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Supporting Information

Synthesis of biphenyl through the C-H bond activation in benzene over a Pd catalyst supported on graphene oxide

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1. Experimental

1.1 Chemicals and Materials:

All solvents and reagents used in the present study were of analytical grade and used as received. Palladium nitrate ($Pd(NO_3)_2 \bullet 2H_2O$), hydrochloric acid (HCl), acetic acid (CH_3COOH), benzene (C_6H_6), acetone (C_3H_6O), anisole (C_7H_8O), toluene (C_7H_8) and nitrobenzene ($C_6H_5NO_2$) were purchased from LobaChemie private limited and graphene oxide was purchased from Platonic Nanotech Private Limited (Mahagama, Godda, Jharkhand, India). Melting points of all the products reported in Table 2 in the manuscript are compared with the data available on these sites.

a) https://pubchem.ncbi.nlm.nih.gov/compound/4_4_-Dimethoxybiphenyl
b) https://www.sigmaaldrich.com/catalog/product/aldrich/d151203?lang=en&region=US
c) https://pubchem.ncbi.nlm.nih.gov/compound/4_4_-Dinitrobiphenyl

1.2 Characterization techniques

The HRTEM analysis was accomplished in FEI Tecnai G2 F30 microscope in which an electron beam is generated from the field emission gun, operated at 300 KeV. X-ray photoelectron spectroscopy (XPS) data were collected using a Thermo Fisher Scientific NEXSA spectrometer. X-

ray powder diffraction (XRD) a characterization technique was performed using a Rigaku D/max 2200V/PC diffractometer. FTIRS analysis was performed by using a Fourier Transform Infrared spectrometer (Agilent Technologies). in the scale of 800-4000 cm^{-1}. The samples were diluted with KBr. An Inductivity Coupled Plasma Mass Spectrometry (ICP-MS) study of the catalyst was performed by using an ELAN DRC-e spectrometer (Perkin Elmer). Thermo-gravimetric analysis/differential scanning calorimetry (TGA/DSC) was performed on a Perkin Elmer, Netzsch Geratebau GmbH apparatus under the nitrogen atmosphere within the temperature range 25-100℃ at a heating rate of 3℃/min. Weight loss percent was calculated by using this formula [$Weight\ loss\ \% = \frac{y1 - y2}{x2 - x1} \times 100$]. A ^{1}H-NMR spectrum was recorded on a JNM ECX-500 spectrometer. The product was measured in $CDCl_3$ at 500 MHz.

2. Tables

Table-S1. Comparison of the present work with literature

Sr. No.	Catalyst	T (°C)	Time of reaction (h)	Yield (%)	References
1.	Pd(II)@GO	80	12	78	This work
2.	$Pd(OAc)_2$molybdovanado-phosphate	90	15	14.3	[1]
3.	Pd-slGO-60, K_2CO_3, EtOH	90	2	66	[2]
4.	Pd/C, HCOONa, NaOH, TBAB, H_2O, MeOH	55-75	0.58	71	[3]
5.	$Pd(OAc)_2/Cu(OTf)_2$, 2-fluoropyridine, CF_3CO_2H, AcOH	80	17	8.0	[4]
6.	Pd catalyst, K_2CO_3,PivOH, PhH/DMA	120	16	83	[5]
7.	$PdCl_2$, $AgNO_3$	80	20	40	[6]
8.	Pd^{II}@PDMS	90	24	26	[7]

