Supplementary Materials: Oscillatory behavior of Pd-Au catalysts in toluene total oxidation

Tarek Barakat [1,2,*], Joanna C. Rooke [1], Dayan Chlala [3], Renaud Cousin[2], Jean-François Lamonier [3], Jean-Marc Giraudon [3], Sandra Casale [4], Pascale Massiani [4], Bao-Lian Su [1,*] and Stéphane Siffert [2,*]

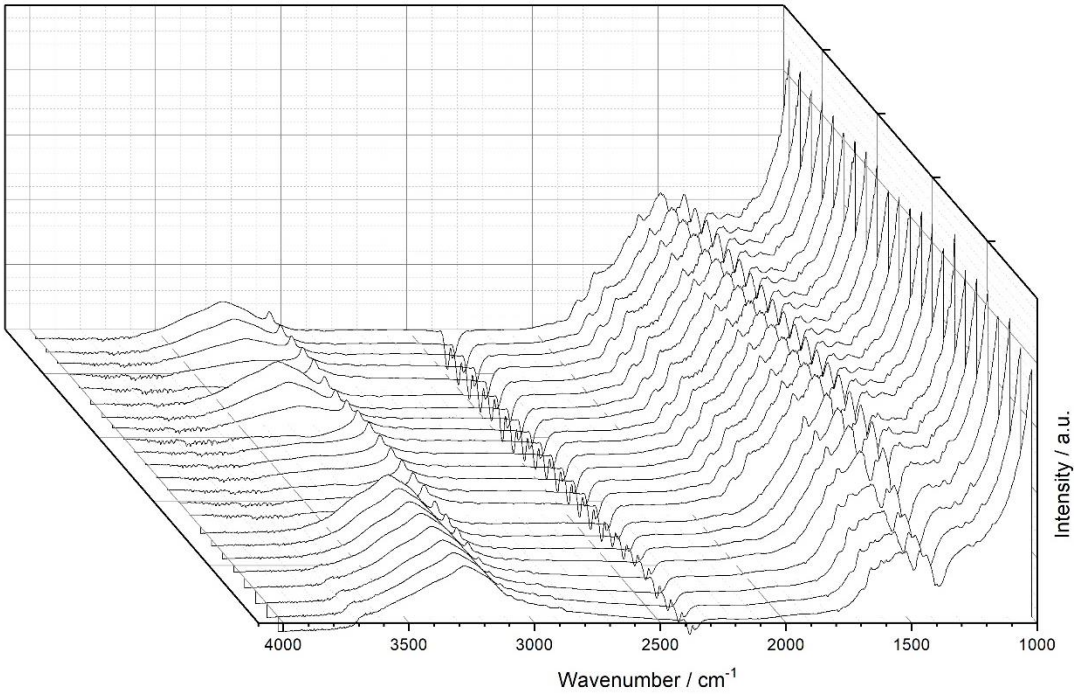

Figure S1. Operando DRIFT results of the PdAu5VTi catalyst.

