Electronic Supplementary Material (ESI) for Faraday Discussions.

Supplementary Information

Methanol synthesis from CO_2 and H_2 using supported Pd alloy catalysts.

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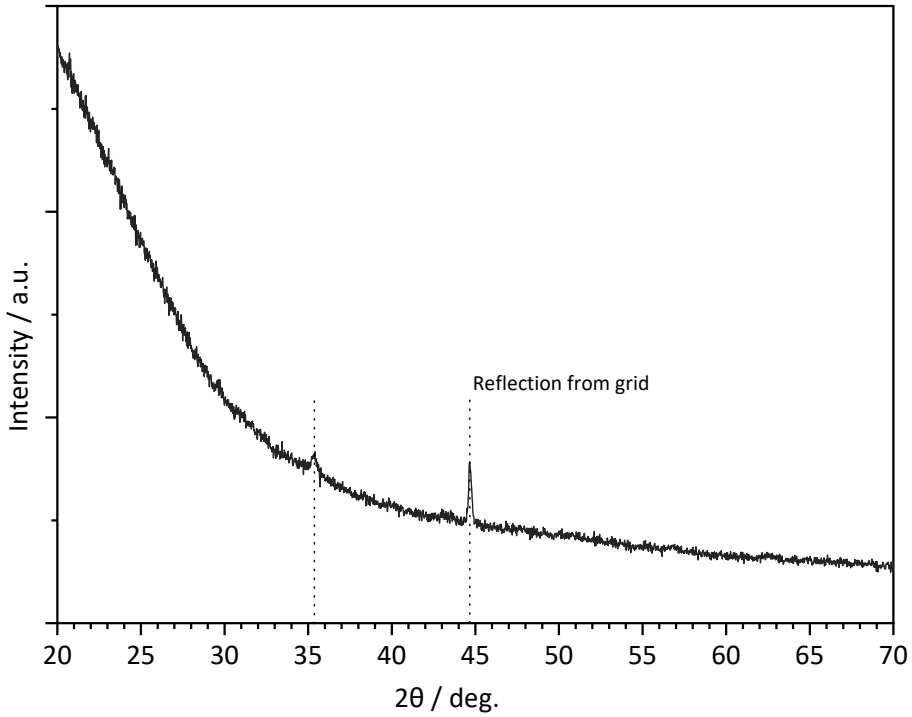

Figure S1: XRD from the SiO_2 blank and the XRD support grid.

Table S1: Tabulated product selectivity for the calcined Pd/Ga_2O_3 catalyst, at different isothermal temperature regions.

Temperature / °C	*Methane*	*CO*	*Methanol*
175	0	86.9	13.1
175	0	87.1	12.9
175	0	85.1	14.9
175	0	83.0	17.0
200	0	86.1	13.9
200	0	78.0	22.0

200	0.2	72.8	27.1
200	0.1	66.1	33.8
225	0.2	48.3	51.5
225	0.1	43.6	56.3
225	0.1	42.1	57.8
225	0.1	40.9	59.0
250	0.1	47.0	52.9
250	0.1	47.2	52.7
250	0.1	47.4	52.5

