Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics. This journal is © the Owner Societies 2023

# **Supporting Information for:**

 $Trends\ in\ adsorbed\ hydroxyl-water\ interactions\ on\ late\ transition\ metal\ nanoparticles$ 

Selwyn Hanselman,<sup>1</sup> Marc T. M. Koper,<sup>1</sup>\* Federico Calle-Vallejo<sup>2,3,4,\*</sup>

<sup>1</sup> Leiden Institute of Chemistry, Leiden University, PO Box 9502, Leiden 2300 RA, The

Netherlands.

<sup>2</sup> Nano-Bio Spectroscopy Group and European Theoretical Spectroscopy Facility (ETSF), Department of Polymers and Advanced Materials: Physics, Chemistry and Technology, University of the Basque Country UPV/EHU, Av. Tolosa 72, 20018 San Sebastián, Spain.

<sup>3</sup> *IKERBASQUE*, *Basque Foundation for Science*, *Plaza de Euskadi 5*, 48009 *Bilbao*, *Spain*.

<sup>4</sup> Department of Materials Science and Chemical Physics & Institute of Theoretical and Computational Chemistry (IQTC), University de Barcelona, Martí i Franquès 1, 08028 Barcelona, Spain.

\*Corresponding authors: <u>m.koper@lic.leidenuniv.nl, federico.calle@ehu.es</u>

# **Table of contents**

S.1. Construction of nanoparticles and micro-solvated *OH and H <sub>2</sub> O configurations	2
S.2. Computational details	4
S.3. Thermodynamics	6
S.4. Formation energy thermodynamics and statistics	8
S.5. Statistical treatment of bivariate normal distributions	16
S.6. Solvation thermodynamics and statistics	18
S.7. Bond lengths and statistics	21
S.8. Excerpts from selected tables	22
S.9. Water bilayer on Au(111)	25
References	25

#### S.1. Construction of nanoparticles and micro-solvated \*OH and H<sub>2</sub>O configurations

The truncated octahedral nanoparticles for each metal were created by relaxing the converged coordinates for Pt nanoparticles found in previous works.<sup>1</sup> Micro-solvated \*OH configurations, more specifically the hydrogen and oxygen atom positions, were taken from the equivalent configurations relaxed in previous works.<sup>1</sup> The OH moiety and water molecules in each configuration were adsorbed onto nanoparticle atoms, equivalent to those on the Pt nanoparticle based on the local coordination environments within the nanoparticle. From these \*OH structures, corresponding H<sub>2</sub>O configurations are generated by replacing the OH moiety by a central H<sub>2</sub>O molecule, moving and rotating this H<sub>2</sub>O molecule away from the surface, and adjusting the orientation and position of the remainder three water molecules to obtain a roughly tetrahedral coordination of the central H<sub>2</sub>O oxygen atom. Ultimately, the central water molecule should form hydrogen bonds with each of the three peripheral water molecules, as shown in Figure 1 in the main text.

Additionally, corresponding \*OH and H<sub>2</sub>O configurations should agree on the features illustrated in Figure S.1: the orientation of the non-binding H atoms of the surface-bound solvent water molecules relative to the mirror plane intersecting the surface-bound solvent and solute adsorption site atom; the (downwards) orientation of one H atom on the non-surface bound water molecule; and (for non-mirror symmetric configurations) the orientation of the second H atom on the non-surface bound water molecule relative to the plane containing the solute O atom, the non-surface bound water molecule O atom and the solute adsorption site.



**Figure S.1.** Features which should be consistent between corresponding micro-solvated OH and  $H_2O$  configurations, in (a) top and (b) lateral views. Nanoparticle atoms are gray or (for the adsorption site) black; solvent oxygen atoms are red, solute oxygen atoms are cyan, and hydrogen atoms are white; relevant planes (perpendicular to the point of view) are shown as dashed lines, while defining displacements relative to these planes are shown using arrows.

#### S.2. Computational details

All calculations were performed using VASP 5.4.4.<sup>2–5</sup> For each calculation, a 450-eV planewave cut-off and a  $10^{-5}$ -eV electronic convergence step cutoff were used, unless specified otherwise. All calculations were performed for the  $\Gamma$ -point only. Free molecules were calculated in an 11 Å cubic unit cell, with  $k_BT = 0.001$  eV and Gaussian smearing of the Fermi level. All systems containing or derived from nanoparticles are calculated using  $k_BT = 0.2$  eV and second-order Methfessel-Paxton smearing of the Fermi level.<sup>6</sup> Systems derived from 38atom nanoparticles are calculated in 17.8 Å cubic unit cells, while systems derived from 79and 201-atom nanoparticles are calculated in 26 Å cubic unit cells. The configurations created in Section S.1 are relaxed using a conjugate gradient algorithm until all atomic forces are smaller than 0.05 eV Å<sup>-1</sup>. After each relaxation, the relaxed configuration is re-assessed according to the rules set out in Section S.1 and, if necessary, corrected by applying mirror transformations to those solvent and solute moieties which are inconsistent.

For each relaxed configuration, vibrational energies are calculated for all O and H atoms through single-atom displacements along each Cartesian unit vector using 0.02 Å steps in both directions to assess the zero-point energies and the vibrational entropies. If no imaginary modes are found, the configuration is considered to be converged and is used for further calculations. If imaginary modes are found, relaxation of the configuration is continued up to 0.02 eV Å<sup>-1</sup>, and another vibrational energy calculation is performed. If more than one imaginary mode persists in the vibrational energy calculation after additional convergence, an additional vibrational calculation is performed using more dense electronic plane wave sampling (600 eV) and stricter electronic convergence (10<sup>-7</sup> eV electronic step size) to reduce noise in the force calculations. Although the stricter criteria may increase forces on configuration ground states converged with the lesser criteria, resulting vibrational modes are sufficiently close to those obtained using the lesser criteria, as shown in Table S.1.

		Au79 k	ink, H <sub>2</sub> O		Ir <sub>79</sub> kink, OH					
	Lax	Strict	Diff		Lax	Strict	Diff			
	(meV)	(meV)	(meV)	$Corr^a$ (-)	(meV)	(meV)	(meV)	$Corr^a$ (-)		
ZPE	2601	2612	11	-	2337	2337	0	-		
TSvib	574	696	122	-	488	528	39	-		
$G_{vib}{}^b$	2027	1916	-111	-	1849	1810	-38	-		
Mode 1	464.8	466.2	1.4	1.00	467.2	466.5	-0.7	1.00		
Mode 2	463.7	465.8	2.1	0.91	462.7	461.9	-0.8	1.00		
Mode 3	463.0	465.4	2.4	0.90	461.2	459.7	-1.6	1.00		
Mode 4	462.1	465.1	3.0	0.99	433.0	431.7	-1.3	1.00		
Mode 5	424.9	426.9	2.0	1.00	416.5	415.4	-1.1	1.00		
Mode 6	419.4	421.7	2.4	1.00	347.4	347.0	-0.4	1.00		
Mode 7	412.6	414.4	1.8	1.00	336.9	336.3	-0.5	1.00		
Mode 8	384.4	385.9	1.5	1.00	199.2	198.9	-0.3	1.00		
Mode 9	202.0	201.7	-0.3	1.00	195.1	194.7	-0.5	0.17		
Mode 10	198.7	199.0	0.3	0.99	195.0	194.3	-0.7	0.17		
Mode 11	198.2	198.4	0.2	0.99	133.1	132.0	-1.0	1.00		
Mode 12	195.6	195.6	0.1	1.00	123.9	123.3	-0.7	0.99		
Mode 13	114.1	114.7	0.6	1.00	121.5	121.2	-0.3	0.99		
Mode 14	94.5	95.5	1.0	0.99	105.1	104.8	-0.3	1.00		
Mode 15	93.1	94.0	0.9	0.99	85.4	85.0	-0.3	1.00		
Mode 16	69.3	69.8	0.5	1.00	81.6	81.1	-0.6	1.00		
Mode 17	60.3	59.8	-0.5	0.99	58.3	57.7	-0.6	0.98		
Mode 18	58.2	58.2	0.0	0.99	56.4	55.4	-1.0	0.83		
Mode 19	51.3	51.6	0.2	0.78	54.5	54.4	-0.1	0.83		
Mode 20	49.3	49.8	0.5	0.78	51.5	49.9	-1.6	0.99		
Mode 21	46.6	46.0	-0.6	0.99	41.1	40.7	-0.5	0.99		
Mode 22	42.2	41.3	-0.9	0.99	39.9	39.4	-0.6	0.79		
Mode 23	41.3	39.9	-1.3	0.99	39.2	38.7	-0.5	0.79		
Mode 24	32.3	32.3	0.0	0.70	30.4	31.2	0.8	0.84		
Mode 25	29.8	29.8	0.0	0.69	29.5	30.4	0.8	0.84		
Mode 26	25.5	25.2	-0.3	0.98	26.1	26.5	0.3	0.90		
Mode 27	24.0	23.0	-1.0	0.98	23.1	23.3	0.2	0.90		
Mode 28	18.5	17.3	-1.2	0.70	15.8	16.6	0.8	0.98		
Mode 29	16.9	16.7	-0.3	0.65	13.3	14.5	1.2	0.92		
Mode 30	15.0	13.9	-1.1	0.94	10.4	13.1	2.7	0.94		
		Au79 k	ink, H <sub>2</sub> O			Ir <sub>79</sub> ki	nk, OH			
	Lax	Strict	Diff		Lax	Strict	Diff			
	(meV)	(meV)	(meV)	$Corr^a$ (-)	(meV)	(meV)	(meV)	$Corr^a$ (-)		
Mode 31	11.5	10.9	-0.5	0.60	9.1	11.8	2.7	0.98		
Mode 32	9.6	8.0	-1.6	0.18	7.3	9.1	1.8	0.84		
Mode 33	8.0	7.0	-1.0	0.40	3.6	7.5	3.8	0.87		
Mode 34	1.2	5.7	4.5	0.48	-	-	-	-		
Mode 35	9.0 i	4.5	-	0.55	-	-	-	-		
Mode 36	9.6 i	3.7	-	0.84	-	-	-	-		

 Table S.1. Vibrational modes for several converged configurations.

*a:* Inner product of lesser and stricter vibrational mode eigenvectors.*b:* Vibrational free energies as defined in Section S.3.

## S.3. Thermodynamics

Individual formation energies were calculated for all OH and H<sub>2</sub>O (deemed OH<sub>x</sub>, x = 1,2) configurations on each nanoparticle at sites *s* in micro-solvated and vacuum environments. Since the full formation energy for micro-solvated H<sub>2</sub>O formation from bulk H<sub>2</sub>O is:

$$^{*} + 4 H_2 0 \rightarrow ^{*} [4 H_2 0]$$
 (S.1)

and its micro-solvated \*OH counterpart is:

$$^{*} + 4H_{2}O \rightarrow ^{*}[OH \cdot 3H_{2}O] + H^{+} + e^{-}$$
 (S.2)

we can use the computational hydrogen electrode to obtain the following formation energies on each metal:<sup>7</sup>

$$\Delta G_{\rm MS}(OH_x;s) = E_{DFT,\rm MS}(OH_x;s) + E_{ZPE,\rm MS}(OH_x;s) - TS_{\rm MS}(OH_x;s) -E_M - 4G_{\rm H_2O} + \frac{(2-x)}{2}G_{\rm H_2}$$
(S.3)

in which  $\Delta E_{DFT,MS}$  is the DFT energy of the specific configuration,  $E_{ZPE,MS}$  is the zero-point energy, *T* is the temperature (300 K),  $S_{MS}$  is the vibrational entropy, and  $E_M$  is the DFT energy of the pristine nanoparticle.  $G_{H_2O}$  and  $G_{H_2}$  are the Gibbs free energies for H<sub>2</sub>O(*l*) and H<sub>2</sub>(*g*) under standard conditions, respectively, defined using entropies and the heat of fusion for H<sub>2</sub>O from literature,<sup>8</sup> as:

$$G_{H_2O(l)} = E_{DFT}(H_2O) + E_{ZPE}(H_2O) + \Delta H_{fus}(H_2O) - TS_{lit}(H_2O(l))$$

which is -2.46 eV with respect to  $G_{H_2}$  and  $G_{O_2}$ , and

$$G_{\mathrm{H}_{2}(g)} = E_{DFT}(\mathrm{H}_{2}) + E_{ZPE}(\mathrm{H}_{2}) - TS_{lit}(\mathrm{H}_{2}(g))$$

Analogously, individual formation energies were calculated for all vacuum (i.e., non-microsolvated) OH configurations, described using:  $^* + H_2O(l) \rightarrow ^*OH + H^+ + e^-$ , as:

$$\Delta G_{\text{vac}}(\text{OH}_{x};s) = E_{DFT,\text{vac}}(\text{OH}_{x};s) + E_{ZPE,\text{vac}}(\text{OH}_{x};s) - TS_{\text{vac}}(\text{OH}_{x};s) -E_{DFT,M} - \Delta G_{\text{H}_{2}\text{O}} + \frac{1}{2}\Delta G_{\text{H}_{2}}$$
(S.4)

From the micro-solvated formation energies, the micro-solvated formation energies for OH are calculated. This micro-solvated formation energy corresponds to the following chemical reaction:

$$*[4H_20] \rightarrow *[0H \cdot 3H_20] + H^+ + e^-$$
 (S.5)

from which we can derive the formation energy relative to analogous to electrochemical formation potentials using the computational hydrogen electrode,<sup>7</sup> as:

$$\Delta G_{f,MS} = \Delta G_{MS}(0H, s) - \Delta G_{MS}(H_2 0, s) + \frac{1}{2} \Delta G_{H_2}$$
(S.6)

Similarly, the vacuum formation energies for OH are calculated with respect to liquid water, as implied above:

$$\Delta G_{f,\text{vac}} = \Delta G_{\text{vac}}(\text{OH}, s) - \Delta G_{\text{H}_2\text{O}} + \frac{1}{2}\Delta G_{H_2}$$
(S.7)

Using these formation energies, we can obtain the (micro)solvation energy for OH on each specific site:

$$\Omega_{OH} = \Delta G_{f,\rm MS} - \Delta G_{f,\rm vac} \tag{S.8}$$

# S.4. Formation energy thermodynamics and statistics

Table S.2. Binding and formation energies.	
--	--

					Micro-s	solvated		Vacuum						
NP	site	CN		$\Delta E$	$\Delta E_{ZPE}$	TS	$\Delta G_{corr}$	$\Delta E$	$\Delta E_{ZPE}$	TS	$\Delta G_{corr}$	$\Delta G_{f, \text{vac}}$	$\Delta G_{f,MS}$	$\Omega_{OH}$
	111	6.00	OH	-0.78	2.22	0.55	-0.06	0.34	0.32	0.11	_	0.55	0.11	0.45
Δσ20	111	0.00	H <sub>2</sub> O	-1.10	2.58	0.68	-0.08	_	-	—	—	0.55	0.11	-0.45
11838	kink	4 00	OH	-1.07	2.26	0.56	-0.06	0.23	0.34	0.11	-	0.46	-0.25	-0.71
·	KIIIK	4.00	H <sub>2</sub> O	-1.00	2.58	0.67	-0.08	_	-	-	—	0.40	0.25	0.71
Ag79	111E	5.00	OH	-0.87	2.26	0.52	-0.06	0.93	0.31	0.12	-0.05	1.06	0.06	-1.00
		0.00	H <sub>2</sub> O	-1.17	2.59	0.60	-0.08	_	-	-	—	1.00	0.00	1100
	111T	6 67	OH	-0.63	2.24	0.60	—	1.04	0.30	0.19	-0.05	1 10	0 19	-0.90
		0.07	H <sub>2</sub> O	-1.11	2.60	0.60	-0.08	-	-	_	_	1.10	0.17	0.90
	kink	4 08	OH	-0.78	2.25	0.54	-0.06	0.93	0.31	0.10	-0.05	1.08	-0.02	-1 11
·			H <sub>2</sub> O	-1.01	2.59	0.70	_	_	-	-	_	1.00	0102	
Ag <sub>201</sub>	100F	5 17	OH	-0.94	2.25	0.55	-0.06	0.86	0.31	0.19	—	0.00	0.01	1.00
	TOOL	5.17	H <sub>2</sub> O	-1.17	2.59	0.72	-	-	-	-	-	0.77	-0.01	-1.00
	100T	6.22	OH	-0.79	2.23	0.52	-0.06	0.39	0.33	0.13	-	0.50	0.12	0.47
	1001	0.33	$H_2O$	-1.11	2.59	0.66	-0.08		-	-	-	0.59	0.12	-0.47
	1115	5.00	OH	-0.99	2.25	0.54	-0.06	0.83	0.31	0.10	-0.05	0.00	0.02	1.01
	THE	5.00	H <sub>2</sub> O	-1.21	$2.60^{a}$	$0.72^{a}$	—	_	-	-	—	0.99	-0.02	-1.01
	11170	7 50	OH	-0.35	2.23	0.54	-0.06	1.14	0.30	0.11	-0.05	1.29	0.25	0.02
	mit	7.50	$H_2O$	-0.91	$2.60^{a}$	$0.76^{a}$	_	I	-	-	_	1.20	0.35	-0.93
	111TM	6.92	OH	-0.64	$2.24^{a}$	$0.54^{a}$	-0.06	-	-	-	-	v	0.10	v
	111111	0.72	H <sub>2</sub> O	-1.06	2.59	0.64	-0.08	-	-	-	-	Λ	0.17	Λ
	kink	4 25	OH	-0.85	2.24	0.60	-0.06	0.82	0.31	0.12	-0.05	0.95	-0.14	-1 10
	KIIIK	1.23	H <sub>2</sub> O	-0.97	2.57	0.65	-0.08	_	-	—	—	0.95	0.11	1.10
Au <sub>38</sub>	111	6.00	OH	-0.66	2.25	0.58	-	х	х	х	-	x	0.33	x
		0.00	H <sub>2</sub> O	-1.22	2.60	0.62	-0.08	-	-	_	_	~	0.55	A
	kink	4.00	OH	-0.98	2.29	0.53	-0.06	0.52	0.32	0.18	-	0.67	0.34	0.32
	KIIIK	4.00	H <sub>2</sub> O	-1.58	2.62	0.67	—	_	_	_	—	0.07	0.54	-0.32
Au <sub>79</sub>	1111	5.00	OH	-0.43	2.29	0.55	-	1.11	0.32	0.12	-0.05	1.20	0.62	
	IIIE	5.00	$H_2O$	-1.23	2.60	0.68	-	-	-	-	-	1.20	0.65	-0.63
	1117	6.67	OH	-0.17	2.26	0.48	-0.06	1.37	0.32	0.18	—	151	0.71	0.90
	1111	0.07	H <sub>2</sub> O	-1.11	2.61	0.58	-0.08	_	_	_	_	1.51	0.71	-0.80
			OH	-0.38	2.30	0.58	_	0.99	0.33	0.15	_		0.40	0.40
	kink	4.08	H <sub>2</sub> O	-1.10	2.62	0.66	_	_	_	_	_	1.17	0.48	-0.69
Au <sub>201</sub>			OH	-0.47	$2.30^{a}$	0.55a	_	1.08	0.33	0.14	_			
	100E	5.17	H <sub>2</sub> O	_1.13	2.60	0.62	-0.08	_	_	_	_	1.27	0.51	-0.76
			011	0.42	2.00	0.524	0.00							
	100T	6.33	OH	-0.42	2.274	0.55*	-0.06	Х	X	X	_	х	0.43	х
			H <sub>2</sub> O	-1.11	$2.62^{a}$	$0.68^{a}$	-	-	-	-	-			
	111E	5.00	OH	-0.56	2.29	0.50	-0.06	1.07	0.32	0.10	-0.05	1.00	0.00	0.04
			H <sub>2</sub> O	-1.16	2.61	0.60	-0.08	-	-	-	-	1.23	0.39	-0.84
	111TC	7.50	OH	0.23	2.27	0.59	-	1.41	0.31	0.11	-0.05			
	-		H <sub>2</sub> O	-0.85	2.59	0.65	-0.08	_	-	-	_	1.56	0.89	-0.67
	111TM	6.92	OH	-0.08	2.27	0.55	-	1.38	0.31	0.11	-0.05	1.53	0.69	-0.84
			H <sub>2</sub> O	-1.00	2.62	0.67	_	-	-	-	-			
	kink	4.25	OH	-0.41	2.28	0.66	-	0.94	0.32	0.11	-0.05	1.10	0.30	-0.80
		-	H <sub>2</sub> O	-0.94	2.58	0.65	-0.08	-	-	-		-	-	
lr <sub>38</sub>	111	6.00	OH	-2.02	2.29	0.46	-	0.43	0.34	0.13	-	0.64	-0.18	-0.82
			H <sub>2</sub> O	-2.10	2.64	0.56	_	-	0.25	0.10	_			
	kink	4.00	UH	-2.54	2.33	0.48	—	-0.46	0.35	0.10	—	-0.21	-0.65	-0.44
Irac				-1.93	2.04	0.34	_	0.00	0.22	0.12	0.05			
1179	111E	5.00	UH	-2.39	2.32	0.47	_	0.09	0.32	0.12	-0.05	0.24	-0.46	-0.69
			$H_2O$	-2.14	2.64	0.58	-	-	-	-	-			