3. Figures

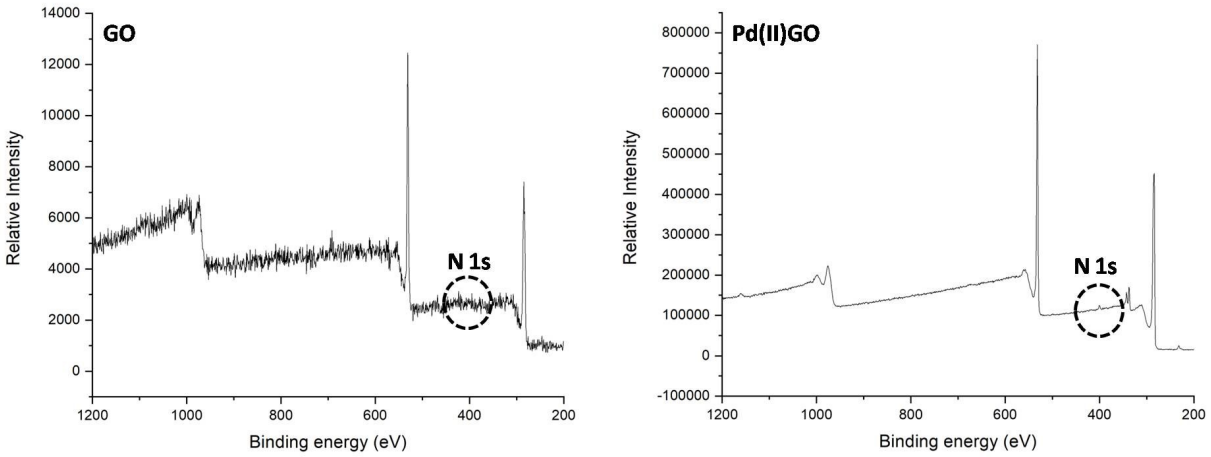

Figure S1. XPS survey spectra of GO and Pd(II)GO.

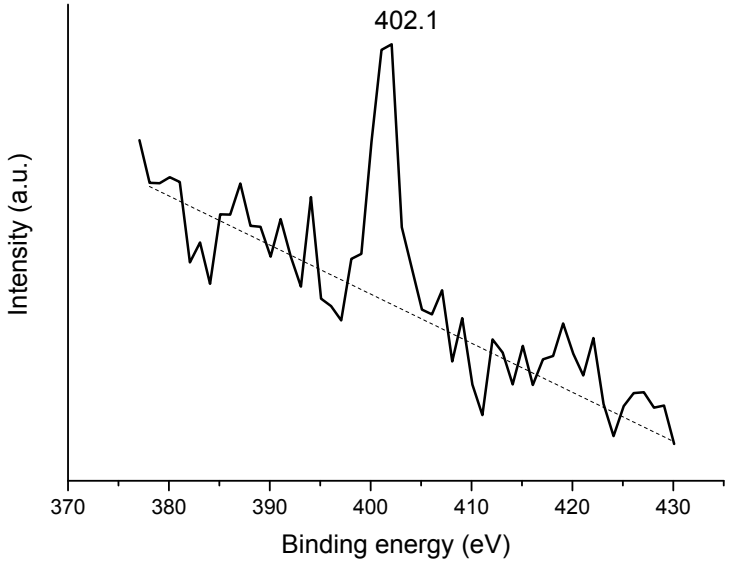

Figure S2. N 1s XPS spectrum extracted from the survey spectrum of Pd(II)@GO

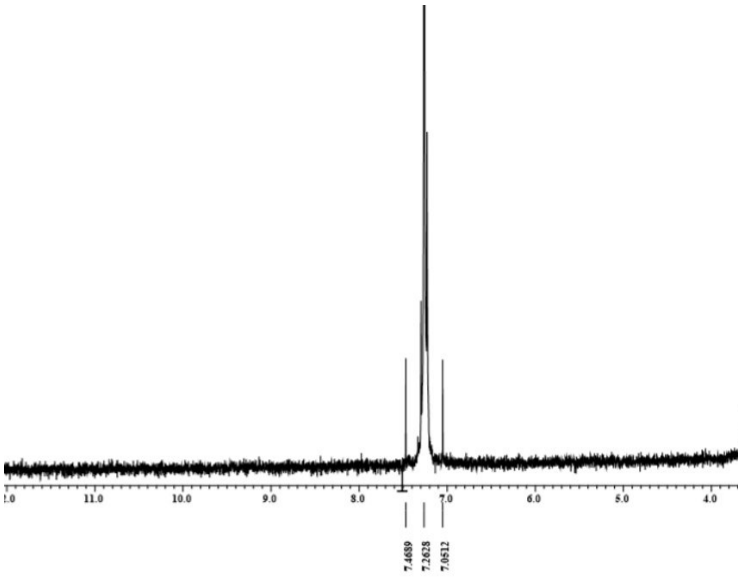

Figure S3. ^{1}H-NMR spectrum of the obtained biphenyl product.

References for Table-S1:

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