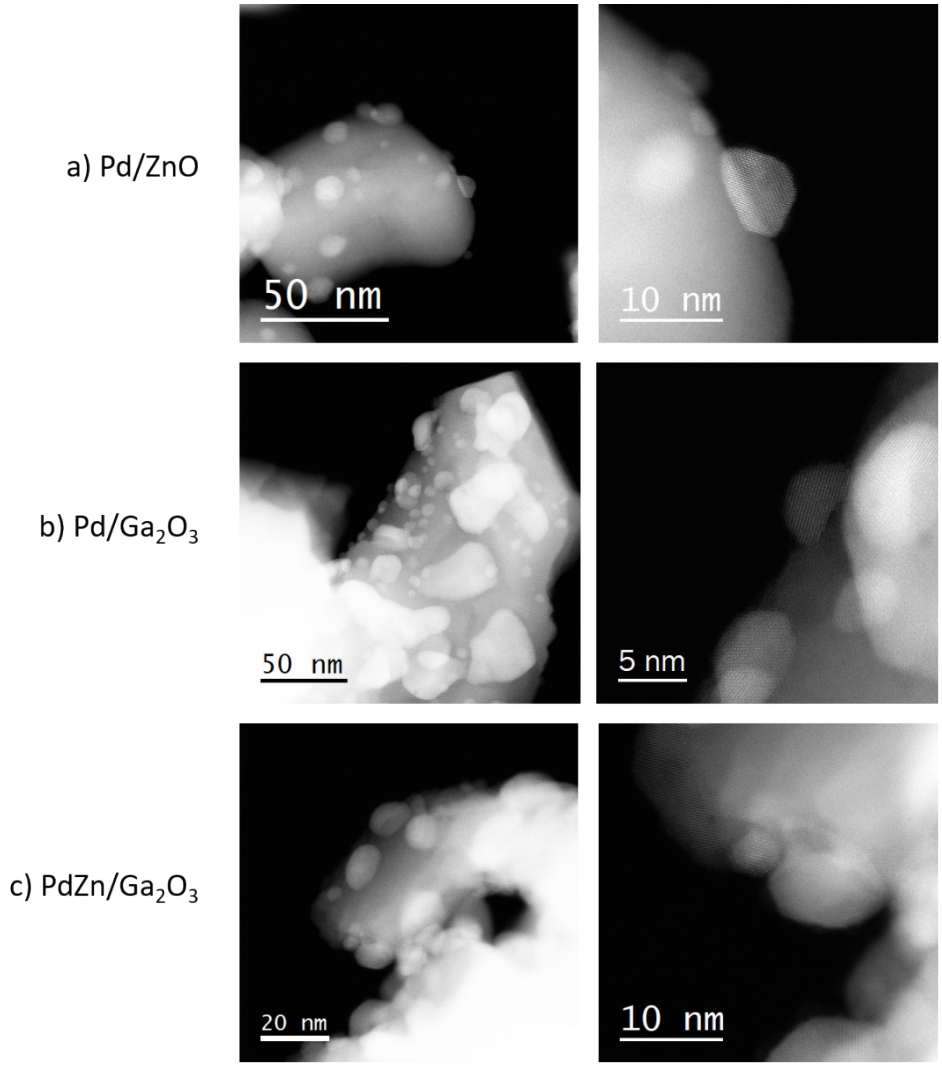

Figure S2: HAADF-STEM images of a) Pd/ZnO, b) Pd/Ga_2O_3 and c) $PdZn/Ga_2O_3$ after reduction at 400°C.

DFT calculations

Table S2: Detailed comparison between experimental and DFT optimised structures, respectively: a_0, b_0, c_0 are lattice parameters (in Å) for structures taken from the ICSD library

before optimisation; and a, b, c are the corresponding relaxed lattice vectors. Similarly, x, y, z are the angles (in degrees) for the structures taken from the ICSD, and x_0, y_0 and z_o are the angles of the optimised cell.

	a_0	b_0	c_0	a	b	c	x_0	y_0	z_0	x	y	z	*Ref*
Pd_2Zn	3.06	3.06	9.57	2.88	2.88	10.28	90	90	90	90	90	90	[1]
PdZn	2.90[2]	2.90	3.38	2.87	2.87	3.37	90	90	90	90	90	90	[2]
$PdZn_2$	7.53	7.36	12.307	7.49	7.47	11.97	90	90	90	90	90	90	[3]
$InPd_3$	4.03	4.03	4.03	4.00	4.00	4.00	90	90	90	90	90	90	[4]
$InPd_2$	5.61	4.22	8.29	5.67	4.23	8.28	90	90	90	90	90	90	[5]
In_3Pd_5	5.60	11.02	4.24	5.65	11.15	4.25	90	90	90	90	90	90	[6]
InPd	3.25	3.25	3.25	3.27	3.27	3.27	90	90	90	90	90	90	[7]
In_3Pd_2	4.52	4.52	4.59	5.42	4.57	4.58	90	90	120	90	90	120	[7]
In_7Pd_3	9.43	9.43	9.43	9.50	9.50	9.50	90	90	90	90	90	90	[8]
Pd_7Ga_3	13.56	4.06	5.44	13.56	4.06	5.49	90	105.2	90	90	105.2	90	[9]
Pd_2Ga	5.48	4.06	7.79	5.51	4.05	7.79	90	90	90	90	90	90	[10]
Pd_5Ga_3	5.42	10.56	4.03	5.45	10.58	4.01	90	90	90	90	90	90	[11]
PdGa	4.90	4.90	4.90	4.89	4.89	4.89	90	90	90	90	90	90	[12]
Pd_3Ga_7	8.77	8.77	8.77	8.76	8.76	8.76	90	90	90	90	90	90	[10]

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