					Micro-s	olvated			Vacu	ium				
NP	site	CN		$\Delta E$	$\Delta E_{ZPE}$	TS	$\Delta G_{corr}$	$\Delta E$	$\Delta E_{ZPE}$	TS	$\Delta G_{corr}$	$\Delta G_{f, \text{vac}}$	$\Delta G_{f,MS}$	$\Omega_{OH}$
Ir79	111T	6 67	OH	-1.52	2.27	0.42	-0.06	0.62	0.34	0.12	-	0.84	-0.01	-0.85
		0.07	H <sub>2</sub> O	-1.83	2.64	0.55	-	-	_	_	-	0.01	0.01	0.05
	kink	4.08	OH	-2.10	2.34	0.49	—	-0.32	0.33	0.14	—	-0.12	-0.60	-0.47
Inc.			H <sub>2</sub> O	-1./1	2.63	0.57	—	-		-	—			
11201	100E	5.17	H <sub>0</sub> O	-2.34	2.32	0.47	_	X	Х	Х	_	х	-0.48	х
			0H	-2.07	2.04	0.38	- 0.06	0.48	0.33	0.13	-			
	100T	6.33	H <sub>2</sub> O	-1.95	2.27	0.40	-0.00	0.40	0.55	0.15		0.68	0.12	-0.57
			OH	-1.93	2.04	0.50	-0.00	0.10	0.35	0.11				
	111E	5.00	H <sub>2</sub> O	-2.40	2.51	0.50	_	-0.10	0.35	0.11	_	0.14	-0.50	-0.63
			OH	_1.06	2.04	0.33		0.68	0.34	0.12				
	111TC	7.50	H <sub>2</sub> O	_1.00	2.52	0.42	_	-	_		_	0.89	0.11	-0.79
	111T		OH	-1.60	2.31	0.46	_	0.53	0.33	0.14	_			
	М	6.92	H <sub>2</sub> O	-1.91	2.65	0.55	_	_	_	_	_	0.72	0.06	-0.66
	1 • 1	1.05	OH	-2.12	2.33	0.44	-0.06	-0.39	0.33	0.13	_	0.10	0.57	0.20
	kink	4.25	$H_2O$	-1.72	2.61	0.54	-0.08	-	_	_	-	-0.19	-0.57	-0.38
Pd <sub>38</sub>	111	6.00	OH	-0.69	2.26	0.47	-0.06	1.05	0.32	0.21	-	1 15	0.50	0.56
	111	0.00	$H_2O$	-1.52	2.61	0.64	-	-	—	—	-	1.15	0.39	-0.30
	kink	4.00	OH	-1.10	2.30	0.55	-	0.60	0.33	0.14	-	0.78	0.10	0.60
	KIIIK	4.00	$H_2O$	-1.42	2.61	0.57	-0.08	-	—	_	-	0.78	0.10	-0.09
Pd79	111F	5.00	OH	-1.31	2.30	0.55	-	0.64	0.32	0.10	-0.05	0.81	0.11	_0.70
	IIIL	5.00	$H_2O$	-1.67	2.61	0.54	-0.08	-	_	_	-	0.01	0.11	0.70
	111T	6.67	OH	-0.93	2.28	0.52	-	0.88	0.32	0.11	-0.05	1.04	0.32	-0.72
		0.07	H <sub>2</sub> O	-1.49	2.61	0.60	-	-	—	-	_	1101	0.02	0.72
	kink	4.08	ОН	-1.07	2.29	0.53	-	0.66	0.32	0.09	-0.05	0.84	0.06	-0.77
			H <sub>2</sub> O	-1.39	2.62	0.59	-	-	-	_	-			
Pd <sub>201</sub>	100E	5.17	OH	-1.12	2.29	0.55	-	0.73	0.33	0.16	-	0.90	0.27	-0.62
			H <sub>2</sub> O	-1.59	2.61	0.68	-	-	-	-	-			
	100T	6.33	ОН	-0.69	2.27	0.54	-	0.94	0.32	0.16	-	1.10	0.53	-0.57
				-1.52	2.62	0.60	_	-	-	-	-			
	111E	5.00	OH	-1.29	2.29	0.48	-0.06	0.67	0.32	0.12	-0.05	0.81	0.11	-0.70
			H <sub>2</sub> O	-1.66	2.62	0.62	-	-	—	-	_			
	111TC	7.50	OH	-0.67	2.29	0.48	_	0.91	0.32	0.11	-0.05	1.06	0.45	-0.62
			H <sub>2</sub> O	-1.30	2.61	0.54	-0.08	-	-	-	_			
	111T	6.92	OH	-0.92	2.28	0.50	—	0.86	0.33	0.15	—	1.04	0.39	-0.65
	M		H <sub>2</sub> O	-1.56	2.62	0.58	-	-	-	-	_	0.75	0.12	0.62
	kink	4.25	ПО	-1.05	2.29	0.48	-0.06	0.59	0.32	0.16	-	0.75	0.13	-0.62
	7.1	1 1 4 1	H <sub>2</sub> O	-1.37	2.59	0.66	—   1'	-	-	_	-			l

| | | |  $H_2O$  | -1.37 2.59 0.66 | - | - - a: Vibrational data obtained using denser plane wave sampling, as described in S.2. *x*: No stable configuration available for this adsorption site.

**Table S.3.** Quality of linear relations of OH formation energies between different metals and adsorption site coordination numbers.

Exclu	uding 3	8–111T, 201–							no
	-	100T, <b>MS</b> <sup>a</sup>	CN	Ag	Au	Ir	Pd	Pt	trend <sup>b</sup>
		R	0.93		0.98	0.96	0.91	0.93	-
	Ag	$max \Delta G_y   x$	0.11	_	0.11	0.12	0.16	0.19	0.27
		ave $\Delta G_y   x$	0.05		0.04	0.06	0.09	0.07	0.13
		R	0.90	0.95		0.94	0.90	0.94	-
	Au	$max \Delta G_y   x$	0.13	0.10	_	0.14	0.19	0.16	0.31
		ave $\Delta G_y   x$	0.07	0.04		0.08	0.09	0.08	0.17
		R	0.99	0.92	0.89		0.96	0.96	-
MS	Ir	$max \Delta G_{v}   x$	0.09	0.17	0.23	_	0.26	0.21	0.42
		ave $\Delta G_{v} x$	0.04	0.10	0.12		0.09	0.08	0.28
		R	0.95	0.83	0.81	0.93		0.95	_
	Pd	$max \Delta G_{y}   x$	0.08	0.12	0.15	0.12	_	0.04	0.22
		ave $\Delta G_{y}   x$	0.04	0.07	0.06	0.04	_	0.03	0.14
		R	0.95	0.87	0.89	0.93	0.90	0.05	_
	Pt	$max \Delta G_{n}   x$	0.11	0.16	0.18	0.13	0.07		0.40
	11	ave $\Delta G_{\mu} _{X}$	0.06	0.10	0.10	0.15	0.07	_	0.21
Fych	iding 3	$\frac{11117}{201}$	0.00	0.10	0.08	0.07	0.05		no
LACI	uning J	100T, <i>vac</i>	CN	Ag	Au	Ir	Pd	Pt	trend <sup>b</sup>
		R	0.66		0.94	0.66	0.60	0.76	_
	Ag	$max \Delta G_{v}   x$	0.38	_	0.13	0.37	0.42	0.32	0.22
	0	ave $\Delta G_{y} x$	0.11		0.07	0.14	0.13	0.10	0.07
		R	0.86	0.97	0.07	0.88	0.82	0.88	_
	Au	$max \Delta G_{2}   x$	0.34	0.18		0.31	0.39	0.28	0.23
	114	ave $\Lambda G_{-1} x$	0.09	0.07	—	0.10	0.09	0.10	0.15
		R	0.98	0.81	0.94	0.10	0.95	0.10	_
vac	Ir	$max \Lambda G_{\perp}   x$	0.14	0.48	0.32		0.23	0.36	0.55
vac		ave $\Delta G   r$	0.14	0.40	0.52	-	0.23	0.50	0.39
		$uve \Delta u_y   x$	0.00	0.29	0.18	0.08	0.11	0.10	0.57
	Dd	$mar \Lambda G   r$	0.06	0.17	0.11	0.07		0.00	0.16
	Fu	$\max \Delta G_y   x$	0.00	0.15	0.11	0.07	-	0.09	0.10
		$ave \Delta G_y   x$	0.03	0.08	0.06	0.03	0.05	0.04	0.11
	D	K K	0.97	0.87	0.94	0.97	0.95		-
	Pt	$\max \Delta G_y   x$	0.10	0.22	0.16	0.16	0.15	-	0.54
		$ave \Delta G_y x$	0.04	0.10	0.09	0.06	0.08		0.17
Exc	luding	38 sites, 201–	<u>CN</u>	Ag	Au	Ir	Pd	Pt	no
		1001, MIS	0.04	-	0 00	0.97	0.02	0.96	trena®
	1 0	$mar \Lambda G   r$	0.09		0.99	0.00	0.12	0.00	0.27
	Ag	$\max \Delta G_y   x$	0.08	-	0.00	0.09	0.15	0.09	0.27
		$uve \Delta u_y   x$	0.04	0.07	0.03	0.05	0.07	0.05	0.15
	•		0.12	0.97		0.95	0.10	0.94	0.21
	Au	$\max \Delta G_y   x$	0.13	0.07	—	0.14	0.18	0.14	0.51
		$ave \Delta G_y   x$	0.07	0.03	0.06	0.08	0.10	0.07	0.15
MS		<u> </u>	0.98	0.93	0.80		0.96	0.97	-
	Ir	$\max \Delta G_y   x$	0.09	0.16	0.23	-	0.26	0.20	0.42
		ave $\Delta G_y   x$	0.05	0.09	0.13	0.0-	0.09	0.07	0.27
		R	0.94	0.84	0.79	0.92		0.95	-
	Pd	$max \Delta G_y   x$	0.09	0.11	0.15	0.12	_	0.05	0.22
		ave $\Delta G_y   x$	0.04	0.06	0.07	0.04		0.03	0.13
		R	0.96	0.92	0.89	0.93	0.90		_
	Pt	$max \Delta G_y   x$	0.11	0.12	0.18	0.13	0.07	_	0.40
		ave $\Delta G_y   x$	0.05	0.08	0.09	0.06	0.05		0.19

Excluding 38 sites, 201–						x	<b>D</b> 1	D	no
	U	100T, <i>vac</i>	CN	Ag	Au	lr	Pd	Pt	trend <sup>b</sup>
		R	0.78		0.80	0.77	0.79	0.87	-
	Ag	$max \Delta G_y   x$	0.10	_	0.09	0.09	0.09	0.10	0.22
		ave $\Delta G_y   x$	0.06		0.05	0.06	0.06	0.04	0.07
		R	0.98	0.89		0.99	0.98	0.95	-
	Au	$max \Delta G_y   x$	0.05	0.18	_	0.04	0.06	0.12	0.23
		ave $\Delta G_y   x$	0.03	0.08		0.02	0.03	0.04	0.15
		R	0.98	0.88	0.99		0.95	0.93	-
vac	Ir	$max \Delta G_y   x$	0.14	0.49	0.10	_	0.24	0.36	0.55
		ave $\Delta G_y   x$	0.07	0.20	0.05		0.10	0.11	0.39
		R	0.95	0.89	0.99	0.98		0.90	-
	Pd	$max \Delta G_y   x$	0.06	0.12	0.05	0.06	_	0.09	0.16
		ave $\Delta G_y   x$	0.03	0.06	0.02	0.03		0.04	0.11
		R	0.97	0.93	0.97	0.97	0.95		-
	Pt	$max \Delta G_y   x$	0.10	0.21	0.13	0.16	0.13	_	0.34
		ave $\Delta G_y   x$	0.04	0.07	0.05	0.06	0.07		0.17
Exclud	ing 38,	79 sites, 201-	$\overline{CN}$	Δσ	Δ11	Ir	Pd	Pt	no
		100T, <b>MS</b>	CIV	лg	Au		1 u	11	<i>trend<sup>b</sup></i>
		R	0.99		0.99	0.98	0.96	0.98	-
	Ag	$max \Delta G_y   x$	0.04	_	0.05	0.07	0.10	0.07	0.28
		ave $\Delta G_y   x$	0.02		0.02	0.05	0.06	0.04	0.16
		R	0.98	0.99		0.97	0.98	0.99	-
	Au	$max \Delta G_y   x$	0.06	0.05	-	0.10	0.08	0.04	0.33
		ave $\Delta G_y   x$	0.04	0.02		0.07	0.06	0.03	0.19
MS	Ir	R	0.98	0.96	0.94		0.96	0.98	-
		$\max \Delta G_y   x$	0.07	0.15	0.16	_	0.21	0.15	0.39
		ave $\Delta G_y   x$	0.05	0.08	0.08		0.09	0.07	0.29
		R	0.94	0.92	0.96	0.92		0.99	-
	Pd	$\max \Delta G_y   x$	0.08	0.09	0.06	0.09	-	0.03	0.18
		ave $\Delta G_y   x$	0.03	0.04	0.03	0.04		0.02	0.12
		R	0.98	0.97	0.99	0.96	0.98		-
	Pt	$max \Delta G_y   x$	0.09	0.11	0.05	0.12	0.05	-	0.35
		ave $\Delta G_y   x$	0.04	0.05	0.03	0.07	0.03		0.22
Exclud	ing 38,	79 sites, 201–	CN	Ag	Au	Ir	Pd	Pt	no
		1001, MIS	0.08		0.06	0.08	0.04	0.00	trend
	1 -	$mar \Lambda G   r$	0.90		0.90	0.90	0.74	0.99	0.23
	Ag	$ava \Delta G   x$	0.03	-	0.05	0.04	0.08	0.03	0.11
		$uve \Delta u_y   x$	0.02	0.08	0.04	0.05	0.04	0.02	0.11
	Δ.,,	$mar \Lambda G   r$	0.02	0.90		0.02	0.99	0.03	0.24
	Au	$ava \Delta G   x$	0.03	0.07	-	0.03	0.04	0.03	0.16
		$uve \Delta u_y   x$	0.02 1 00	0.04	1 00	0.02	0.02	0.02	0.10
MS	La	$mar \Lambda G   r$	1.00	0.33	0.06		0.99	0.99	0.58
	Iľ	$ave \Lambda C \downarrow x$	0.05	0.12	0.00	-	0.08	0.07	0.30
		$uve \Delta u_y   \lambda$	0.03	0.08	0.04 1 00	0.00	0.06	0.04	0.42
	٤đ	mar AC Inc	0.90	0.97	1.00	0.99		0.20	0.16
	Pa	$\max \Delta G_{y}   x$	0.04	0.00	0.03	0.03	-	0.04	0.10
		$ave \Delta G_y   x$	0.02	0.03	0.01	0.02	0 00	0.02	0.11
	D4	mar AC 1	1.00	0.99	0.99	1.00	0.99		0.31
	Γl	$av \Delta G_{y x}$	0.01	0.03	0.04	0.04	0.08	-	0.21
	1		0.01	0.05	0.05	0.02	0.04		0.21

*a*: All  $\Delta G_y$  in this table are in eV.

