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Addition/Correction

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Correction to Theoretical Study of Dioxygen Induced Inhibition of [FeFe]-Hydrogenase

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We here report misprints that occurred at the type-setting stage of our paper that we had overlooked in the galley proof. We are grateful to Adam Kubas from University College London for drawing our attention to these issues.

Page 7130. The calculated bond distances in Table 1 are a direct copy of the data given in Table 2. Our originally submitted Table 1 is given here. Note that the bond angles given in the original paper are the correct ones. Also, Table 2 contains a minor issue: the bond distances $Fe_d \cdots C(CO_\mu)$ are listed under "Angles".

Page 7136. In Table 9, protonation energies of O_2 adducts of the H cluster are given. Four of the external protonation energies in the published article are positive. Clearly, all of these external protonation energies must be exothermic, and thus the negative sign is missing four times (the correct energies are −221.3, −173.1, −193.1, and −173.5 kcal/mol). Also, note that the last sentence of section 7 should read: "Furthermore, protonation of the emerging species turns out to be highly favorable by more than −210 kcal/mol for the transfer of a first and by more than −170 kcal/mol for the transfer of a second proton."

Page 7139. We clarify a possible labeling issue in Figure 10. The first compound is referred to as the CO_2-*deprived* structure **4a**−$[Fe_p(II)Fe_d(IV)]^-$ in the caption as well as in the describing text in section 8. This structure is then labeled as **4a**−$[Fe_p(II)Fe_d(III)]^-$ in Figure 10, which might cause misunderstandings because the *product* of CO_2 ejection was already labeled by the number 6 (**6**−$[Fe_p(II)Fe_d(III)]^-$) in Figure 9 on p 7138 but must not be confused with compounds **6**−$[Fe_p(II)Fe_d(IV)]^-$ and **6**−$[Fe_p(II)Fe_d(III)]^{2-}$ in Figure 10.

Table 1. Structural Features of the DFT-Optimized H-Clusters Shown in Figure 3[a]

		1−$[Fe_p(II)Fe_d(II)]^{2-}$			**1(NH)**−$[Fe_p(II)Fe_d(II)]^{2-}$		
	exp.	BP86	B3LYP	TPSS	BP86	B3LYP	TPSS
Distances							
$Fe_p \cdots Fe_d$	2.55	2.57	2.55	2.56	2.57	2.58	2.56
$Fe_d \cdots O(H_2O)$	2.38	2.19	2.12	2.14	2.20	2.10	2.15
$Fe_p \cdots S_{\mu_1}$	2.29	2.37	2.36	2.36	2.38	2.40	2.36
$Fe_p \cdots S_{\mu_2}$	2.30	2.32	2.31	2.32	2.32	2.35	2.32
$Fe_p \cdots C(O)$	1.74	1.76	1.77	1.77	1.76	1.80	1.77
$Fe_p \cdots C(N)$	1.83	1.91	1.93	1.93	1.91	1.95	1.93
$Fe_d \cdots S_{\mu_1}$	2.32	2.35	2.34	2.34	2.35	2.37	2.34
$Fe_d \cdots S_{\mu_2}$	2.30	2.36	2.35	2.34	2.35	2.36	2.34
$Fe_d \cdots C(O)$	1.77	1.75	1.77	1.77	1.75	1.80	1.77
$Fe_d \cdots C(N)$	1.93	1.91	1.93	1.93	1.91	1.95	1.92
$Fe_p \cdots S_{\mu_b}$	2.39	2.41	2.41	2.41	2.38	2.39	2.39
$Fe_p \cdots C(CO_\mu)$	1.91	1.96	1.96	1.96	1.96	1.93	1.96
$Fe_d \cdots C(CO_\mu)$	1.99	1.94	1.97	1.96	1.95	2.09	1.97
Angles							
$Fe_p - S_{\mu_b} - Fe_1$	117.1	122.7	125.4	122.2	127.9	127.2	124.3
$Fe_4 - Fe_1 - S_{\mu_b} - Fe_p$	−87.4	−79.8	−79.2	−81.2	−68.6	−69.4	−74.5

[a] For all optimizations, the TZVP basis set was used. The charge of the cluster is −2 elementary charges in each case, corresponding to a $[Fe_p(II)Fe_d(II)]$-pair at the $[2Fe]_H$ subsite.

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