Supplementary Information

Table S1. DFT-derived parameters used to determine the free energy of water and solvated O_2 at the Pt(111) surface. These values were calculated using DFT and the double reference method by applying a quadratic fit for energy versus potential using the following equation.

$$G(U) = AU^2 + BU + C + ZPVE - TS_{vib} \quad (1)$$

where A, B, and C are the quadratic fit parameters determined by the double reference method, ZPVE is the zero-point vibrational energy (ZPVE), and S_{vib} is the vibrational entropy at 300K.

Systems	Density (g cm^{-3})	A	B	C	ZPVE (eV)	TS_{vib} (eV)
24 H_2O	1.0	-0.614	0.814	-617.3	0.67	0.06
	0.86	-0.430	0.427	-618.1	0.68	0.06
	0.68	-0.316	0.308	-616.4	0.67	0.06
O_2+23 H_2O	1.0	-0.604	0.737	-613.2	0.12	0.03
	0.86	-0.478	0.335	-613.9	0.13	0.05
	0.68	-0.41	0.054	-612.4	0.12	0.05
36 H_2O	1.0	-0.374	0.528	-792.2	0.68	0.06
	0.86	-0.273	0.333	-793.7	0.68	0.06
	0.68	-0.175	0.163	-790.9	0.68	0.06
O_2+35 H_2O	1.0	-0.411	0.555	-788.2	0.13	0.04
	0.86	-0.277	0.262	-789.5	0.13	0.04
	0.68	-0.189	0.119	-786.9	0.13	0.04