*b*: Null hypothesis, in which deviations are relative to the average as opposed to linear regression.

**Table S.4.** Parameters for linear regressions of OH formation energies between different metals and adsorption site coordination numbers.

					ĺ		Metal <i>x</i>		
		Metal y	Parameters <sup>a</sup>	ĊN	Ag	Au	Ir	Pd	Pt
Excluding 38-	MS	Ag	a	0.13	_	0.91	0.55	1.07	0.72
1111, 201–1001			b	-0.67 0.13	1.00	-0.46	0.23	-0.19 1.10	-0.08 0.77
		Au	b	-0.17	0.51	-	0.74	0.31	0.43
		Ir	а	0.23	1.53	1.40	_	1.97	1.28
			b	-1.59	-0.40	-1.11	0.43	-0.77	-0.55
		Pd	a b	-0.35	0.19	-0.12	0.45	-	0.62
		Dt	a	0.16	1.05	1.02	0.68	1.50	
		- Ti	b	-0.72	0.12	-0.40	0.39	-0.17	_
	vac	Ag	a b	0.12	-	0.80	0.36	-0.08	0.85
			a	0.18	1.09	0.01	0.56	1.85	1.08
		Au	b	0.27	0.14	_	1.09	-0.39	0.42
		Ir	a	0.33	1.22	1.39	_	3.42	1.85
			b a	-1.50 0.09	-0.98	-1.45 0.36	0.27	-2.76	-1.16 0.49
		Pd	b	0.41	0.58	0.44	0.81	-	0.51
		Pt	a	0.17	0.67	0.71	0.48	1.66	_
F 1 1 20 1	140	11	b	-0.12	0.07	-0.12	0.64	-0.70	0.73
Excluding 38 sites, 201–100T	MS	Ag	a b	0.12 -0.58	-	<b>0.81</b> 0.39	0.49	<b>0.91</b> -0.14	<b>0.63</b> -0.04
			a	0.13	1.17	0.57	0.54	1.03	0.73
		Au	b	-0.15	0.49	_	0.74	0.34	0.45
		Ir	a	0.23	1.78	1.38	_	1.91	1.22
			b a	-1.60 0.11	-0.44	-1.10 <b>0.60</b>	0.44	-0.75	-0.52 0.61
		Pd	b	-0.37	0.17	-0.12	0.37	_	0.12
		Pt	а	0.17	1.35	1.08	0.71	1.54	_
			b	-0.79	0.08	-0.44	0.39	-0.18	0.49
	vac	Ag	a b	0.70	-	0.51	1.02	0.75	0.69
		A	a	0.14	1.24	0110	0.41	1.41	0.80
		Au	b	0.57	-0.02	_	1.19	0.05	0.69
		Ir	a	0.32	3.14	2.37	-	3.26	1.89
			a	0.09	<b>0.86</b>	0.68	0.28	-2.00	0.53
		Pd	b	0.39	-0.03	0.00	0.81	-	0.48
		Pt	a	0.16	1.59	1.12	0.46	1.54	_
Excluding 38-79	MS		b	-0.08	-0.92	-0.69	0.65	<u>-0.58</u>	0.53
sites, 201–100T	ms	Ag	b a	-0.73	-	-0.32	0.18	-0.17	-0.07
		Δu	a	0.15	1.15	_	0.44	0.75	0.51
			b	-0.37	0.44	1.07	0.63	0.30	0.38
		Ir	a b	<b>0.25</b> -1.70	-0.35	1.07 _0.78	-	1.84 _0.79	1.13 _0.54
		D I	a	0.11	0.76	0.46	0.47	0.77	0.58
		Pa	b	-0.36	0.25	0.07	0.41	-	0.14
		Pt	a	0.21	1.43	0.90	0.82	1.67	_
	vac		D a	-0.93 0.05	0.18	-0.19 <b>0.76</b>	0.47	-0.23 -0.25	0.05
		Ag	b	0.68	-	0.08	0.93	1.19	0.92
		An	а	0.14	1.21	_	0.45	1.43	0.79
			b	0.51	0.02	2.22	1.18	0.03	0.67
		Ir	a h	<b>0.33</b> -1.55	0.18	<b>2.22</b> -2.62	-	2.74 -2.17	<b>1./ð</b> -1.17
		יח	a	0.11	-0.10	0.69	0.34	,	0.59
		rd	b	0.32	1.02	-0.01	0.80	-	0.43
		Pt	a 1.	0.19	0.05	1.24	0.56	1.60	_
	I	l	b	-0.23	0.79	-0.82	0.66	-0.64	

*a*: Parameters for linear regressions  $\overline{\Delta G_y} = a\Delta G_x + b$ , for which  $\overline{\Delta G_y}, \Delta G_x, a$ , and *b* are in eV.

	Site		MS	5, 38		MS, 79				$M_{2}^{*}$	S, 201		
	$(\overline{CN})$	Parameters <sup>a</sup>	111	kink	111E	111T	kink	100E	100T	111E	111TC	111TM	kink
MS,		R		0.84	0.65	0.61	0.71	0.84	0.79	0.77	0.60	0.68	0.86
38	111	$max \Delta G_{} x$		0.25	0.36	0.35	0.33	0.26	0.21	0.29	0 39	0.34	0.22
	(6.00)	$ave \Lambda G   r$	-	0.10	0.16	0.55	0.55	0.10	0.14	0.14	0.15	0.14	0.10
		$ave \Delta u_y _X$	0.04	0.10	0.10	0.17	0.15	1.00	0.14	0.14	0.15	0.14	0.10
	kink		0.04		0.94	0.92	0.95	1.00	0.75	0.97	0.94	0.90	0.99
	(4.00)	$\max \Delta G_y   x$	0.32	-	0.16	0.16	0.16	0.06	0.35	0.14	0.22	0.13	0.08
	. ,	ave $\Delta G_y x$	0.15		0.11	0.12	0.09	0.02	0.20	0.07	0.09	0.09	0.04
MS,	1111	R	0.65	0.94		0.97	0.99	0.95	0.49	0.98	0.95	0.93	0.94
79	(5.00)	$max \Delta G_y   x$	0.46	0.14	-	0.13	0.05	0.14	0.49	0.10	0.16	0.22	0.19
	(5.00)	ave $\Delta G_{y} x$	0.22	0.11		0.06	0.03	0.10	0.27	0.05	0.09	0.11	0.09
		R	0.61	0.92	0.97		0.96	0.92	0.50	0.94	0.96	0.96	0.91
	111T	$max \Delta G_{y}   x$	0.35	0.14	0.09	_	0.10	0.14	0.37	0.11	0.13	0.12	0.15
	(6.67)	ave $\Delta G_{n}   x$	0.14	0.08	0.04		0.06	0.09	0.16	0.07	0.05	0.05	0.09
		R	0.71	0.95	0.99	0.96	0.00	0.97	0.52	1.00	0.93	0.92	0.97
	kink	$max \Lambda G_{-}   x$	0.41	0.16	0.05	0.15		0.10	0.45	0.05	0.16	0.24	0.14
	(4.08)	$ave \Lambda G   r$	0.71	0.10	0.03	0.15	-	0.10	0.75	0.03	0.10	0.11	0.14
MC		$uve \Delta u_y _{\lambda}$	0.21	1.00	0.05	0.09	0.07	0.08	0.20	0.03	0.11	0.11	0.07
201	100E		0.04	1.00	0.95	0.92	0.97		0.71	0.98	0.95	0.94	0.99
201	(5.17)	$\max \Delta G_y   x$	0.31	0.06	0.15	0.18	0.10	-	0.34	0.09	0.21	0.15	0.06
	. /	ave $\Delta G_y x$	0.15	0.02	0.10	0.12	0.08		0.21	0.06	0.10	0.10	0.03
	100T	R	0.79	0.75	0.49	0.50	0.52	0.71		0.57	0.64	0.71	0.68
	(6 33)	$max \Delta G_y   x$	0.22	0.20	0.26	0.27	0.26	0.21	-	0.25	0.20	0.20	0.24
	(0.55)	ave $\Delta G_y   x$	0.09	0.12	0.17	0.17	0.16	0.12		0.15	0.15	0.14	0.12
	1115	R	0.77	0.97	0.98	0.94	1.00	0.98	0.57		0.92	0.92	0.99
	111E (5.00)	$max \Delta G_{y} x$	0.31	0.12	0.09	0.14	0.05	0.08	0.34	_	0.14	0.18	0.07
	(5.00)	ave $\Delta G_{y} x$	0.16	0.06	0.04	0.09	0.02	0.05	0.21		0.10	0.10	0.04
		R	0.60	0.94	0.95	0.96	0.93	0.93	0.64	0.92		0.98	0.90
	111TC	$max \Delta G x$	0.35	0.16	0.12	0.14	0.13	0.16	0.36	0.12		0.07	0.18
	(7.50)	ave $\Lambda G   r$	0.17	0.10	0.06	0.14	0.15	0.10	0.17	0.00	-	0.07	0.10
		$uve \Delta u_y _X$	0.17	0.07	0.00	0.00	0.08	0.08	0.17	0.09	0.08	0.04	0.10
	111TM	mar AC In	0.00	0.90	0.95	0.90	0.94	0.54	0.71	0.92	0.90		0.92
	(6.92)	$\max \Delta G_y   x$	0.28	0.08	0.15	0.11	0.10	0.10	0.29	0.15	0.06	-	0.11
		ave $\Delta G_y   x$	0.13	0.06	0.06	0.05	0.07	0.07	0.12	0.08	0.03		0.08
	kink	R	0.86	0.99	0.94	0.91	0.97	0.99	0.68	0.99	0.90	0.92	
	(4.08)	$max \Delta G_y   x$	0.26	0.06	0.17	0.17	0.13	0.05	0.30	0.08	0.23	0.15	-
	(1100)	ave $\Delta G_y   x$	0.12	0.04	0.09	0.11	0.07	0.02	0.19	0.04	0.11	0.11	
vac,	111	R		0.61	0.38	0.61	0.42	0.57	0.60	0.50	0.32	0.56	0.63
38	(6.00)	$max \Delta G_y   x$	_	0.25	0.33	0.25	0.32	0.27	0.28	0.29	0.36	0.29	0.23
	(0.00)	ave $\Delta G_{y} x$		0.18	0.18	0.18	0.18	0.18	0.15	0.18	0.18	0.17	0.17
vac,		R	0.93		0.81	0.73	0.87	0.93	0.67	0.90	0.73	0.75	0.94
38	kink	$max \Delta G_{y}   x$	0.17	_	0.32	0.33	0.27	0.18	0.38	0.22	0.37	0.30	0.17
	(4.00)	ave $\Delta G_{y}   x$	0.11		0.17	0.22	0.15	0.12	0.24	0.13	0.21	0.21	0.11
vac.		R	0.56	0.81		0.83	0.94	0.85	0.29	0.92	0.81	0.74	0.85
79	111E	$max \Delta G x$	0.35	0.37		0.36	0.23	0.32	0.48	0.25	0.37	0.42	0.31
	(5.00)	ave $\Lambda G   \mathbf{x}$	0.33	0.17	_	0.14	0.00	0.15	0.10	0.10	0.15	0.12	0.15
		are $\Delta a_y   x$	0.27	0.17	0.00	0.14	0.09	0.13	0.30	0.10	0.15	0.18	0.15
	111T	max AC 1v	0.37	0.74	0.17		0.10	0.22	0.42	0.00	0.00	0.25	0.22
	(6.67)	$ave \Lambda C I \propto$	0.41	0.24	0.17	-	0.10	0.25	0.43	0.19	0.27	0.23	0.22
		$uve \Delta u_y   \lambda$	0.19	0.15	0.09	0.74	0.11	0.15	0.19	0.12	0.11	0.13	0.15
	kink	R Mar AC Le	0.04	0.79	0.40	0.70		0.40	0.28	0.90	0.72	0.07	0.40
	(4.08)	$\max \Delta G_y   x$	0.51	0.55	0.40	0.53	-	0.49	0.68	0.40	0.54	0.60	0.48
		ave $\Delta G_y x$	0.34	0.22	0.19	0.24		0.20	0.39	0.16	0.28	0.27	0.19
vac,	100E	R	0.08	0.52	0.88	0.82	0.89		0.39	0.85	0.61	0.55	0.65
201	(5.17)	$max \Delta G_y   x$	0.31	0.23	0.13	0.16	0.14	-	0.31	0.16	0.26	0.25	0.18
	(0.177)	ave $\Delta G_y   x$	0.15	0.16	0.07	0.10	0.07		0.15	0.09	0.13	0.15	0.15
	100T	R	0.80	0.80	0.50	0.72	0.51	0.73		0.57	0.73	0.89	0.70
	(6.33)	$max \Delta G_y   x$	0.21	0.23	0.32	0.27	0.32	0.27	_	0.31	0.24	0.16	0.27
	(0.55)	ave $\Delta G_{y} x$	0.11	0.12	0.16	0.13	0.16	0.13		0.16	0.12	0.09	0.14
		R	0.62	0.84	0.94	0.85	0.96	0.88	0.32		0.82	0.76	0.89
	111E	$max \Delta G_{\nu}   x$	0.37	0.36	0.24	0.35	0.22	0.32	0.50	_	0.36	0.43	0.30
	(5.00)	ave $\Delta G_{y} x$	0.28	0.17	0.10	0.14	0.09	0.15	0.31		0.17	0.18	0.15
		R	0.34	0.75	0.93	0.88	0.90	0.78	0.19	0.86	0.17	0.78	0.76
	111TC	$max \Lambda G_{-1}x$	0.34	0.22	0.14	0.18	0.17	0.22	0.35	0.20		0.22	0.24
	(7.50)	$av = \Delta g \mu a$	0.10	0.12	0.07	0.10	0.17	0.12	0.00	0.10	-	0.22	0.12
		D	0.19	0.13	0.07	0.08	0.08	0.12	0.20	0.10	0.06	0.15	0.12
	111TM	K Mar AC Is	0.34	0.91	0.99	0.99	0.97	0.91	0.49	0.95	0.10		0.10
	(6.92)	$\max \Delta G_y   x$	0.40	0.16	0.07	0.05	0.11	0.16	0.44	0.14	0.10	-	0.19
		ave $\Delta G_y   x$	0.20	0.11	0.04	0.02	0.06	0.11	0.22	0.08	0.05		0.11

