ERRATA

Erratum: “The UBI–QEP Method: Basic Formalism and Applications to Chemisorption Phenomena on Transition Metal Surfaces. Chemisorption Energetics”
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1. On p. 6, the second sentence in the subsection *Two-Center M–A Potential: Quadratic Exponential Potential* should read:

Our first assumption is that the two-center M–A interaction between the metal and adsorbate atoms is also quasi-spherical and, therefore, the M–A bond energy (Q) depends only on the M–A distance (r_b) or some function $x(r_b)$ of this distance, in terms of which the M–A potential $E(x)$ can be expressed accurately and conveniently, for instance, in polynomial form.

2. On p. 8, Table 2 should read as follows:

Table 2. Atomic oxygen and nitrogen binding energies (kcal/mol) for bridging (B) and hollow (H) sites on some fcc(111), fcc(100), and bcc W(100) surfaces: comparison of calculated DFT and UBI–QEP values

Surface	H	B	H/B ratio of binding energies		Ratio of energies for (100) and (111) at H sites	
	DFT		DFT	UBI–QEP	DFT	UBI–QEP
Oxygen						
Cu(111) [63]	96.9	86.5	1.12	1.11		
Ag(111) [64]	86.3					
Ag(100) [64]	95.3	77.5	1.23	1.17	1.10	1.05
Ni(111) [59]	114.3	102.0	1.12	1.11		
Ni(111) [65]	114.7				1.12	1.05
Ni(100) [65]	129.1					
Pt(111) [66]	98.3	83.7	1.17	1.11		
Pt(111) [67]	75.7	63.0	1.20	1.11		
Nitrogen						
W(100) [68]	170	147	1.16	1.20		

Note: DFT calculations were performed for low coverages ($\theta \leq 1/n$). These correspond to ZCL values. In [65], calculations were performed by an ab initio (but not DFT) method.

3. On p. 11, the second sentence after Eq. 17 should read:

Also, if there are three or more bonds, which are all nonequivalent, some M–A (or M–B) bond indices may formally become negative [30, 76] (cf. Eq. (16)).

4. On p. 14, the last sentence in the left column should read:

In recent DFT calculations [93], the accuracy is rather high— $Q_{\text{CO}} = 33.3$ kcal/mol for the on-top site and $Q_{\text{CO}} = 32.3$ kcal/mol for the hollow fcc site—whereas the best experimental estimate is $Q_{\text{CO}} = 35.5$ kcal/mol.

5. On p. 14, right column, the sentence in lines 11 and 12 from the bottom should begin as follows:

The maximal value of the $M_{(1)}\text{--}A$ bond energy (a) will be smaller than the initial...

6. On p. 15, Table 5 should read:

Table 5. Binding energies Q_{AB} (kcal/mol): comparison with the experiment

AB	Surface	Site	Coordination type	Q_{0A}	Q_{AB}	
					UBI–QEP	experiment
CH ₃ OH	Pt(111)	on-top	mono-O	51.0	10.6	11.4 [98]
CH ₃ OH	Rh(111)	on-top	mono-O	61.2	14.5	14 [99]
OH	Pt(111)	hollow	mono-O	51.0	58.6*	60 [100, 101]
OH	Ag(111)	hollow	mono-O	48.0	55.2*	55 [102]
OH	Pd(111)	hollow	mono-O	52.3	60.2*	60 [103, 104, 105]
H ₂ O	Pt(111)	on-top	mono-O	51.0	10.1	9.6 [98]
H ₂ O	Cu(111)	on-top	mono-O	61.8	13.5	9.8 [106]
H ₂ O	Ag(111)	on-top	mono-O	48.0	8.6	9–10 [102]
NO	Pd(111)	bridge	mono-N	78.0	32	31 [107]
NO	Pt(111)	bridge	mono-N	69.6	26	27 [107]
O ₂	Pt(111)	bridge	di-O	51.0	11	9 [108]
N ₂	Pt(111)	bridge	di-N	69.6	11	9 [109]
SCH ₃	Au(111)	hollow	mono-S	48.0	44	44 [110]
NH ₃	Ni(111)	on-top	mono-N	81.0	18	20 [111]
NH ₃	Pt(111)	on-top	mono-N	69.6	11–14	12 [112]
NH ₂	Pt(111)	hollow	mono-N	69.6	39–47	>42 [113]
NH	Pt(111)	hollow	mono-N	69.6	71	71–74 [113]
HCOOH	Ag(111)	bridge	di-O	48.0	12	13 [114, 115]

* The value corrected for the formation of hydrogen bonds, see [39, 116].

7. On p. 16, the last sentence in the paragraph after Eq. (47) should read:

Some examples of calculated BIs for TS ($x_{\text{AB, TS}}$) can be found in Table 4 from [27].

8. On p. 17, in Table 6, the entry in the first row and fourth column should read: (43).

9. The footnote to Table 6 should read:

* $Q_{\text{OH}} \sim 60$ kcal/mol (taking into account the hydrogen-bond correction) [27].

10. On p. 19, the last line in the right column should read:

take as the value of D in Eq. (43).

11. On p. 21, left column, the third line from the bottom should read:

However, if $m = m' = 0$, one should use Eqs. (39a) and (39b).

12. On p. 22, Eq. (65) should read as follows:

$$Q_{\text{A2(X)}} = 2a_{\text{X}} = (3/2)a'.$$

13. On p. 23, the last sentence in the first paragraph in the left column should read:

Section A3.2 of the Appendix discusses this in detail.

14. On p. 26, Eq. (A24b) should read:

$$Q_i^* = 0.199Q_0.$$