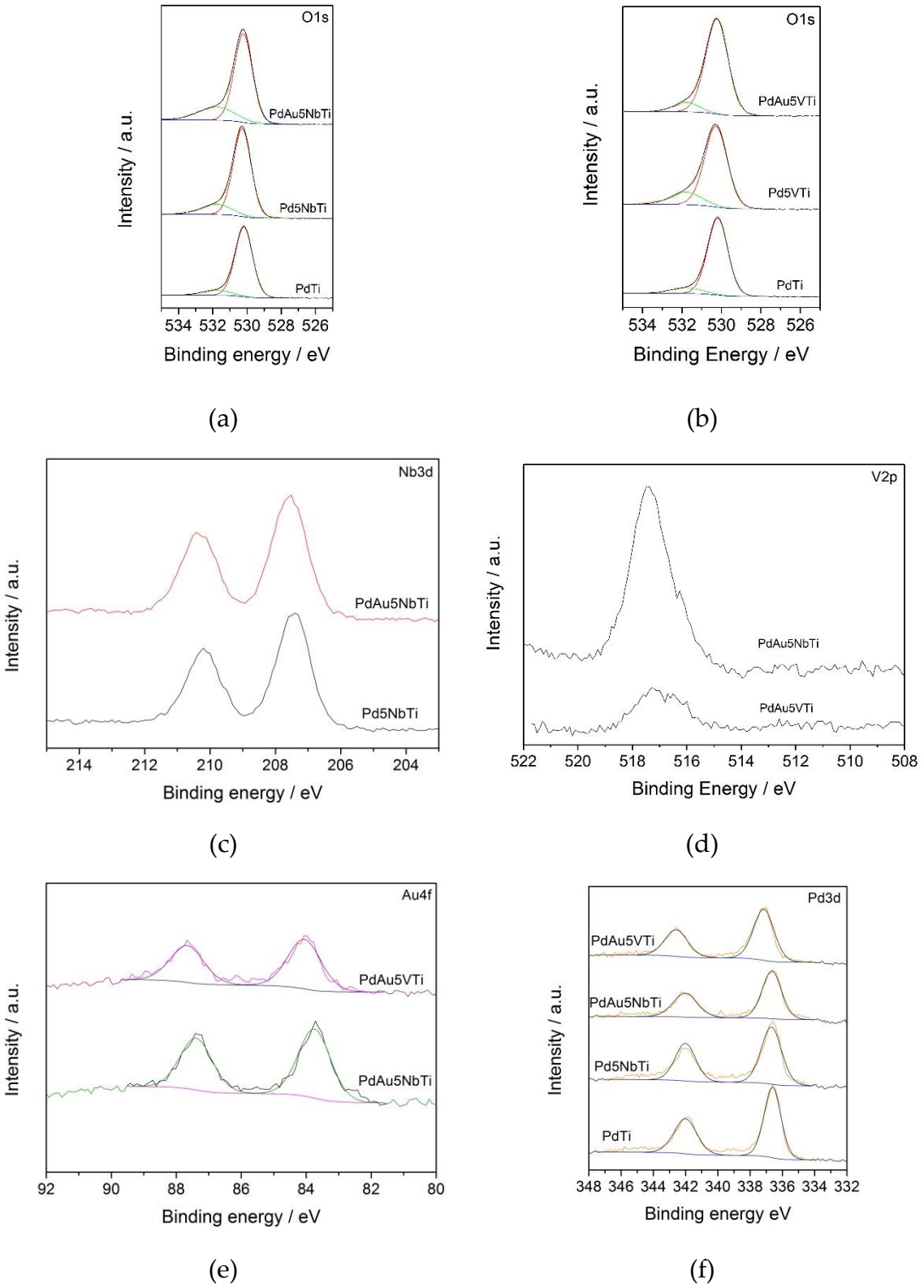

Figure S2. XPS spectra of mono and bimetallic Nb- (a, c and e) and V-doped (b, d and f) TiO_2 samples.

Table S1. BET surface area measurements, noble metal content and T50 values for the oxidation of toluene of bimetallic loaded doped catalysts compared to a previously tested $PdAu/TiO_2$ sample.

Samples	BET surface area measurements (m^2 g^{-1})		Noble metal content (wt %)		T_{50} (°C)
	Before test	After test	Au	Pd	
PdAu5NbTi	160	152	0.42	0.37	214
PdAu5VTi	163	150	0.27	0.38	221
$PdAu/TiO_2$	151	127 [1]	0.80	0.39	219

Table S2. Observed DRIFT absorption bands and their assignments for the PdAu5NbTi and PdAu5VTi catalysts as seen in Figures 2 and S1 respectively.

PdAu5VTi	PdAu5NbTi			
Bands (cm^{-1})	Bands (cm^{-1})	Assignment	Intensity	Type of vibration
3500–3100	3500–3100	O-H (Ti-OH)	Strong	Stretching
3068	3068	C-H sp^3 (aromatic)	Strong	Stretching
2939	2943	C-H sp^3	Strong	Asymmetric stretching
2897	2903	C-H sp^3	Strong	Symmetric stretching
1839	1853	C=O	Strong	Stretching
1776	1784	α and β-unsaturated aliphatic	Strong	Stretching
1676	-			
1639	1641	C=C	Medium	Stretching
1599	1599	C=C in ring	Medium	
-	1584	C=C in-plane	Strong	Stretching
1526	1526	C-C olefin	Strong	Stretching
1513	1513	C-C in ring	Strong	
1445	1444	C-O-H	Medium	Bending
1417	1411	C=O	Strong	Stretching
1324	1327	O-H	Medium	Bending (in-plane)
1305, 1243	1304, 1247	C-O	Strong	Stretching
-	1181	C-O-C	Medium	Bending

Table S3. Binding energy and quantitative analysis values of XPS experiments conducted on mono and bimetallic Nb- and V-doped catalysts.

Samples	Binding Energies (eV)									Quantitative analysis					
	O 1s		Pd 3d		Au 4f		Nb 3d		V 2p	O/Ti	$O_I/(O_I+O_{II})$	$O_{II}/(O_I+O_{II})$	Pd/(Ti+A)*	Au/(Ti+A)*	Pd/Au
	O_I	O_{II}	$3d_{5/2}$	$3d_{3/2}$	$4f_{7/2}$	$4f_{5/2}$	$2p_{5/2}$	$2p_{3/2}$	$2p_{3/2}$						
PdTi	530.2	531.2	336.6	341.9	-	-	-	-	-	1.5	0.90	0.10	0.020	-	-
Pd5NbTi	530.3	531.8	336.7	342.0	-	-	207.4	210.2	-	1.7	0.84	0.16	0.016	-	-
PdAu5NbTi	530.2	531.8	336.7	342.0	83.7	87.4	207.9	210.6	-	1.8	0.77	0.23	0.011	0.0027	4
Pd5VTi	530.3	531.8	336.8	342.1	-	-	-	-	517.0	1.6	0.86	0.14	0.021	-	-
PdAu5VTi	530.3	531.5	337.1	342.6	84.0	87.7	-	-	517.3	1.6	0.90	0.10	0.013	0.0026	5

* A = Nb or V

References

1. Hosseini, M.; Siffert, S.; Tidahy, H.L.; Cousin, R.; Lamonier, J.-F.; Aboukaïs, A.; Vantomme, A.; Roussel, M.; Su, B.-L. Promotional effect of gold added to palladium supported on a new mesoporous TiO2 for total oxidation of volatile organic compounds. *Catal. Today* **2007**, *122*, 391–396, doi:10.1016/j.cattod.2007.03.012.