**Table S.5.** Quality of linear relations between formation site binding energies.

	Site		MS	. 38		MS. 79				MS	5. 201		
	$(\overline{CN})$	Parameters <sup>a</sup>	111	kink	111E	111T	kink	100E	100T	111E	111TC	111TM	kink
vac,		R	0.67	0.82	0.90	0.78	0.93	0.87	0.35	0.92	0.76	0.71	
201	k1nk	$max \Delta G_{y} x$	0.45	0.49	0.34	0.47	0.32	0.44	0.64	0.34	0.48	0.56	_
	(4.08)	ave $\Delta G_{y} x$	0.32	0.20	0.17	0.22	0.13	0.17	0.36	0.14	0.25	0.25	
					•			•					
	Site		vac	, 38		vac, 79				va	c, 201		
	$(\overline{CN})$	Parameters <sup>a</sup>	111	kink	111E	111T	kink	100E	100T	111E	111TC	111TM	kink
MS,	111	R		0.93	0.56	0.37	0.64	0.08	0.80	0.62	0.34	0.54	0.67
38	(6.00)	$max \Delta G_y   x$	-	0.13	0.38	0.39	0.33	0.27	0.20	0.35	0.42	0.37	0.33
	(0.00)	ave $\Delta G_y   x$		0.08	0.18	0.20	0.17	0.14	0.16	0.17	0.19	0.20	0.16
	kink	R	0.61		0.81	0.72	0.79	0.52	0.80	0.84	0.75	0.91	0.82
	(4.00)	$\max \Delta G_y   x$	0.36	-	0.35	0.32	0.38	0.32	0.27	0.33	0.33	0.20	0.36
MS		$ave \Delta G_y x$	0.19	0.91	0.17	0.21	0.18	0.16	0.14	0.16	0.20	0.15	0.16
79	111E	$max \Lambda G_{n}   x$	0.36	0.36		0.90	0.00	0.18	0.30	0.21	0.93	0.99	0.90
	(5.00)	ave $\Delta G_{y} x$	0.18	0.15	_	0.12	0.12	0.10	0.15	0.09	0.11	0.05	0.11
		R	0.61	0.73	0.83	0.12	0.76	0.82	0.72	0.85	0.88	0.99	0.78
	111T	$max \Delta G_{y} x$	0.16	0.30	0.23	_	0.24	0.19	0.13	0.22	0.19	0.04	0.23
	(6.67)	ave $\Delta G_y   x$	0.08	0.13	0.10		0.11	0.10	0.07	0.09	0.09	0.02	0.10
	kink	R	0.42	0.87	0.94	0.87		0.89	0.51	0.96	0.90	0.97	0.93
	(4.08)	$max \Delta G_y   x$	0.39	0.31	0.22	0.28	-	0.16	0.34	0.19	0.26	0.14	0.22
	(1.00)	ave $\Delta G_y   x$	0.19	0.12	0.09	0.14		0.08	0.18	0.08	0.12	0.08	0.09
MS, 201	100E	R	0.57	0.93	0.85	0.74	0.84		0.73	0.88	0.78	0.91	0.87
201	(5.17)	$\max \Delta G_y   x$	0.39	0.21	0.30	0.34	0.33	-	0.31	0.28	0.33	0.21	0.31
		$ave \Delta G_y x$	0.19	0.10	0.15	0.20	0.16	0.20	0.15	0.14	0.18	0.15	0.14
	100T	$max \Lambda G   x$	0.00	0.07	0.29	0.12	0.20	0.39		0.32	0.19	0.49	0.33
	(6.33)	ave $\Delta G_{y} x$	0.15	0.11	0.17	0.19	0.17	0.15	-	0.17	0.18	0.16	0.16
		R	0.50	0.90	0.92	0.83	0.90	0.85	0.57	0.17	0.86	0.95	0.92
	111E	$max \Delta G_{v} x$	0.33	0.23	0.20	0.25	0.22	0.15	0.29	_	0.25	0.16	0.20
	(5.00)	ave $\Delta G_y   x$	0.17	0.09	0.09	0.13	0.10	0.08	0.16		0.12	0.09	0.08
	111TC	R	0.32	0.73	0.81	0.80	0.72	0.61	0.73	0.82	-	0.98	0.76
	(7.50)	$max \Delta G_y   x$	0.23	0.29	0.27	0.27	0.27	0.23	0.16	0.25		0.10	0.26
	(7.50)	ave $\Delta G_y x$	0.13	0.15	0.11	0.12	0.15	0.15	0.11	0.12		0.05	0.14
	111TM	R	0.56	0.75	0.74	0.77	0.67	0.55	0.89	0.76	0.78		0.71
	(6.92)	$\max \Delta G_y   x$	0.19	0.23	0.27	0.21	0.28	0.24	0.10	0.26	0.23	-	0.27
		$ave \Delta G_y x$	0.09	0.12	0.11	0.12	0.12	0.12	0.06	0.11	0.12	0.80	0.11
	kink	$max \Lambda G_{\rm cl} x$	0.05	0.94	0.05	0.75	0.05	0.05	0.70	0.09	0.70	0.22	
	(4.08)	ave $\Delta G_{y} x$	0.17	0.08	0.13	0.17	0.13	0.11	0.16	0.11	0.15	0.13	-
		yi	0.17	0.00	0.15	0.17	0.15	0.11	0.10	0.11	0.12	0.12	
	Site		vac	, 38		vac, 79				va	ıc, 201		
	$(\overline{CN})$	Parameters <sup>a</sup>	111	kink	111E	111T	kink	100E	100T	111E	111TC	111TM	kink
vac,	111	R		0.60	0.06	0.22	0.19	0.06	0.75	0.18	0.23	0.54	0.21
38	(6.00)	$max \Delta G_y   x$	-	0.24	0.39	0.36	0.37	0.36	0.23	0.38	0.38	0.25	0.37
	(0.00)	ave $\Delta G_y   x$		0.17	0.20	0.18	0.19	0.24	0.11	0.19	0.19	0.16	0.19
	kink	R	0.60		0.81	0.56	0.86	0.29	0.62	0.84	0.60	0.72	0.88
	(4.00)	$\max \Delta G_y   x$	0.48	-	0.36	0.46	0.27	0.20	0.42	0.31	0.46	0.40	0.27
vac		R	0.24	0.81	0.18	0.24	0.10	0.10	0.20	1 00	0.22	0.24	0.14
79	111E	max $\Delta G_{y} x$	0.48	0.30	_	0.31	0.11	0.10	0.46	0.06	0.17	0.09	0.11
	(5.00)	ave $\Delta G_v   x$	0.24	0.18		0.16	0.06	0.05	0.23	0.03	0.11	0.07	0.04
	1117	R	0.22	0.56	0.83		0.77	0.99	0.11	0.85	0.92	0.93	0.76
	(6.67)	$max \Delta G_y   x$	0.15	0.35	0.19	-	0.26	0.06	0.14	0.19	0.15	0.16	0.25
	(0.07)	ave $\Delta G_y   x$	0.09	0.15	0.12		0.14	0.03	0.10	0.12	0.09	0.08	0.14
	kink	R	0.19	0.86	0.98	0.77		0.93	0.13	0.99	0.85	0.93	1.00
	(4.08)	$\max \Delta G_y   x$	0.67	0.34	0.15	0.48	-	0.14	0.67	0.11	0.35	0.29	0.07
	( )	ave $\Delta G_y   x$	0.34	0.22	0.09	0.27	0.02	0.07	0.37	0.07	0.22	0.15	0.03
vac, 201	100E	K max AC 1x	0.06	0.29	0.95	0.99	0.93		0.73	0.99	0.89	0.94	0.90
	(5.17)	ave $\Lambda G_{y x}$	0.15	0.28	0.09	0.03	0.11	_	0.10	0.04	0.14	0.10	0.09
		R	0.75	0.10	0.00	0.03	0.13	0.73	0.00	0.17	0.07	0.00	0.20
	100T	$max \Delta G_{v} x$	0.25	0.30	0.29	0.26	0.30	0.22	_	0.31	0.24	0.03	0.31
	(6.33)	ave $\Delta G_v   x$	0.13	0.15	0.22	0.22	0.21	0.15		0.21	0.22	0.02	0.21
	1111	R	0.18	0.84	1.00	0.85	0.99	0.99	0.17		0.92	0.97	0.99
	(5 00)	$max \Delta G_y   x$	0.49	0.27	0.06	0.33	0.10	0.04	0.48	-	0.23	0.15	0.09
	(3.00)	ave $\Delta G_y   x$	0.25	0.18	0.03	0.18	0.05	0.02	0.25		0.12	0.08	0.05
	111TC	R	0.23	0.60	0.93	0.92	0.85	0.89	0.08	0.92		0.99	0.86
	(7.50)	$\max \Delta G_y   x$	0.22	0.28	0.11	0.12	0.18	0.13	0.21	0.15	-	0.06	0.17
		ave $\Delta G_y x$	0.11	0.14	0.07	0.08	0.09	0.07	0.12	0.07		0.03	0.09

Site		vac	2, 38		vac, 79				va	c, 201		
$(\overline{CN})$	Parameters <sup>a</sup>	111	kink	111E	111T	kink	100E	100T	111E	111TC	111TM	kink
111 <b>TM</b>	R	0.54	0.72	0.98	0.93	0.93	0.94	0.99	0.97	0.99		0.93
(6.02)	$max \Delta G_y   x$	0.17	0.32	0.07	0.16	0.17	0.10	0.03	0.11	0.07	-	0.15
(0.92)	ave $\Delta G_y   x$	0.11	0.16	0.06	0.08	0.09	0.07	0.02	0.06	0.04		0.10
1	R	0.21	0.88	0.98	0.76	1.00	0.96	0.20	0.99	0.86	0.93	
KIIIK (4.08)	$max \Delta G_y   x$	0.67	0.29	0.14	0.49	0.06	0.09	0.65	0.10	0.33	0.26	-
(4.08)	ave $\Delta G_y   x$	0.33	0.19	0.06	0.27	0.03	0.04	0.33	0.06	0.20	0.16	

*a*: All  $\Delta G_y$  are in eV.

#### S.5. Statistical treatment of bivariate normal distributions

We modeled formation energies for each metal *M* using bivariate normal distributions. These distributions are described in Equation S.10, with  $x = \Delta G_{f,MS}$  and  $y = \Delta G_{f,vac}$ :

$$P_{M}(x,y) = \frac{1}{2\pi\sigma_{M1}\sigma_{M2}} \exp\left(-\frac{(\cos\theta_{M}(x-\bar{x}_{M})+\sin\theta_{M}(y-\bar{y}_{M}))^{2}}{2\sigma_{M1}^{2}} - \frac{(-\sin\theta_{M}(x-\bar{x}_{M})+\cos\theta_{M}(y-\bar{y}_{M}))^{2}}{2\sigma_{M2}^{2}}\right) (S.10)$$

where  $\bar{x}_M$  and  $\bar{y}_M$  are the mean formation energies for each metal,  $\theta_M$  is the angle along which the first component of the distribution is oriented (perpendicular to the second component), and  $\sigma_{M1}$  and  $\sigma_{M2}$  are the standard deviations of respective components.  $\theta_M$  is defined using the net orientation of the known x, y of the metal, so:

$$\theta_M = \tan^{-1} \left( 2 \frac{\overline{(x-\bar{x})(y-\bar{y})}}{\overline{(x-\bar{x})^2} - \overline{(y-\bar{y})^2}} \right) \tag{S.11}$$

Subsequently,  $\sigma_{M1}$  and  $\sigma_{M2}$  are optimized such that  $\prod_{site_M} P_M(x_{site_M}, y_{site_M})$  is maximized, ensuring the bivariate normal distribution is closest to the observed distribution of formation energies.

The equally weighted average of resulting  $P_M$  for Au, Ir, Pd, and Pt is compared to the linear fit of all  $\bar{y}_M$  with respect to  $\bar{x}_M$ . We obtained the correlation coefficient of the distributions with respect to this linear fit by analytically evaluating the expression in Equation S.12:

$$R_{dist} = \sqrt{1 - \frac{\sum_{M} \iint_{-\infty}^{\infty} (y - ax - b)^{2} P_{M}(x, y) \, dx \, dy}{\sum_{M} \iint_{-\infty}^{\infty} (y - \bar{\bar{y}})^{2} P_{M}(x, y) \, dx \, dy}}$$
(S.12)

Here, ax + b is the equation corresponding to the linear fit of  $\bar{y}_M$  with respect to  $\bar{x}_M$ , and  $\bar{y}$  is the average across all  $\bar{y}_M$ . The corresponding MAE is calculated by numerically evaluating the integral in Equation S.13 using the 2D adaptive quadrature method implemented in GNU Octave 7.2.0:<sup>9</sup>

$$MAE = \sum_{M} \iint_{-\infty}^{\infty} |y - ax - b| P_M(x, y) \, dx \, dy \tag{S.13}$$

The  $P_M$  parameters and corresponding MAE are listed below in Table S.6.

Metal	$\overline{x}_M$ (eV)	$\overline{y}_M$ (eV)	$\boldsymbol{\theta}_{M}\left(^{\circ} ight)$	<b>σ</b> <sub>1</sub> (eV)	<b>σ</b> <sub>2</sub> (eV)	MAE (eV)
Ag	0.074	1.063	31.1	0.194	0.052	0.32
Au	0.574	1.328	42.8	0.254	0.123	0.15
Ir	-0.305	0.356	-35.3	0.065	0.303	0.09
Pd	0.231	0.904	39.8	0.188	0.076	0.09
Pt	0.178	0.806	42.2	0.311	0.128	0.16

**Table S.6.** Bivariate normal distribution parameters.

# S.6. Solvation energy statistics

**Table S.7.** Parameters for linear regressions of solvation energies between different metals and adsorption site

 coordination numbers.

	Metal v	Parameters <sup>a</sup>	$\overline{CN}$	Δσ	Au	Ĭr	Pd	Pt
Excluding 38_	inetai y	1 drameters	0.02	115	0.54	_0.14	0.02	0.90
111. 201–100T	Ag	h a	-1.05	_	-0.60	-1.05	_0.95	-0.42
,			-0.05	0.98	0.00	0.33	-0.58	1.17
	Au	b	-0.44	0.26	—	-0.50	-1.10	0.01
	Ŧ	а	-0.10	-0.25	0.30		-0.25	0.64
	Ir	b	-0.07	-0.85	-0.40	_	-0.78	-0.22
	۲u	a	0.02	0.00	-0.06	-0.02		0.21
	Pa	b	-0.76	-0.67	-0.72	-0.70	_	-0.55
	D+	a	0.00	0.40	0.26	0.14	0.44	
	Ρl	b	-0.59	-0.23	-0.43	-0.54	-0.32	_
Excluding 38	Δa	а	0.06		-0.02	-0.45	0.23	0.18
sites, 201–100T	Ag	b	-1.30	_	-1.02	-1.29	-0.85	-0.89
	Δ11	а	-0.01	-0.02	_	-0.05	-0.22	-0.08
	Au	b	-0.72	-0.76		-0.79	-0.90	-0.81
	Ir	а	-0.10	-2.09	-0.19	_	-0.13	-0.04
		b	-0.09	-2.74	-0.78		-0.73	-0.66
	Pd	а	0.02	0.14	-0.10	-0.02	_	0.46
		b	-0.76	-0.53	-0.75	-0.69		-0.38
	Pt	a	0.01	0.14	-0.05	0.00	0.57	_
		b	-0.71	-0.49	-0.67	-0.64	-0.25	
Excluding 38,	Ag	a	0.04	_	0.66	-0.40	0.07	0.34
79 sites, 201–		b	-1.25	0.77	-0.50	-1.25	-0.96	-0.80
1001	Au	a	0.02	0.77	_	-0.23	1.26	0.84
		Ď	-0.93	0.01	0.00	-0.93	0.03	-0.27
	Ir		-0.10	-2.45	- <b>0.99</b>	_	0.50	-0.75
		<i>b</i>	-0.03	-5.08	-1.39 0.36	0.03	-0.23	-1.07
	Pd		-0.66	-0.61	_0.30	_0.03	_	_0.33
			-0.00 0.01	0.01	0.50	-0.03 -0.07	1 45	-0.50
	Pt	b a	-0.68	-0.24	-0.12	-0.68	0.32	_

*a*: Parameters for linear regressions  $\overline{\Delta G_y} = a\Delta G_x + b$ , for which  $\overline{\Delta G_y}, \Delta G_x, a$ , and *b* are in eV.

		Metal y	Statistics <sup>a</sup>	<u>CN</u>	Ag	Au	Ir	Pd	Pt	no trend <sup>b</sup>
			R	0.16		0.73	-0.19	0.01	0.60	-
		Ag	$max \Delta G_y   x$	0.27	-	0.14	0.29	0.25	0.13	0.49
			ave $\Delta G_y   x$	0.08		0.07	0.10	0.09	0.08	0.13
			R	-0.39	0.73		0.31	-0.19	0.60	-
		Au	$max \Delta G_y   x$	0.31	0.19	-	0.32	0.37	0.23	0.13
			ave $\Delta G_y   x$	0.11	0.09		0.13	0.11	0.10	0.07
Ex	cluding		R	-0.84	-0.19	0.31		-0.08	0.29	-
31	8–111T,	Ir	$max \Delta G_y   x$	0.12	0.22	0.26	-	0.25	0.23	0.28
20	01-100T		ave $\Delta G_y   x$	0.07	0.15	0.12		0.13	0.12	0.12
			R	0.38	0.01	-0.19	-0.08		0.00	-
		Pd	$max \Delta G_y   x$	0.07	0.09	0.09	0.08	-	0.09	0.11
			ave $\Delta G_y   x$	0.04	0.05	0.04	0.04		0.04	0.05
			R	-0.06	0.60	0.55	0.29	0.00		-
		Pt	$max \Delta G_y   x$	0.13	0.11	0.14	0.12	0.14	-	0.19
			ave $\Delta G_y   x$	0.06	0.05	0.05	0.06	0.05		0.06
		Metal y	Statistics <sup>a</sup>	<u>CN</u>	Ag	Au	Ir	Pd	Pt	no trend <sup>b</sup>
		Ag	R	0.91	_	-0.02	-0.97	0.18	0.16	_

Table S.8. Quality of linear relations between solvation energies on different metals.

