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Supplementary Information

On the key role of hydroxyl groups on platinum-catalysed alcohol oxidation in aqueous medium.

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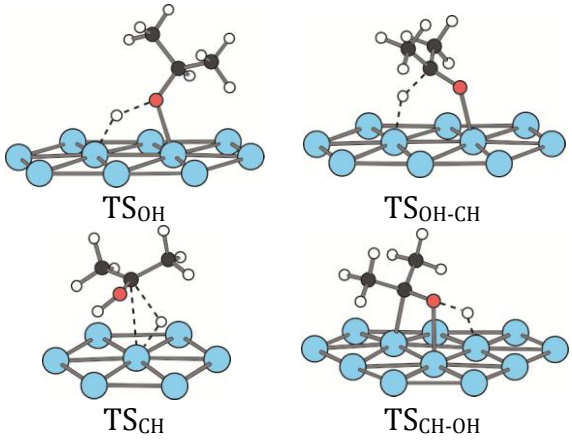

Figure S1. Transition states structures of the isopropanol oxidation at a bare Pt(111)

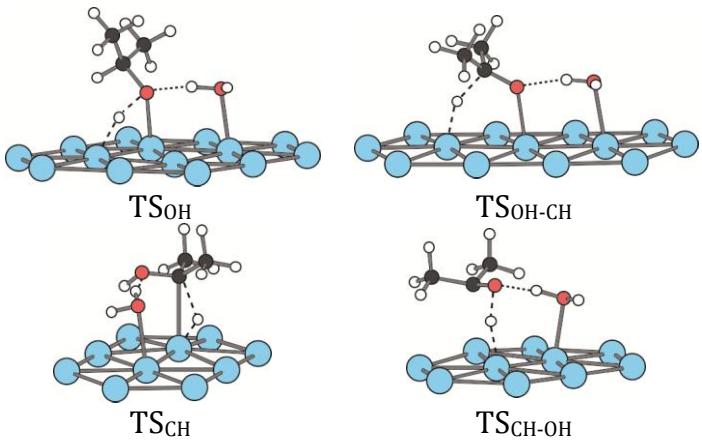

Figure S2. Transition states structures of the isopropanol oxidation at a H_2O@Pt(111) surface.

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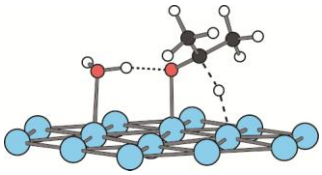

Figure S3. Transition state structure of the isopropanol oxidation at a OH@Pt(111) surface

	ΔE	ΔE‡	N	X-H	Pt-X	Pt-H	H...O
OH							
Pt(111)	0.72	0.93	4	1.64	2.07	1.64	
H_2O@Pt(111)	0.59	0.85	4	1.62	2.17	1.64	1.61
OH-CH							
Pt(111)	-0.64	0.08	5	1.44	3.02	1.71	
H_2O@Pt(111)	-0.46	0.28	5	1.50	3.09	1.68	1.76
CH							
Pt(111)	0.00	0.81	3	1.98	3.03	1.61	
H_2O@Pt(111)	0.16	1.13	3	1.72	2.60	1.62	1.73
CH-OH							
Pt(111)	0.47	0.81	4	1.66	2.24	1.61	
H_2O@Pt(111)	-0.08	0.65	6	1.47	3.05	1.66	1.50
OH@Pt(111)	-0.43	0.27	5	1.49	3.08	1.68	1.62

Table S1. Energetics and main geometrical characteristics of the transition state structures for the isopropanol oxidation at the bare platinum surface (Pt(111)), at the hydrated platinum surface (H_2O@Pt(111)) and at the hydroxylated surface (OH@Pt(111)). The CH step is the first step of Route C. The CH-OH step is the second step of route C. The OH step is the first step of route O. The OH-CH is the second step of route O. The reaction energy ΔE and the activation energy ΔE‡ of each step are provided in eV. The transition state structures are characterized by the number of involved atoms (N). The main distances are given in Å: X-H is the breaking bond; Pt-Y corresponds to the Pt-C (resp. Pt-O) bond for the CH bond scission (resp. OH bond scission). In the case of reaction at the hydrated and the hydroxylated surfaces, C or O is not adsorbed in the final product. H...O corresponds to the hydrogen bonds.