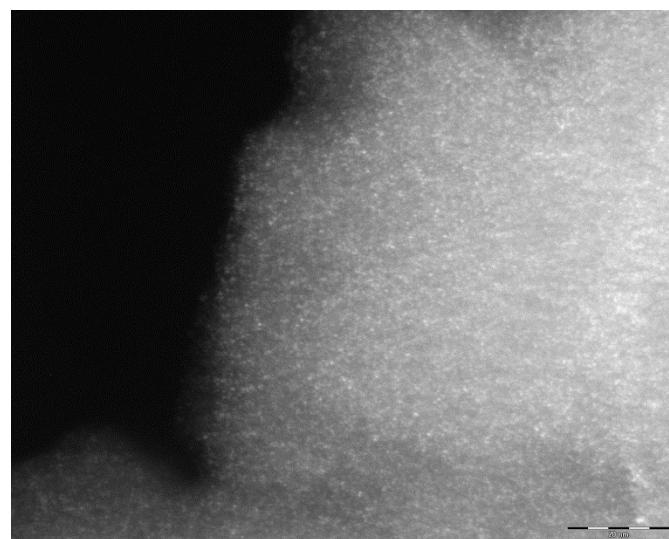
<sup>1</sup>H-<sup>13</sup>C cross-polarization (125.721 MHz) on Poly PPh<sub>3</sub> + Pd(acac)<sub>2</sub>(Phenyl caps)  
MAS: 10kHz & 12kHz, T: RT, Relaxation delay: 5s  
500MHz



**Figure S9** 1D (<sup>1</sup>H-<sup>13</sup>C) CP (cross polarization) spectra of 0.52Pd@1 with a contact time of 1 ms. Spectra were recorded with MAS rates of 10 and 12 kHz and are overlaid to identify spinning side bands (\*).

### ***Characterization of 1.07Pd@1***

#### ***TEM Image***



**Figure S10** Dark field TEM image of 1.07Pd@1.