		$max \Delta G_y   x$	0.04		0.11	0.17	0.12	0.11	0.11
		ave $\Delta G_y   x$	0.03		0.06	0.07	0.05	0.06	0.05
		R	-0.09	-0.02		-0.10	-0.15	0.16	-
	Au	$max \Delta G_y   x$	0.12	0.11	-	0.12	0.12	0.12	0.13
		ave $\Delta G_y   x$	0.07	0.07		0.08	0.07	0.07	0.07
Excluding 38		R	-0.81	-0.97	-0.10		-0.04	-0.01	-
sites, 201-	Ir	$max \Delta G_y   x$	0.12	0.06	0.25	-	0.26	0.26	0.26
100T		ave $\Delta G_y   x$	0.08	0.03	0.12		0.12	0.12	0.12
		R	0.36	0.18	-0.15	-0.04		0.00	-
	Pd	$max \Delta G_y   x$	0.07	0.08	0.09	0.09	-	0.10	0.10
		ave $\Delta G_y   x$	0.04	0.05	0.05	0.04		0.03	0.05
		R	0.29	0.16	-0.06	-0.01	0.00		-
	Pt	$max \Delta G_y   x$	0.09	0.10	0.10	0.09	0.09	-	0.10
		ave $\Delta G_y   x$	0.05	0.05	0.04	0.04	0.04		0.04
			ĈN	Δα	Δu	Ir	Pd	Pt	no trend <sup>b</sup>
			011	115	7 <b>u</b>	11	14	11	no nond
		R	0.91	11g	0.71	-0.99	0.05	0.35	-
	Ag	$R$ $max \Delta G_{y} x$	<b>0.91</b> 0.03	-	<b>0.71</b> 0.07	- <b>0.99</b> 0.16	<b>0.05</b> 0.09	<b>0.35</b> 0.08	- 0.49
	Ag	$R$ $max \Delta G_y   x$ $ave \Delta G_y   x$	<b>0.91</b> 0.03 0.02	-	0.71 0.07 0.03	- <b>0.99</b> 0.16 0.09	0.05 0.09 0.04	0.35 0.08 0.05	- 0.49 0.13
	Ag	$R$ $max \Delta G_{y} x$ $ave \Delta G_{y} x$ $R$	0.91 0.03 0.02 0.48	- 0.71	<b>0.71</b> 0.07 0.03	-0.99 0.16 0.09 -0.47	0.05 0.09 0.04 0.67	0.35 0.08 0.05 0.35	- 0.49 0.13 -
	Ag	$R$ $max \Delta G_{y} x$ $ave \Delta G_{y} x$ $R$ $max \Delta G_{y} x$	0.03 0.02 0.48 0.09	- 0.71 0.07	<b>0.71</b> 0.07 0.03	- <b>0.99</b> 0.16 0.09 - <b>0.47</b> 0.08	0.05 0.09 0.04 0.67 0.08	0.35 0.08 0.05 0.35 0.08	- 0.49 0.13 - 0.13
	Ag Au	$R$ $max \Delta G_y   x$ $ave \Delta G_y   x$ $R$ $max \Delta G_y   x$ $ave \Delta G_y   x$	0.03 0.02 0.48 0.09 0.05	- 0.71 0.07 0.04	<b>0.71</b> 0.07 0.03	- <b>0.99</b> 0.16 0.09 - <b>0.47</b> 0.08 0.06	0.05 0.09 0.04 0.67 0.08 0.04	0.35 0.08 0.05 0.35 0.08 0.04	- 0.49 0.13 - 0.13 0.07
Excluding	Ag Au	$R$ $max \Delta G_{y} x$ $ave \Delta G_{y} x$ $R$ $max \Delta G_{y} x$ $ave \Delta G_{y} x$ $R$ $R$	0.91 0.03 0.02 0.48 0.09 0.05 -0.87	- 0.71 0.07 0.04 -0.99	<b>0.71</b> 0.07 0.03 - - <b>0.47</b>	- <b>0.99</b> 0.16 0.09 - <b>0.47</b> 0.08 0.06	0.05 0.09 0.04 0.67 0.08 0.04 0.04 0.14	0.35 0.08 0.05 0.35 0.08 0.04 -0.23	- 0.49 0.13 - 0.13 0.07 -
Excluding 38, 79 sites,	Ag Au Ir	$R$ $max \Delta G_y   x$ $ave \Delta G_y   x$ $R$ $max \Delta G_y   x$ $ave \Delta G_y   x$ $R$ $max \Delta G_y   x$	0.91 0.03 0.02 0.48 0.09 0.05 -0.87 0.11	- 0.71 0.07 0.04 -0.99 0.03	<b>0.71</b> 0.07 0.03 - - <b>0.47</b> 0.22	- <b>0.99</b> 0.16 0.09 - <b>0.47</b> 0.08 0.06	0.05 0.09 0.04 0.67 0.08 0.04 0.14 0.22	0.35 0.08 0.05 0.35 0.08 0.04 -0.23 0.24	- 0.49 0.13 - 0.13 0.07 - 0.28
Excluding 38, 79 sites, 201–100T	Ag Au Ir	$R$ $max \Delta G_{y} x$ $ave \Delta G_{y} x$ $R$ $max \Delta G_{y} x$ $ave \Delta G_{y} x$ $R$ $max \Delta G_{y} x$ $ave \Delta G_{y} x$	0.91 0.03 0.02 0.48 0.09 0.05 -0.87 0.11 0.06	- 0.71 0.07 0.04 -0.99 0.03 0.02	<b>0.71</b> 0.07 0.03 - - <b>0.47</b> 0.22 0.11	- <b>0.99</b> 0.16 0.09 - <b>0.47</b> 0.08 0.06	0.05 0.09 0.04 0.67 0.08 0.04 0.14 0.22 0.11	0.35 0.08 0.05 0.35 0.08 0.04 -0.23 0.24 0.12	0.49 0.13 0.13 0.07 - 0.28 0.12
Excluding 38, 79 sites, 201–100T	Ag Au Ir	$R$ $max \Delta G_{y} x$ $ave \Delta G_{y} x$ $R$ $max \Delta G_{y} x$ $ave \Delta G_{y} x$ $R$ $max \Delta G_{y} x$ $R$ $max \Delta G_{y} x$ $R$ $R$	0.91 0.03 0.02 0.48 0.09 0.05 -0.87 0.11 0.06 0.15	- <b>0.71</b> 0.07 0.04 - <b>0.99</b> 0.03 0.02 <b>0.05</b>	••••••••••••••••••••••••••••••••••••••	-0.99 0.16 0.09 -0.47 0.08 0.06 - 0.14	0.05 0.09 0.04 0.67 0.08 0.04 0.14 0.22 0.11	0.35 0.08 0.05 0.35 0.08 0.04 -0.23 0.24 0.12 0.00	0.49 0.13 - 0.13 0.07 - 0.28 0.12 -
Excluding 38, 79 sites, 201–100T	Ag Au Ir Pd	$R$ $max \Delta G_{y} x$ $ave \Delta G_{y} x$ $R$ $max \Delta G_{y} x$ $ave \Delta G_{y} x$ $R$ $max \Delta G_{y} x$ $R$ $max \Delta G_{y} x$ $R$ $max \Delta G_{y} x$	0.91 0.03 0.02 0.48 0.09 0.05 -0.87 0.11 0.06 0.15 0.06	- <b>0.71</b> 0.07 0.04 - <b>0.99</b> 0.03 0.02 <b>0.05</b> 0.06	••••••••••••••••••••••••••••••••••••••	- <b>0.99</b> 0.16 0.09 - <b>0.47</b> 0.08 0.06 - <b>0.14</b> 0.06	0.05 0.09 0.04 0.67 0.08 0.04 0.14 0.22 0.11	0.35 0.08 0.05 0.35 0.08 0.04 -0.23 0.24 0.12 0.00 0.03	0.49 0.13 - 0.13 0.07 - 0.28 0.12 - 0.11
Excluding 38, 79 sites, 201–100T	Ag Au Ir Pd	$R$ $max \Delta G_{y} x$ $ave \Delta G_{y} x$ $R$ $max \Delta G_{y} x$ $ave \Delta G_{y} x$ $R$ $max \Delta G_{y} x$ $R$ $max \Delta G_{y} x$ $R$ $max \Delta G_{y} x$	0.91 0.03 0.02 0.48 0.09 0.05 -0.87 0.11 0.06 0.15 0.06 0.03	- 0.71 0.07 0.04 -0.99 0.03 0.02 0.05 0.06 0.03	•	-0.99 0.16 0.09 -0.47 0.08 0.06 - 0.14 0.06 0.03	0.05 0.09 0.04 0.67 0.08 0.04 0.14 0.22 0.11	0.35 0.08 0.05 0.35 0.08 0.04 -0.23 0.24 0.12 0.00 0.03 0.01	0.49 0.13 - 0.13 0.07 - 0.28 0.12 - 0.11 0.05
Excluding 38, 79 sites, 201–100T	Ag Au Ir Pd	$R$ $max \Delta G_{y} x$ $ave \Delta G_{y} x$ $R$ $max \Delta G_{y} x$ $ave \Delta G_{y} x$ $R$ $max \Delta G_{y} x$ $R$ $R$	0.91 0.03 0.02 0.48 0.09 0.05 -0.87 0.11 0.06 0.15 0.06 0.03 0.26		0.71 0.07 0.03 − − 0.47 0.22 0.11 0.67 0.04 0.02 0.72	-0.99 0.16 0.09 -0.47 0.08 0.06 - 0.14 0.06 0.03 -0.23	0.05 0.09 0.04 0.67 0.08 0.04 0.14 0.22 0.11 - 0.00	0.35 0.08 0.05 0.35 0.08 0.04 -0.23 0.24 0.12 0.00 0.03 0.01	0.49 0.13 0.13 0.07 0.28 0.12 0.11 0.05 -
Excluding 38, 79 sites, 201–100T	Ag Au Ir Pd Pt	$R$ $max \Delta G_{y} x$ $ave \Delta G_{y} x$ $R$ $max \Delta G_{y} x$ $ave \Delta G_{y} x$ $R$ $max \Delta G_{y} x$	0.91 0.03 0.02 0.48 0.09 0.05 -0.87 0.11 0.06 0.15 0.06 0.03 0.26 0.08	- 0.71 0.07 0.04 -0.99 0.03 0.02 0.05 0.06 0.03 0.35 0.09	0.71 0.07 0.03 − − 0.47 0.22 0.11 0.67 0.04 0.02 0.72 0.06	-0.99 0.16 0.09 -0.47 0.08 0.06 - - 0.14 0.06 0.03 -0.23 0.07	0.05 0.09 0.04 0.67 0.08 0.04 0.14 0.22 0.11 - 0.00 0.04	0.35 0.08 0.05 0.35 0.08 0.04 -0.23 0.24 0.12 0.00 0.03 0.01	0.49 0.13 0.13 0.07 0.28 0.12 0.11 0.05 0.19

*a*: All  $\Delta G_y$  are in eV.

b: Null hypothesis, in which deviations are relative to the average as opposed to linear regression.

	Metal y	Statistics <sup>a</sup>	<u>CN</u>	Ag	Au	Ir	Pd	no trend <sup>b</sup>
		R	0.22		0.78	0.92	0.96	-
	Ag	$max \Delta G_y   x$	0.12	-	0.08	0.05	0.04	0.13
		ave $\Delta G_y   x$	0.07		0.05	0.03	0.02	0.07
		R	0.48	0.78		0.86	0.95	_
	Au	$max \Delta G_y   x$	0.14	0.11	-	0.10	0.11	0.17
$H_2O$ ,		ave $\Delta G_y   x$	0.08	0.05		0.04	0.04	0.08
MS		R	0.48	0.92	0.86		0.95	-
	Ir	$max \Delta G_y   x$	0.33	0.19	0.23	-	0.15	0.53
		ave $\Delta G_y   x$	0.21	0.09	0.12		0.06	0.20
		R	0.26	0.96	0.83	0.95		-
	Pd	$max \Delta G_y   x$	0.19	0.08	0.14	0.08	-	0.20
		ave $\Delta G_y   x$	0.11	0.03	0.06	0.03		0.11
	Metal y	Statistics <sup>a</sup>	ĊN	Ag	Au	Ir	Pd	no trend <sup>b</sup>
	Metal y	Statistics <sup>a</sup> R	CN 0.82	Ag	Au <b>0.98</b>	Ir <b>0.96</b>	Pd <b>0.90</b>	no trend <sup>b</sup>
	Metal y Ag	$\frac{\text{Statistics}^{a}}{R}$ $\max \Delta G_{y} x$	CN 0.82 0.18	Ag —	Au <b>0.98</b> 0.08	Ir <b>0.96</b> 0.10	Pd <b>0.90</b> 0.16	no trend <sup>b</sup> - 0.40
	Metal y Ag	$\frac{\text{Statistics}^{a}}{R}$ $\max \Delta G_{y}   x$ $ave \Delta G_{y}   x$	CN           0.82           0.18           0.09	Ag —	Au 0.98 0.08 0.04	Ir <b>0.96</b> 0.10 0.04	Pd <b>0.90</b> 0.16 0.06	no trend <sup>b</sup> - 0.40 0.16
	Metal y Ag	$\frac{Statistics^{a}}{R}$ $\max \Delta G_{y}   x$ $ave \Delta G_{y}   x$ $R$	CN           0.82           0.18           0.09           0.89	Ag - 0.98	Au 0.98 0.08 0.04	Ir 0.96 0.10 0.04 0.96	Pd 0.90 0.16 0.06 0.91	no trend <sup>b</sup> - 0.40 0.16 -
	Metal y Ag Au	$\frac{\text{Statistics}^{a}}{R}$ $\max \Delta G_{y}   x$ $ave \Delta G_{y}   x$ $R$ $\max \Delta G_{y}   x$	CN           0.82           0.18           0.09           0.89           0.18	Ag - <b>0.98</b> 0.08	Au 0.98 0.08 0.04	Ir 0.96 0.10 0.04 0.96 0.12	Pd 0.90 0.16 0.06 0.91 0.19	no trend <sup>b</sup> - 0.40 0.16 - 0.47
ОН,	Metal y Ag Au	$Statistics^{a}$ $R$ $max \Delta G_{y}   x$ $ave \Delta G_{y}   x$ $R$ $max \Delta G_{y}   x$ $ave \Delta G_{y}   x$	CN           0.82           0.18           0.09           0.89           0.18           0.08	Ag - 0.98 0.08 0.04	Au 0.98 0.08 0.04	Ir 0.96 0.10 0.04 0.96 0.12 0.05	Pd 0.90 0.16 0.06 0.91 0.19 0.07	no trend <sup>b</sup> - 0.40 0.16 - 0.47 0.20
OH, MS	Metal y Ag Au	$Statistics^{a}$ $R$ $max \Delta G_{y}   x$ $ave \Delta G_{y}   x$ $R$ $max \Delta G_{y}   x$ $ave \Delta G_{y}   x$ $R$	CN           0.82           0.18           0.09           0.89           0.18           0.08           0.85	Ag - 0.98 0.08 0.04 0.96	Au 0.98 0.08 0.04 - 0.96	Ir 0.96 0.10 0.04 0.96 0.12 0.05	Pd 0.90 0.16 0.06 0.91 0.19 0.07 0.97	no trend <sup>b</sup> - 0.40 0.16 - 0.47 0.20 -
OH, MS	Metal y Ag Au Ir	$Statistics^{a}$ $R$ $max \Delta G_{y} x$ $ave \Delta G_{y} x$ $R$ $max \Delta G_{y} x$ $ave \Delta G_{y} x$ $R$ $max \Delta G_{y} x$	CN           0.82           0.18           0.09           0.89           0.18           0.08           0.85           0.35	Ag - 0.98 0.08 0.04 0.96 0.27	Au 0.98 0.08 0.04 - 0.96 0.22	Ir 0.96 0.10 0.04 0.96 0.12 0.05	Pd 0.90 0.16 0.06 0.91 0.19 0.07 0.97 0.19	no trend <sup>b</sup> - 0.40 0.16 - 0.47 0.20 - 0.95
OH, MS	Metal y Ag Au Ir	$Statistics^{a}$ $R$ $max \Delta G_{y} x$ $ave \Delta G_{y} x$ $R$ $max \Delta G_{y} x$ $ave \Delta G_{y} x$ $R$ $max \Delta G_{y} x$ $ave \Delta G_{y} x$ $ave \Delta G_{y} x$	CN           0.82           0.18           0.09           0.89           0.18           0.08           0.85           0.35           0.23	Ag - 0.98 0.08 0.04 0.96 0.27 0.10	Au 0.98 0.08 0.04 - 0.96 0.22 0.10	Ir 0.96 0.10 0.04 0.96 0.12 0.05	Pd 0.90 0.16 0.06 0.91 0.19 0.07 0.97 0.19 0.11	no trend <sup>b</sup> - 0.40 0.16 - 0.47 0.20 - 0.95 0.42
OH, MS	Metal y Ag Au Ir	$Statistics^{a}$ $R$ $max \Delta G_{y} x$ $ave \Delta G_{y} x$ $R$ $max \Delta G_{y} x$ $ave \Delta G_{y} x$ $R$ $max \Delta G_{y} x$ $ave \Delta G_{y} x$ $R$ $R$ $R$	CN           0.82           0.18           0.09           0.89           0.18           0.08           0.85           0.35           0.23           0.75	Ag - 0.98 0.08 0.04 0.96 0.27 0.10 0.90	Au 0.98 0.08 0.04 - 0.96 0.22 0.10 0.91	Ir 0.96 0.10 0.04 0.96 0.12 0.05 - 0.97	Pd 0.90 0.16 0.06 0.91 0.19 0.07 0.97 0.19 0.11	no trend <sup>b</sup> - 0.40 0.16 - 0.47 0.20 - 0.95 0.42 -
OH, MS	Metal y Ag Au Ir Pd	$Statistics^{a}$ $R$ $max \Delta G_{y} x$ $ave \Delta G_{y} x$ $R$ $max \Delta G_{y} x$ $ave \Delta G_{y} x$ $R$ $max \Delta G_{y} x$ $ave \Delta G_{y} x$ $R$ $max \Delta G_{y} x$ $R$ $max \Delta G_{y} x$	CN           0.82           0.18           0.09           0.89           0.18           0.08           0.35           0.23           0.75           0.20	Ag - 0.98 0.08 0.04 0.96 0.27 0.10 0.90 0.21	Au 0.98 0.08 0.04 - 0.96 0.22 0.10 0.91 0.19	Ir 0.96 0.10 0.04 0.96 0.12 0.05 - 0.97 0.09	Pd 0.90 0.16 0.06 0.91 0.19 0.07 0.97 0.19 0.11	no trend <sup>b</sup> - 0.40 0.16 - 0.47 0.20 - 0.95 0.42 - 0.42

*a*: All  $\Delta G_y$  are in eV.

b: Null hypothesis, in which deviations are relative to the average as opposed to linear regression.

	Metal y	Parameters <sup>a</sup>	<u>CN</u>	Ag	Au	Ir	Pd
	٨٥	а	0.02		0.67	0.30	0.63
	Ag	b	0.72	-	0.23	0.75	0.50
	A.11	а	0.04	0.91		0.33	0.63
$H_2O$ ,	Au	b	0.61	0.12	_	0.79	0.55
MS	Ţ.,	а	0.10	2.75	2.23		1.87
	п	b	-0.38	-2.02	-1.71	-	-0.71
	Di	а	0.03	1.47	1.09	0.49	
	Pd	b	0.33	-0.70	-0.45	0.39	-
			ĊN	Ag	Au	Ir	Pd
	٨٥	а	CN 0.13	Ag	Au 0.81	Ir <b>0.40</b>	Pd 0.81
	Ag	a b	<b>CN</b> <b>0.13</b> 0.14	Ag -	Au <b>0.81</b> -0.28	Ir <b>0.40</b> 0.92	Pd <b>0.81</b> 0.30
	Ag	a b a	CN           0.13           0.14           0.17	Ag - 1.17	Au <b>0.81</b> -0.28	Ir 0.40 0.92 0.47	Pd 0.81 0.30 0.98
ОН,	Ag Au	a b a b	CN           0.13           0.14           0.17           0.46	Ag - <b>1.17</b> 0.40	Au <b>0.81</b> -0.28 -	Ir 0.40 0.92 0.47 1.48	Pd 0.81 0.30 0.98 0.73
OH, MS	Ag Au	a b a b a	CN           0.13           0.14           0.17           0.46           0.34	Ag - 1.17 0.40 2.35	Au <b>0.81</b> -0.28 - <b>1.95</b>	Ir 0.40 0.92 0.47 1.48	Pd 0.81 0.30 0.98 0.73 2.12
OH, MS	Ag Au Ir	a b a b a b	<b>CN 0.13</b> 0.14 <b>0.17</b> 0.46 <b>0.34</b> −1.98	Ag - 1.17 0.40 2.35 -2.18	Au <b>0.81</b> -0.28 - <b>1.95</b> -2.90	Ir 0.40 0.92 0.47 1.48 –	Pd 0.81 0.30 0.98 0.73 2.12 -1.62
OH, MS	Ag Au Ir	a b a b a b a	CN           0.13           0.14           0.17           0.46           0.34           -1.98           0.14	Ag - 1.17 0.40 2.35 -2.18 1.00	Au <b>0.81</b> -0.28 - <b>1.95</b> -2.90 <b>0.84</b>	Ir 0.40 0.92 0.47 1.48 - 0.44	Pd 0.81 0.30 0.98 0.73 2.12 -1.62

**Table S.10.** Parameters for linear regressions between micro-solvated  $OH_x$  (x = 1,2) energies on different metals.

*a*: Parameters for linear regressions  $\overline{\Delta G_y} = a\Delta G_x + b$ , for which  $\overline{\Delta G_y}, \Delta G_x, a$ , and *b* are in eV.

## S.7. Bond lengths and statistics

Table S.11. Bond length statistics.

			J	•	•	<b>O</b>	्
Madal	G						
Metal	Species	Parameters			2,110	0.07(	
Ag	011	mean bond length			2.119	0.976	
	OH, vac	max deviation	-	-	0.121	0.001	-
		average deviation	1 0 5 2	1 504	0.037	0.001	0.01/
		mean bond length	1.053	1.506	2.253	0.983	2.016
	OH, MS	max deviation	0.008	0.035	0.042	0.003	0.092
		average deviation	0.005	0.020	0.023	0.002	0.048
		mean bond length	0.992	1.870		1.008	1.693
	$H_2O, MS$	max deviation	0.003	0.050	-	0.004	0.034
		average deviation	0.001	0.017	2 00 4	0.002	0.020
Au	OU	mean bond length			2.094	0.977	
	OH, vac	max deviation	-	—	0.207	0.001	-
		average deviation			0.046	0.000	
		mean bond length	1.044	1.542	2.223	0.988	1.913
	OH, MS	max deviation	0.022	0.066	0.063	0.003	0.047
		average deviation	0.008	0.037	0.036	0.001	0.022
		mean bond length	0.994	1.863		1.009	1.686
	$H_2O, MS$	max deviation	0.006	0.081	-	0.005	0.038
		average deviation	0.001	0.021		0.003	0.019
Ir		mean bond length			1.966	0.979	
	OH, vac	max deviation	-	-	0.046	0.001	-
		average deviation			0.030	0.000	
		mean bond length	1.050	1.547	2.103	1.002	1.775
	OH, MS	max deviation	0.087	0.213	0.055	0.008	0.105
		average deviation	0.021	0.085	0.029	0.003	0.045
		mean bond length	1.002	1.845		1.019	1.640
	$H_2O, MS$	max deviation	0.008	0.161	-	0.010	0.066
		average deviation	0.004	0.059		0.004	0.030
Pd		mean bond length			1.974	0.979	
	OH, vac	max deviation	-	-	0.017	0.001	-
		average deviation			0.009	0.000	
		mean bond length	1.044	1.538	2.105	0.992	1.858
	OH, MS	max deviation	0.013	0.071	0.018	0.007	0.108
		average deviation	0.006	0.030	0.009	0.003	0.045
		mean bond length	0.997	1.836		1.015	1.657
	$H_2O, MS$	max deviation	0.004	0.101	-	0.007	0.048
		average deviation	0.002	0.031		0.003	0.023
Pt		mean bond length			2.119	0.976	
	OH, vac	max deviation	-	_	0.121	0.001	-
		average deviation			0.037	0.001	
		mean bond length	1.053	1.506	2.253	0.983	2.016
	OH, MS	max deviation	0.008	0.035	0.042	0.003	0.092
		average deviation	0.005	0.020	0.023	0.002	0.048
		mean bond length	0.992	1.870		1.008	1.693
	$H_2O, MS$	max deviation	0.003	0.050	-	0.004	0.034
		average deviation	0.001	0.017		0.002	0.020

*a:* All values are in Å. Values for all metals and bond lengths are included to enable analysis of the effects different metal nanoparticles have on surface-bound water and (solvated) adsorbates. Specifically, all statistics are listed using 3 decimal places to enable a comparison of maximum and average deviations between metals and bonds.

#### S.8. Excerpts from selected tables

The tables S.NE below contain the data from respective tables S.N which are discussed in the main body.

			Ag			Au			Ir			Pd	
NP	site	$\Delta G_{f, \text{vac}}$	$\Delta G_{f,MS}$	$\Omega_{OH}$	$\Delta G_{f, \text{vac}}$	$\Delta G_{f,MS}$	$\Omega_{OH}$	$\Delta G_{f, \text{vac}}$	$\Delta G_{f,MS}$	$\Omega_{OH}$	$\Delta G_{f, \text{vac}}$	$\Delta G_{f,MS}$	$\Omega_{OH}$
M38	111	0.55	0.11	-0.45	х	0.33	х	0.64	-0.18	-0.82	1.15	0.59	-0.56
	kink	0.46	-0.25	-0.71	0.67	0.34	-0.32	-0.21	-0.65	-0.44	0.78	0.10	-0.69
M79	111E	1.06	0.06	-1.00	1.26	0.63	-0.63	0.24	-0.46	-0.69	0.81	0.11	-0.70
	111T	1.10	0.19	-0.90	1.51	0.71	-0.80	0.84	-0.01	-0.85	1.04	0.32	-0.72
	kink	1.08	-0.02	-1.11	1.17	0.48	-0.69	-0.12	-0.60	-0.47	0.84	0.06	-0.77
M <sub>201</sub>	100E	0.99	-0.01	-1.00	1.27	0.51	-0.76	х	-0.48	Х	0.90	0.27	-0.62
	100T	0.59	0.12	-0.47	х	0.43 <sup><i>ab</i></sup>	х	0.68	0.12	-0.57	1.10	0.53	-0.57
	111E	0.99	$-0.02^{a}$	-1.01	1.23	0.39	-0.84	0.14	-0.50	-0.63	0.81	0.11	-0.70
	111TC	1.28	0.35 <sup><i>a</i></sup>	-0.93	1.56	0.89	-0.67	0.89	0.11	-0.79	1.06	0.45	-0.62
	111TM	х	0.19 <sup>b</sup>	x	1.53	0.69	-0.84	0.72	0.06	-0.66	1.04	0.39	-0.65
	kink	0.95	-0.14	-1.10	1.10	0.30	-0.80	-0.19	-0.57	-0.38	0.75	0.13	-0.62

Table S.2E. Binding and formation energies.

*a*: Vibrational data for  $4^{*}H_{2}O$  obtained using denser plane wave sampling, as described in S.2. *b*: Vibrational data for  $*OH+3^{*}H_{2}O$  obtained using denser plane wave sampling, as described in S.2.

*x*: No stable configuration available for this adsorption site.

Table S.4E. Parameters for linear regressions of OH formation energies between different metals and adsorption site coordination numbers.

						Metal <i>x</i>		
	Metal y	Parameters <sup>a</sup>	CN	Ag	Au	Ir	Pd	Pt
MS	<b>A</b>	а	0.12		0.81	0.49	0.91	0.63
	Ag	b	-0.58	_	-0.39	0.22	-0.14	-0.04
	A.11	а	0.13	1.17		0.54	1.03	0.73
	Au	b	-0.15	0.49	_	0.74	0.34	0.45
	Ţ.,	а	0.23	1.78	1.38		1.91	1.22
	Ir	b	-1.60	-0.44	-1.10	-	-0.75	-0.52
	DJ	а	0.11	0.77	0.60	0.44		0.61
	ru	b	-0.37	0.17	-0.12	0.37	_	0.12
	D4	а	0.17	1.35	1.08	0.71	1.54	
	rι	b	-0.79	0.08	-0.44	0.39	-0.18	-
vac	٨a	а	0.07		0.51	0.19	0.73	0.48
	Ag	b	0.70	_	0.40	1.02	0.42	0.69
	4.11	а	0.14	1.24		0.41	1.41	0.80
	Au	b	0.57	-0.02	_	1.19	0.05	0.69
	Ţ.,	а	0.32	3.14	2.37		3.26	1.89
	п	b	-1.47	-3.08	-2.81	_	-2.60	-1.19
	Dd	а	0.09	0.86	0.68	0.28		0.53
	ru	b	0.39	-0.03	0.00	0.81	_	0.48
	Df	а	0.16	1.59	1.12	0.46	1.54	
	Γι	b	-0.08	-0.92	-0.69	0.65	-0.58	—

*a*: Parameters for linear regressions  $\overline{\Delta G_y} = a\Delta G_x + b$ , for which  $\overline{\Delta G_y}, \Delta G_x, a$ , and *b* are in eV.

Table S.5E. Pearson *R* values for linear relations between formation site binding energies.

		MS	, 38		<i>MS</i> , 79				$M_{s}^{2}$	S, 201		
	Site	111	kink	111E	111T	kink	100E	100T	111E	111TC	111TM	kink
<i>MS</i> , 38	111	х	0.84	0.65	0.61	0.71	0.84	0.79	0.77	0.60	0.68	0.86
	kink	0.84	х	0.94	0.92	0.95	1.00	0.75	0.97	0.94	0.96	0.99
<i>MS</i> , 79	111E	0.65	0.94	Х	0.97	0.99	0.95	0.49	0.98	0.95	0.93	0.94
	111T	0.61	0.92	0.97	Х	0.96	0.92	0.50	0.94	0.96	0.96	0.91
	kink	0.71	0.95	0.99	0.96	х	0.97	0.52	1.00	0.93	0.92	0.97
MS, 201	100E	0.84	1.00	0.95	0.92	0.97	Х	0.71	0.98	0.93	0.94	0.99
	100T	0.79	0.75	0.49	0.50	0.52	0.71	х	0.57	0.64	0.71	0.68
	111E	0.77	0.97	0.98	0.94	1.00	0.98	0.57	х	0.92	0.92	0.99
	111TC	0.60	0.94	0.95	0.96	0.93	0.93	0.64	0.92	Х	0.98	0.90
	111TM	0.68	0.96	0.93	0.96	0.92	0.94	0.71	0.92	0.98	Х	0.92
	kink	0.86	0.99	0.94	0.91	0.97	0.99	0.68	0.99	0.90	0.92	х
vac, 38	111	х	0.61	0.38	0.61	0.42	0.57	0.60	0.50	0.32	0.56	0.63
	kink	0.93	х	0.81	0.73	0.87	0.93	0.67	0.90	0.73	0.75	0.94
vac, 79	111E	0.56	0.81	х	0.83	0.94	0.85	0.29	0.92	0.81	0.74	0.85
	111T	0.37	0.72	0.90	х	0.87	0.74	0.12	0.83	0.80	0.77	0.75
	kink	0.64	0.79	0.88	0.76	х	0.84	0.28	0.90	0.72	0.67	0.85
vac, 201	100E	0.08	0.52	0.88	0.82	0.89	х	0.39	0.85	0.61	0.55	0.65
	100T	0.80	0.80	0.50	0.72	0.51	0.73	х	0.57	0.73	0.89	0.70
	111E	0.62	0.84	0.94	0.85	0.96	0.88	0.32	х	0.82	0.76	0.89
	111TC	0.34	0.75	0.93	0.88	0.90	0.78	0.19	0.86	Х	0.78	0.76
	111TM	0.54	0.91	0.99	0.99	0.97	0.91	0.49	0.95	0.98	Х	0.89
	kink	0.67	0.82	0.90	078	0.93	0.87	0 35	0.92	0.76	0.71	x
	KIIK	0.07	0.02	0.20	0.70	0.75	0.07	0.55	0.72	0.70	0.71	
	Site	vac	, 38	0.20	vac, 79	0.75	0.07	0.55	va	c, 201	0.71	
	Site	vac 111	, 38 kink	111E	<i>vac</i> , 79 111	kink	111E	111	va kink	c, 201 111E	111	kink
<i>MS</i> , 38	Site 111	vac 111 x	6.62 , 38 kink 0.93	111E 0.56	<i>vac</i> , 79 111 0.37	kink 0.64	111E 0.08	111 0.80	va kink 0.62	c, 201 111E 0.34	111 0.54	kink 0.67
<i>MS</i> , 38	Site 111 kink	vac 111 x 0.61	0.02 , 38 kink 0.93 x	111E 0.56 0.81	vac, 79 111 0.37 0.72	kink 0.64 0.79	111E 0.08 0.52	111 0.80 0.80	vac kink 0.62 0.84	c, 201 111E 0.34 0.75	111 0.54 0.91	kink 0.67 0.82
<i>MS</i> , 38 <i>MS</i> , 79	Site 111 kink 111E	vac 111 x 0.61 0.38	, 38 kink 0.93 x 0.81	111E 0.56 0.81 x	vac, 79 111 0.37 0.72 0.90	kink 0.64 0.79 0.88	111E 0.08 0.52 0.88	111 0.80 0.80 0.50	vac kink 0.62 0.84 0.94	c, 201 111E 0.34 0.75 0.93	111 0.54 0.91 0.99	kink 0.67 0.82 0.90
<i>MS</i> , 38 <i>MS</i> , 79	Site 111 kink 111E 111T	vac 111 x 0.61 0.38 0.61	0.02 , 38 kink 0.93 x 0.81 0.73	111E 0.56 0.81 x 0.83	vac, 79 111 0.37 0.72 0.90 x	kink 0.64 0.79 0.88 0.76	111E 0.08 0.52 0.88 0.82	111           0.80           0.80           0.50           0.72	vav kink 0.62 0.84 0.94 0.85	c, 201 111E 0.34 0.75 0.93 0.88	111 0.54 0.91 0.99 0.99	kink 0.67 0.82 0.90 0.78
<i>MS</i> , 38 <i>MS</i> , 79	Site 111 kink 111E 111T kink	vac 111 x 0.61 0.38 0.61 0.42	0.02 x, 38 kink 0.93 x 0.81 0.73 0.87	111E 0.56 0.81 x 0.83 0.94	vac, 79 111 0.37 0.72 0.90 x 0.87	kink 0.64 0.79 0.88 0.76 x	111E 0.08 0.52 0.88 0.82 0.89	111 0.80 0.80 0.50 0.72 0.51	vav kink 0.62 0.84 0.94 0.85 0.96	c, 201           111E           0.34           0.75           0.93           0.88           0.90	111 0.54 0.91 0.99 0.99 0.97	kink 0.67 0.82 0.90 0.78 0.93
<i>MS</i> , 38 <i>MS</i> , 79 <i>MS</i> , 201	Site 111 kink 111E 111T kink 100E	vac 111 x 0.61 0.38 0.61 0.42 0.57	0.81 0.87 0.93	111E 0.56 0.81 x 0.83 0.94 0.85	vac, 79 111 0.37 0.72 0.90 x 0.87 0.74	kink 0.64 0.79 0.88 0.76 x 0.84	111E 0.08 0.52 0.88 0.82 0.89 x	111           0.80           0.80           0.50           0.72           0.51           0.73	va kink 0.62 0.84 0.94 0.95 0.96 0.88	0.10           c, 201           111E           0.34           0.75           0.93           0.88           0.90           0.78	111 0.54 0.91 0.99 0.99 0.97 0.91	kink 0.67 0.82 0.90 0.78 0.93 0.87
<i>MS</i> , 38 <i>MS</i> , 79 <i>MS</i> , 201	Site 111 kink 111E 111T kink 100E 100T	vac 111 x 0.61 0.38 0.61 0.42 0.57 0.60	o.02           , 38           kink           0.93           x           0.81           0.73           0.87           0.93           0.67	111E 0.56 0.81 x 0.83 0.94 0.85 0.29	vac, 79           111           0.37           0.72           0.90           x           0.87           0.74	kink 0.64 0.79 0.88 0.76 x 0.84 0.28	111E 0.08 0.52 0.88 0.82 0.89 x 0.39	111 0.80 0.80 0.50 0.72 0.51 0.73 x	va kink 0.62 0.84 0.94 0.85 0.96 0.88 0.32	$\begin{array}{r} 0.10 \\ \hline 0.10 \\ \hline 0.201 \\ \hline 111E \\ \hline 0.34 \\ \hline 0.75 \\ \hline 0.93 \\ \hline 0.88 \\ \hline 0.90 \\ \hline 0.78 \\ \hline 0.19 \end{array}$	111 0.54 0.91 0.99 0.99 0.97 0.91 0.49	kink 0.67 0.82 0.90 0.78 0.93 0.87 0.35
<i>MS</i> , 38 <i>MS</i> , 79 <i>MS</i> , 201	Site 111 kink 111E 111T kink 100E 100T 111E	vac 111 x 0.61 0.38 0.61 0.42 0.57 0.60 0.50	0.02           , 38           kink           0.93           x           0.81           0.73           0.87           0.93           0.67           0.90	111E 0.56 0.81 x 0.83 0.94 0.85 0.29 0.92	0.70           vac, 79           111           0.37           0.72           0.90           x           0.87           0.74           0.12           0.83	kink 0.64 0.79 0.88 0.76 x 0.84 0.28 0.90	111E 0.08 0.52 0.88 0.82 0.89 x 0.39 0.85	111 0.80 0.50 0.72 0.51 0.73 x 0.57	va kink 0.62 0.84 0.94 0.85 0.96 0.88 0.32 x	$\begin{array}{r} c, 201 \\ \hline 111E \\ 0.34 \\ 0.75 \\ 0.93 \\ 0.88 \\ 0.90 \\ 0.78 \\ 0.19 \\ 0.86 \end{array}$	111 0.54 0.91 0.99 0.99 0.97 0.91 0.49 0.95	kink 0.67 0.82 0.90 0.78 0.93 0.87 0.35 0.92
<i>MS</i> , 38 <i>MS</i> , 79 <i>MS</i> , 201	Site 111 kink 111E 111T kink 100E 100T 111E 111TC	vac           111           x           0.61           0.38           0.61           0.42           0.57           0.60           0.50           0.32	0.02           , 38           kink           0.93           x           0.81           0.73           0.87           0.93           0.67           0.90           0.73	111E 0.56 0.81 x 0.83 0.94 0.85 0.29 0.92 0.92 0.81	vac, 79 111 0.37 0.72 0.90 x 0.87 0.74 0.12 0.83 0.80	kink 0.64 0.79 0.88 0.76 x 0.84 0.28 0.90 0.72	111E 0.08 0.52 0.88 0.82 0.89 x 0.39 0.85 0.61	111 0.80 0.50 0.72 0.51 0.73 x 0.57 0.73	va kink 0.62 0.84 0.94 0.85 0.96 0.88 0.32 x 0.82	0.100           c, 201           111E           0.34           0.75           0.93           0.88           0.90           0.78           0.19           0.86           x	111 0.54 0.91 0.99 0.99 0.97 0.91 0.49 0.95 0.98	kink 0.67 0.82 0.90 0.78 0.93 0.87 0.35 0.92 0.76
<i>MS</i> , 38 <i>MS</i> , 79 <i>MS</i> , 201	Site 111 kink 111E 111T kink 100E 100T 111E 111TC 111TM	vac           111           x           0.61           0.38           0.61           0.42           0.57           0.60           0.50           0.32           0.56	0.02           , 38           kink           0.93           x           0.81           0.73           0.93           0.67           0.90           0.73           0.75	111E 0.56 0.81 x 0.83 0.94 0.85 0.29 0.92 0.81 0.74	0.70           vac, 79           111           0.37           0.72           0.90           x           0.87           0.74           0.12           0.83           0.80           0.77	kink 0.64 0.79 0.88 0.76 x 0.84 0.28 0.90 0.72 0.67	111E 0.08 0.52 0.88 0.82 0.89 x 0.39 0.85 0.61 0.55	111 0.80 0.80 0.72 0.51 0.73 x 0.57 0.73 0.89	va kink 0.62 0.84 0.94 0.85 0.96 0.88 0.32 x 0.82 0.76	0.78           0.111           0.34           0.75           0.93           0.88           0.90           0.78           0.19           0.86           x           0.78	111 0.54 0.91 0.99 0.99 0.97 0.91 0.49 0.95 0.98 x	kink 0.67 0.82 0.90 0.78 0.93 0.87 0.35 0.92 0.76 0.71
<i>MS</i> , 38 <i>MS</i> , 79 <i>MS</i> , 201	Kink           Site           111           kink           111E           111T           kink           100E           100T           111E           111TC           111TC           111TM           kink	vac           111           x           0.61           0.38           0.61           0.42           0.57           0.60           0.50           0.32           0.56           0.63	0.02           , 38           kink           0.93           x           0.81           0.73           0.87           0.93           0.67           0.90           0.73           0.75           0.92	111E 0.56 0.81 x 0.83 0.94 0.85 0.29 0.92 0.81 0.74 0.85	0.70 vac, 79 111 0.37 0.72 0.90 x 0.87 0.74 0.12 0.83 0.80 0.77 0.75 0.75	kink 0.64 0.79 0.88 0.76 x 0.84 0.28 0.90 0.72 0.67 0.67 0.85	111E 0.08 0.52 0.88 0.82 0.89 x 0.39 0.85 0.61 0.55 0.65	111 0.80 0.80 0.50 0.72 0.51 0.73 x 0.57 0.73 0.89 0.70	va kink 0.62 0.84 0.94 0.85 0.96 0.88 0.32 x 0.82 0.76 0.89	c, 201 111E 0.34 0.75 0.93 0.88 0.90 0.78 0.19 0.86 x 0.78 0.78 0.78 0.78 0.78 0.78 0.76	111 0.54 0.91 0.99 0.99 0.97 0.91 0.49 0.95 0.98 x 0.89	kink 0.67 0.82 0.90 0.78 0.93 0.87 0.35 0.92 0.76 0.71 x
MS, 38 MS, 79 MS, 201 vac, 38	Kink           Site           111           kink           111E           111T           kink           100E           100T           111E           111T           111E           111T           kink           111TK           kink           111TM           kink           1111	vac           111           x           0.61           0.38           0.61           0.42           0.57           0.60           0.50           0.32           0.56           0.63           x	0.02           , 38           kink           0.93           x           0.81           0.73           0.87           0.93           0.67           0.90           0.73           0.75           0.94	111E 0.56 0.81 x 0.83 0.94 0.85 0.29 0.92 0.81 0.74 0.85 0.06	vac, 79           111           0.37           0.72           0.90           x           0.87           0.74           0.12           0.83           0.80           0.775           0.22	kink 0.64 0.79 0.88 0.76 x 0.84 0.28 0.90 0.72 0.67 0.85 0.19	111E 0.08 0.52 0.88 0.82 0.89 x 0.39 0.85 0.61 0.55 0.65 0.065	111           0.80           0.50           0.72           0.51           0.73           x           0.57           0.73           0.73           0.75           0.70	va kink 0.62 0.84 0.94 0.85 0.96 0.88 0.32 x 0.82 0.76 0.89 0.18	c, 201 111E 0.34 0.75 0.93 0.88 0.90 0.78 0.19 0.86 x 0.78 0.76 0.23	111 0.54 0.91 0.99 0.99 0.97 0.91 0.49 0.95 0.98 x 0.89 0.54	kink 0.67 0.82 0.90 0.78 0.93 0.87 0.35 0.92 0.76 0.71 x 0.21
<i>MS</i> , 38 <i>MS</i> , 79 <i>MS</i> , 201 <i>vac</i> , 38	Site 111 kink 111E 111T kink 100E 100T 111E 111TC 111TM kink 111 kink	vac 111 x 0.61 0.38 0.61 0.42 0.57 0.60 0.50 0.32 0.56 0.63 x 0.63 x	0.02           , 38           kink           0.93           x           0.81           0.73           0.93           0.67           0.90           0.73           0.75           0.94           0.60           x	111E           0.56           0.81           x           0.83           0.94           0.85           0.29           0.92           0.81           0.74           0.85           0.06           0.81	vac, 79           111           0.37           0.72           0.90           x           0.87           0.74           0.12           0.83           0.70           0.75           0.22           0.26	kink 0.64 0.79 0.88 0.76 x 0.84 0.28 0.90 0.72 0.67 0.85 0.19 0.85	111E 0.08 0.52 0.88 0.82 0.89 x 0.39 0.85 0.61 0.55 0.65 0.65 0.06 0.29	111           0.80           0.50           0.51           0.72           0.51           0.73           x           0.57           0.73           0.73           0.73           0.75           0.75           0.75           0.75           0.75	va kink 0.62 0.84 0.94 0.85 0.96 0.88 0.32 x 0.82 0.76 0.89 0.18 0.84	c, 201 111E 0.34 0.75 0.93 0.88 0.90 0.78 0.19 0.86 x 0.78 0.76 0.23 0.60	111 0.54 0.91 0.99 0.99 0.97 0.91 0.49 0.95 0.98 x 0.89 0.54 0.54 0.72	kink 0.67 0.82 0.90 0.78 0.93 0.87 0.35 0.92 0.76 0.71 x 0.21 0.21 0.20
MS, 38 MS, 79 MS, 201 vac, 38 vac, 79	Kink           Site           111           kink           111E           111T           kink           100E           100T           111E           111TC           111TC           111TC           111TM           kink           111           kink           111E	vac           111           x           0.61           0.38           0.61           0.42           0.57           0.60           0.50           0.32           0.56           0.63           x           0.60           0.22	0.02           , 38           kink           0.93           x           0.81           0.73           0.93           0.67           0.90           0.73           0.75           0.94           0.60           x	111E 0.56 0.81 x 0.83 0.94 0.85 0.29 0.92 0.81 0.74 0.85 0.06 0.81 x 0.22	$\begin{array}{c} 0.76\\ \hline vac, 79\\ \hline 111\\ \hline 0.37\\ \hline 0.72\\ \hline 0.90\\ \hline x\\ \hline 0.90\\ \hline x\\ \hline 0.83\\ \hline 0.74\\ \hline 0.12\\ \hline 0.83\\ \hline 0.80\\ \hline 0.77\\ \hline 0.75\\ \hline 0.22\\ \hline 0.56\\ \hline 0.83\\ \end{array}$	kink 0.64 0.79 0.88 0.76 x 0.84 0.28 0.90 0.72 0.67 0.85 0.19 0.86 0.98	111E 0.08 0.52 0.88 0.82 0.89 x 0.39 0.85 0.61 0.55 0.65 0.065 0.29 0.95	111           0.80           0.50           0.72           0.51           0.73           x           0.57           0.73           0.75           0.62           0.11	va kink 0.62 0.84 0.94 0.85 0.96 0.88 0.32 x 0.82 0.76 0.89 0.18 0.84 1.00	$\begin{array}{c} 0.76\\ \hline 0.76\\ \hline 0.34\\ \hline 0.75\\ \hline 0.93\\ \hline 0.93\\ \hline 0.93\\ \hline 0.90\\ \hline 0.78\\ \hline 0.19\\ \hline 0.86\\ \hline x\\ 0.78\\ \hline 0.78\\ \hline 0.78\\ \hline 0.76\\ \hline 0.23\\ \hline 0.60\\ \hline 0.93\\ \hline 0.92\\ \end{array}$	111 0.54 0.91 0.99 0.99 0.99 0.97 0.91 0.49 0.95 0.98 x 0.89 0.54 0.72 0.98	kink 0.67 0.82 0.90 0.78 0.93 0.87 0.35 0.92 0.76 0.71 x 0.21 0.88 0.98 0.76
MS, 38 MS, 79 MS, 201 vac, 38 vac, 79	Kink           Site           111           kink           111E           111T           kink           100E           100T           111E           111TC           111TM           kink           1111           kink           1111           kink           1111           kink           1111           kink	vac           111           x           0.61           0.38           0.61           0.42           0.57           0.60           0.50           0.32           0.56           0.63           x           0.60           0.22	0.02           , 38           kink           0.93           x           0.81           0.73           0.93           0.67           0.90           0.73           0.75           0.94           0.60           x           0.81           0.56	111E 0.56 0.81 x 0.83 0.94 0.85 0.29 0.92 0.81 0.74 0.85 0.06 0.81 x 0.83 0.62	0.70           vac, 79           111           0.37           0.72           0.90           x           0.87           0.74           0.12           0.83           0.75           0.22           0.56           0.83           x	kink 0.64 0.79 0.88 0.76 x 0.84 0.28 0.90 0.72 0.67 0.85 0.19 0.86 0.98 0.77	111E 0.08 0.52 0.88 0.82 0.89 x 0.39 0.85 0.61 0.55 0.65 0.06 0.29 0.95 0.99	111           0.80           0.50           0.72           0.51           0.73           x           0.57           0.73           0.73           0.73           0.73           0.73           0.71           0.72           0.73           0.73           0.73           0.73           0.73           0.70           0.75           0.62           0.11           0.12	val           kink           0.62           0.84           0.94           0.85           0.96           0.88           0.32           x           0.82           0.76           0.89           0.18           0.84           1.00           0.85	$\begin{array}{c} 0.76\\ \hline 0.76\\ \hline 0.34\\ \hline 0.75\\ \hline 0.93\\ \hline 0.93\\ \hline 0.90\\ \hline 0.78\\ \hline 0.90\\ \hline 0.78\\ \hline 0.19\\ \hline 0.86\\ \hline x\\ 0.78\\ \hline 0.78\\ \hline 0.78\\ \hline 0.76\\ \hline 0.23\\ \hline 0.60\\ \hline 0.93\\ \hline 0.92\\ \hline 0.92\\ \hline 0.5\\ \hline$	111 0.54 0.99 0.99 0.99 0.99 0.97 0.91 0.49 0.95 0.98 x 0.89 0.54 0.72 0.98 0.93 0.62	kink 0.67 0.82 0.90 0.78 0.93 0.87 0.35 0.92 0.76 0.71 x 0.21 0.88 0.98 0.76 1.60
MS, 38 MS, 79 MS, 201 vac, 38 vac, 79	Kink           Site           111           kink           111E           111T           kink           100E           100T           111E           111TC           111TM           kink           111T           kink           111E           111TM           kink           111E           111TK	vac           111           x           0.61           0.38           0.61           0.42           0.57           0.60           0.50           0.32           0.56           0.63           x           0.60           0.22           0.19	0.02           , 38           kink           0.93           x           0.81           0.73           0.87           0.93           0.67           0.90           0.73           0.75           0.94           0.60           x           0.81           0.56           0.86	111E 0.56 0.81 x 0.83 0.94 0.85 0.29 0.92 0.81 0.74 0.85 0.06 0.81 x 0.83 0.98	0.70           vac, 79           111           0.37           0.72           0.90           x           0.87           0.74           0.12           0.83           0.75           0.22           0.56           0.83           x           0.77	kink 0.64 0.79 0.88 0.76 x 0.84 0.28 0.90 0.72 0.67 0.85 0.19 0.86 0.98 0.77 x x	111E           0.08           0.52           0.88           0.82           0.89           x           0.39           0.85           0.61           0.55           0.65           0.065           0.99           0.93	111           0.80           0.50           0.72           0.51           0.73           x           0.57           0.73           0.73           0.73           0.73           0.73           0.73           0.73           0.73           0.73           0.73           0.73           0.73           0.73           0.73           0.73           0.74           0.75           0.62           0.11           0.13	val           kink           0.62           0.84           0.94           0.85           0.96           0.88           0.32           x           0.82           0.76           0.89           0.18           0.84           1.00           0.85           0.99	c. 201           111E           0.34           0.75           0.93           0.88           0.90           0.78           0.19           0.86           x           0.76           0.23           0.60           0.93           0.960	111 0.54 0.99 0.99 0.99 0.97 0.91 0.49 0.95 0.98 x 0.89 0.54 0.72 0.98 0.93 0.93 0.93	kink 0.67 0.82 0.90 0.78 0.93 0.87 0.35 0.92 0.76 0.71 x 0.21 0.88 0.98 0.76 1.00
<i>MS</i> , 38 <i>MS</i> , 79 <i>MS</i> , 201 <i>vac</i> , 38 <i>vac</i> , 79 <i>vac</i> , 201	Kink           Site           111           kink           111E           111T           kink           100E           100T           111E           111TC           111TM           kink           111           kink           111E           111TM           kink           111E           111TM           kink           111E           111T           kink           111T           kink	vac           111           x           0.61           0.38           0.61           0.42           0.57           0.60           0.50           0.32           0.56           0.63           x           0.60           0.22           0.19           0.06	0.02           , 38           kink           0.93           x           0.81           0.73           0.87           0.93           0.67           0.90           0.73           0.75           0.94           0.60           x           0.81           0.56           0.86           0.262	111E           0.56           0.81           x           0.83           0.94           0.85           0.29           0.92           0.81           0.74           0.85           0.06           0.81           x           0.83           0.92	0.70           vac, 79           111           0.37           0.72           0.90           x           0.87           0.74           0.12           0.83           0.80           0.77           0.75           0.22           0.56           0.83           x           0.77           0.99           0.11	kink 0.64 0.79 0.88 0.76 x 0.84 0.28 0.90 0.72 0.67 0.85 0.19 0.86 0.98 0.77 x 0.93 0.12	111E           0.08           0.52           0.88           0.82           0.89           x           0.39           0.85           0.61           0.55           0.65           0.06           0.29           0.95           0.99           0.93           x	111           0.80           0.50           0.72           0.51           0.73           x           0.57           0.73           0.70           0.75           0.62           0.11           0.13           0.73	val           kink           0.62           0.84           0.94           0.85           0.96           0.88           0.32           x           0.82           0.76           0.89           0.18           0.84           1.00           0.85           0.99           0.99	c. 201           111E           0.34           0.75           0.93           0.88           0.90           0.78           0.19           0.86           x           0.78           0.78           0.78           0.90           0.86           x           0.78           0.78           0.93           0.93           0.93           0.92           0.85           0.89           0.60	111 0.54 0.99 0.99 0.99 0.97 0.91 0.49 0.95 0.98 x 0.89 0.54 0.72 0.98 0.93 0.93 0.94 0.92	kink 0.67 0.82 0.90 0.78 0.93 0.87 0.35 0.92 0.76 0.71 x 0.21 0.88 0.98 0.76 1.00 0.96 0.26
<i>MS</i> , 38 <i>MS</i> , 79 <i>MS</i> , 201 <i>vac</i> , 38 <i>vac</i> , 79 <i>vac</i> , 201	Kink           Site           111           kink           111E           111T           kink           100E           100T           111E           111TC           111TM           kink           111           kink           111E           111TM           kink           111E           111TM           kink           111E           111T           kink           100E           1000E           100T           111TF	vac           111           x           0.61           0.38           0.61           0.42           0.57           0.60           0.50           0.52           0.56           0.63           x           0.60           0.22           0.19           0.06           0.75	0.02           , 38           kink           0.93           x           0.81           0.73           0.87           0.93           0.67           0.90           0.73           0.75           0.94           0.60           x           0.81           0.56           0.86           0.29           0.62	1111E 0.56 0.81 x 0.83 0.94 0.85 0.29 0.92 0.81 0.74 0.85 0.06 0.81 x 0.83 0.98 0.95 0.11 1.00	0.70           vac, 79           111           0.37           0.72           0.90           x           0.87           0.74           0.12           0.83           0.75           0.22           0.56           0.83           x           0.77           0.99           0.11           0.25	kink 0.64 0.79 0.88 0.76 x 0.84 0.28 0.90 0.72 0.67 0.85 0.19 0.86 0.98 0.77 x 0.93 0.13 0.63	1111E 0.08 0.52 0.88 0.82 0.89 x 0.39 0.85 0.61 0.55 0.65 0.65 0.06 0.29 0.95 0.99 0.93 x 0.73 0.62	111           0.80           0.50           0.72           0.51           0.73           x           0.57           0.73           0.89           0.70           0.75           0.62           0.11           0.13           0.73	val           kink           0.62           0.84           0.94           0.85           0.96           0.88           0.32           x           0.82           0.76           0.89           0.18           0.84           1.00           0.85           0.99           0.17	$\begin{array}{c} 0.16\\ \hline 0.16\\ \hline 0.201\\ \hline 1111E\\ \hline 0.34\\ \hline 0.75\\ \hline 0.93\\ \hline 0.93\\ \hline 0.90\\ \hline 0.78\\ \hline 0.90\\ \hline 0.78\\ \hline 0.19\\ \hline 0.86\\ \hline x\\ 0.76\\ \hline 0.23\\ \hline 0.76\\ \hline 0.23\\ \hline 0.60\\ \hline 0.93\\ \hline 0.92\\ \hline 0.85\\ \hline 0.89\\ \hline 0.08\\ \hline 0.08\\ \hline 0.22\\ \hline 0.82\\ \hline 0.$	111 0.54 0.99 0.99 0.99 0.97 0.91 0.49 0.95 0.98 x 0.89 0.54 0.72 0.98 0.93 0.93 0.94 0.99 0.97	kink 0.67 0.82 0.90 0.78 0.93 0.87 0.35 0.92 0.76 0.71 x 0.21 0.88 0.98 0.76 1.00 0.96 0.20
MS, 38 MS, 79 MS, 201 vac, 38 vac, 79 vac, 201	Kink           Site           111           kink           111E           111T           kink           100E           100T           111E           111TC           111TM           kink           111E           111TM           kink           111E           111T           kink           111T           kink           111T           kink           100E           100T           111E           1100E           100T           111E	vac           111           x           0.61           0.38           0.61           0.42           0.57           0.60           0.50           0.32           0.56           0.63           x           0.60           0.22           0.19           0.06           0.75           0.18           0.22	0.62           , 38           kink           0.93           x           0.81           0.73           0.93           0.67           0.90           0.73           0.75           0.94           0.60           x           0.81           0.56           0.82           0.81           0.56           0.86           0.29           0.62           0.84           0.50	111E 0.56 0.81 x 0.83 0.94 0.85 0.29 0.92 0.81 0.74 0.85 0.06 0.81 x 0.83 0.98 0.95 0.11 1.00 0.62	0.70           vac, 79           111           0.37           0.72           0.90           x           0.87           0.74           0.12           0.83           0.75           0.22           0.56           0.83           x           0.77           0.99           0.11           0.85           0.22	kink 0.64 0.79 0.88 0.76 x 0.84 0.28 0.90 0.72 0.67 0.85 0.19 0.86 0.98 0.77 x 0.93 0.13 0.93 0.55	1111E 0.08 0.52 0.88 0.82 0.89 x 0.39 0.85 0.61 0.55 0.65 0.65 0.65 0.06 0.29 0.95 0.99 0.93 x 0.73 0.99 0.90	111           0.80           0.50           0.51           0.51           0.73           x           0.57           0.73           0.89           0.70           0.75           0.62           0.11           0.13           0.73           x	val           kink           0.62           0.84           0.94           0.85           0.96           0.88           0.32           x           0.82           0.76           0.89           0.18           0.84           1.00           0.85           0.99           0.17           x           0.62	$\begin{array}{c} c, 201 \\ \hline 111E \\ 0.34 \\ 0.75 \\ 0.93 \\ 0.88 \\ 0.90 \\ 0.78 \\ 0.78 \\ 0.19 \\ 0.86 \\ x \\ 0.78 \\ 0.76 \\ 0.23 \\ 0.60 \\ 0.93 \\ 0.92 \\ 0.85 \\ 0.89 \\ 0.08 \\ 0.92 \\ 0$	111           0.54           0.91           0.99           0.97           0.91           0.49           0.95           0.98           x           0.72           0.98           0.93           0.93           0.94           0.97	kink 0.67 0.82 0.90 0.78 0.93 0.87 0.35 0.92 0.76 0.71 x 0.21 0.88 0.98 0.76 1.00 0.96 0.20 0.99 0.26
MS, 38 MS, 79 MS, 201 vac, 38 vac, 79 vac, 201	Kink           Site           111           kink           111E           111T           kink           100E           100T           111E           111TC           111TM           kink           111E           111T           kink           111E           111TE           111TC	vac           111           x           0.61           0.38           0.61           0.42           0.57           0.60           0.52           0.56           0.63           x           0.60           0.22           0.19           0.06           0.75           0.18           0.23	0.02           , 38           kink           0.93           x           0.81           0.73           0.93           0.67           0.90           0.73           0.75           0.94           0.60           x           0.81           0.56           0.86           0.29           0.62           0.84           0.60	111E 0.56 0.81 x 0.83 0.94 0.85 0.29 0.92 0.81 0.74 0.85 0.06 0.81 x 0.83 0.98 0.95 0.11 1.00 0.93 0.92	0.70           111           0.37           0.72           0.90           x           0.87           0.74           0.12           0.83           0.75           0.22           0.56           0.83           x           0.77           0.99           0.11           0.85           0.92           0.62	kink 0.64 0.79 0.88 0.76 x 0.84 0.28 0.90 0.72 0.67 0.85 0.19 0.86 0.98 0.77 x 0.93 0.13 0.99 0.85 0.22	111E 0.08 0.52 0.88 0.82 0.89 x 0.39 0.85 0.61 0.55 0.65 0.06 0.29 0.95 0.99 0.93 x 0.73 0.99 0.89 0.89	111           0.80           0.50           0.72           0.51           0.73           x           0.57           0.73           0.73           0.73           0.73           0.73           0.73           0.73           0.75           0.62           0.11           0.13           0.73           x           0.73           0.73           0.73           0.73	val           kink           0.62           0.84           0.94           0.85           0.96           0.88           0.32           x           0.82           0.76           0.89           0.18           0.84           1.00           0.85           0.99           0.17           x           0.92           0.92	$\begin{array}{c} 0.76\\ \hline 0.76\\ \hline 0.34\\ \hline 0.75\\ \hline 0.93\\ \hline 0.93\\ \hline 0.93\\ \hline 0.90\\ \hline 0.78\\ \hline 0.90\\ \hline 0.78\\ \hline 0.78\\ \hline 0.19\\ \hline 0.86\\ \hline x\\ 0.78\\ \hline 0.92\\ \hline 0.85\\ \hline 0.89\\ \hline 0.08\\ \hline 0.92\\ \hline x\\ 0.00\\ \hline 0.92\\ \hline x\\ 0.00\\ \hline 0.92\\ \hline 0.85\\ \hline 0.89\\ \hline 0.08\\ \hline 0.92\\ \hline x\\ 0.00\\ \hline 0.92\\ \hline 0.85\\ \hline 0.89\\ \hline 0.08\\ \hline 0.92\\ \hline 0.00\\ \hline 0.0$	0.91 111 0.54 0.99 0.99 0.99 0.99 0.97 0.91 0.49 0.95 0.98 x 0.89 0.54 0.72 0.98 0.54 0.72 0.98 0.93 0.93 0.93 0.94 0.99 0.97	kink 0.67 0.82 0.90 0.78 0.93 0.87 0.35 0.92 0.76 0.71 x 0.21 0.88 0.98 0.76 1.00 0.96 0.20 0.99 0.86 0.02
MS, 38 MS, 79 MS, 201 vac, 38 vac, 79 vac, 201	Kink           Site           111           kink           111E           111T           kink           100E           100T           111E           111TC           111TM           kink           111E           111T           kink           111E           111T           kink           111E           111T           kink           111E           111TE           111TE           111TC           111TC           111TC	vac           111           x           0.61           0.38           0.61           0.42           0.57           0.60           0.50           0.32           0.56           0.63           x           0.60           0.22           0.19           0.06           0.75           0.18           0.23	0.82           , 38           kink           0.93           x           0.81           0.73           0.93           0.67           0.90           0.73           0.75           0.94           0.60           x           0.81           0.56           0.86           0.29           0.62           0.84           0.60	111E           0.56           0.81           x           0.83           0.94           0.85           0.29           0.92           0.81           0.74           0.85           0.06           0.81           x           0.83           0.98           0.95           0.11           1.00           0.93           0.98	0.70           vac, 79           111           0.37           0.72           0.90           x           0.87           0.74           0.12           0.83           0.75           0.22           0.56           0.83           x           0.77           0.99           0.11           0.85           0.92           0.93	kink 0.64 0.79 0.88 0.76 x 0.84 0.28 0.90 0.72 0.67 0.85 0.19 0.85 0.77 x 0.93 0.13 0.99 0.85 0.93 1.02	111E 0.08 0.52 0.88 0.82 0.89 x 0.39 0.85 0.61 0.55 0.65 0.65 0.06 0.29 0.95 0.99 0.93 x 0.73 0.99 0.89 0.89 0.89	111           0.80           0.50           0.72           0.51           0.73           x           0.57           0.73           x           0.75           0.62           0.11           0.13           0.73           x           0.75           0.62           0.11           0.13           0.73           x           0.73           0.73	val           kink           0.62           0.84           0.94           0.85           0.96           0.88           0.32           x           0.82           0.76           0.89           0.18           0.84           1.00           0.85           0.99           0.17           x           0.92           0.97           0.97	c, 201 111E 0.34 0.75 0.93 0.88 0.90 0.78 0.19 0.86 x 0.78 0.79 0.86 0.23 0.60 0.93 0.92 0.85 0.89 0.08 0.92 x 0.99 0.92 x 0.92 0.85	111 0.54 0.99 0.99 0.99 0.99 0.97 0.91 0.49 0.95 0.98 x 0.89 0.54 0.72 0.98 0.54 0.72 0.98 0.93 0.93 0.93 0.94 0.99 0.97 0.99 0.99 0.99 0.97 0.99 0.97 0.99 0.98 0.93 0.93 0.93 0.94 0.99 0.93 0.93 0.94 0.99 0.93 0.93 0.94 0.95 0.93 0.93 0.94 0.95 0.93 0.92 0.94 0.93 0.93 0.94 0.99 0.93 0.94 0.95 0.93 0.94 0.95 0.93 0.94 0.95 0.93 0.94 0.95 0.93 0.94 0.95 0.93 0.94 0.95 0.93 0.94 0.99 0.97 0.99 0.93 0.97 0.99 0.97 0.99 0.93 0.97 0.99 0.97 0.99 0.97 0.99 0.92 0.92 0.92 0.93 0.93 0.95 0.55	kink 0.67 0.82 0.90 0.78 0.93 0.87 0.35 0.92 0.76 0.71 x 0.21 0.88 0.98 0.76 1.00 0.96 0.20 0.99 0.86 0.93

**Table S.6E.** Parameters for linear regressions of solvation energies between different metals and adsorption site

 coordination numbers.

Metal y	Parameters <sup>a</sup>	<u>CN</u>	Ag	Au	Ir	Pd	Pt
٨a	a	0.06		-0.02	-0.45	0.23	0.18
Ag	b	-1.30	_	-1.02	-1.29	-0.85	-0.89
۸.,	а	-0.01	-0.02		-0.05	-0.22	-0.08
Au	b	-0.72	-0.76	_	-0.79	-0.90	-0.81
Ĭn	a	-0.10	-2.09	-0.19		-0.13	-0.04
II	b	-0.09	-2.74	-0.78	_	-0.73	-0.66
DJ	a	0.02	0.14	-0.10	-0.02		0.46
Pu	b	-0.76	-0.53	-0.75	-0.69	_	-0.38
D4	a	0.01	0.14	-0.05	0.00	0.57	
Pt	b	-0.71	-0.49	-0.67	-0.64	-0.25	_

*a*: Parameters for linear regressions  $\overline{\Delta G_y} = a\Delta G_x + b$ , for which  $\overline{\Delta G_y}$ ,  $\Delta G_x$ , *a*, and *b* are in eV.

Table S.7E. Q	Juality of l	inear relations	between s	solvation	energies	on different	metals.
---------------	--------------	-----------------	-----------	-----------	----------	--------------	---------

	Metal y	Statistics <sup>a</sup>	<u>CN</u>	Ag	Au	Ir	Pd	Pt	no trend <sup>b</sup>
Excluding 38 sites, 201–100T	Ag	R	0.91		-0.02	-0.97	0.18	0.16	-
		$max \Delta G_y   x$	0.04	-	0.11	0.17	0.12	0.11	0.11
		ave $\Delta G_y   x$	0.03		0.06	0.07	0.05	0.06	0.05
	Au	R	-0.09	-0.02		-0.10	-0.15	0.16	-
		$max \Delta G_y   x$	0.12	0.11	_	0.12	0.12	0.12	0.13
		ave $\Delta G_y   x$	0.07	0.07		0.08	0.07	0.07	0.07
	Ir	R	-0.81	-0.97	-0.10		-0.04	-0.01	-
		$max \Delta G_y   x$	0.12	0.06	0.25	-	0.26	0.26	0.26
		ave $\Delta G_y   x$	0.08	0.03	0.12		0.12	0.12	0.12
	Pd	R	0.36	0.18	-0.15	-0.04		0.00	-
		$max \Delta G_y   x$	0.07	0.08	0.09	0.09	-	0.10	0.10
		ave $\Delta G_y   x$	0.04	0.05	0.05	0.04		0.03	0.05
	Pt	R	0.29	0.16	-0.06	-0.01	0.00		-
		$max \Delta G_y   x$	0.09	0.10	0.10	0.09	0.09	-	0.10
		ave $\Delta G_y   x$	0.05	0.05	0.04	0.04	0.04		0.04
in eV		-							

*a*: All  $\Delta G_y$  are in eV.

b: Null hypothesis, in which deviations are relative to the average as opposed to linear regression.

**Table S.8E.** Quality of linear relations between micro-solvated  $OH_x$  (x = 1,2) energies on different metals.

	Metal y	Statistics <sup>a</sup>	CN	Ag	Au	Ir	Pd	no trend <sup>b</sup>
H2O, MS	٨٥	R	0.22	-	0.78	0.92	0.96	-
	Ag	$max \Delta G_y   x$	0.12		0.08	0.05	0.04	0.13
	A 11	R	0.48	0.78	-	0.86	0.95	-
	Au	$max \Delta G_y   x$	0.14	0.11		0.10	0.11	0.17
	Ť.,	R	0.48	0.92	0.86	_	0.95	-
	п	$max \Delta G_y   x$	0.33	0.19	0.23		0.15	0.53
	Pd	R	0.26	0.96	0.83	0.95	-	-
		$max \Delta G_y   x$	0.19	0.08	0.14	0.08		0.20
OH, MS	٨٥	R	0.82		0.98	0.96	0.90	-
	Ag	$max \Delta G_y   x$	0.18	_	0.08	0.10	0.16	0.40
	A 11	R	0.89	0.98		0.96	0.91	-
	Au	$max \Delta G_y   x$	0.18	0.08	-	0.12	0.19	0.47
	Ť.,	R	0.85 0.96		0.96		0.97	-
	Ir	$max \Delta G_y   x$	0.35	0.27	0.22	-	0.19	0.95
	ЪI	R	0.75	0.90	0.91	0.97		-
	Pa	$max \Delta G_y   x$	0.20	0.21	0.19	0.09	-	0.42

*a*: All  $\Delta G_y$  are in eV.

b: Null hypothesis, in which deviations are relative to the average as opposed to linear regression.

## **S.9.** Water bilayer on Au(111)

We computed the solvation of \*OH within a water bilayer on Au(111) that appears in Table 1 in the main text using a  $\sqrt{3} \times \sqrt{3}$  R30° (111) supercell. In it, the adsorption energies of atop \*OH in vacuum and surrounded by water are 1.65 and 0.97 eV, such that  $\Omega_{OH} = -0.68 \ eV$ . The ZPE and TS (at T = 298.15 K) of \*OH are 0.32 and 0.17 eV in vacuum, and 1.02 and 0.25 eV withing the half-dissociated water bilayer. In turn, the ZPE and TS of the full water bilayer are 1.31 and 0.32 eV.

## References

- Calle-Vallejo, F.; F. de Morais, R.; Illas, F.; Loffreda, D.; Sautet, P. Affordable Estimation of Solvation Contributions to the Adsorption Energies of Oxygenates on Metal Nanoparticles. J. Phys. Chem. C 2019, 123 (9), 5578–5582. https://doi.org/10.1021/acs.jpcc.9b01211.
- (2) Kresse, G.; Furthmüller, J. Efficiency of Ab-Initio Total Energy Calculations for Metals and Semiconductors Using a Plane-Wave Basis Set. *Comput. Mater. Sci.* **1996**, *6* (1), 15–50. https://doi.org/10.1016/0927-0256(96)00008-0.
- (3) Kresse, G.; Furthmüller, J. Efficient Iterative Schemes for Ab Initio Total-Energy Calculations Using a Plane-Wave Basis Set. *Phys. Rev. B* **1996**, *54* (16), 11169–11186. https://doi.org/10.1103/PhysRevB.54.11169.
- (4) Kresse, G.; Hafner, J. Ab Initio Molecular Dynamics for Liquid Metals. *Phys. Rev. B* **1993**, 47 (1), 558–561. https://doi.org/10.1103/PhysRevB.47.558.
- (5) Kresse, G.; Hafner, J. Ab Initio Molecular-Dynamics Simulation of the Liquid-Metal--Amorphous-Semiconductor Transition in Germanium. *Phys. Rev. B* **1994**, *49* (20), 14251–14269. https://doi.org/10.1103/PhysRevB.49.14251.
- (6) Methfessel, M.; Paxton, A. T. High-Precision Sampling for Brillouin-Zone Integration in Metals. *Phys. Rev. B* **1989**, *40* (6), 3616–3621. https://doi.org/10.1103/PhysRevB.40.3616.
- (7) Nørskov, J. K.; Rossmeisl, J.; Logadottir, A.; Lindqvist, L.; Kitchin, J. R.; Bligaard, T.; Jónsson, H. Origin of the Overpotential for Oxygen Reduction at a Fuel-Cell Cathode. *J. Phys. Chem. B* 2004, *108* (46), 17886–17892. https://doi.org/10.1021/jp047349j.
- (8) Lide, D. R. CRC Handbook of Chemistry and Physics, 84th ed.; CRC Press, 2003.
- (9) Shampine, L. F. Matlab Program for Quadrature in 2D. *Appl. Math. Comput.* **2008**, 202 (1), 266–274. https://doi.org/10.1016/j.amc.2008.02.012.