

Correction

Correction: Anders et al. First Principle Surface Analysis of YF₃ and Isostructural HoF₃. *Materials* 2022, 15, 6048

Jennifer Anders , Niklas Limberg  and Beate Paulus

Institute for Chemistry and Biochemistry, Freie Universität Berlin, Arnimallee 22, 14195 Berlin, Germany

* Correspondence: jennifer.anders@fu-berlin.de

In the original publication [1], there was a mistake in **Table 2** and **Figure 2** as published. Within **Table 2**, the coordination numbers of the two stoichiometric terminations of surface (011) have been flipped [showing (011)-1 and (011)-2 with 6,6,8,8 and 7,7,9,9, respectively]. **Figure 2** showed the surface of (011)-2 in the first row, third image with the same incorrect coordination numbers of 7,7,9,9 instead of 6,6,8,8. The authors state that the scientific conclusions are unaffected. This correction was approved by the Academic Editor. The original publication has also been updated.

Table 2. The YF₃ (PBE) and HoF₃ (PBE+U_d/3 eV/4f-in-core) surfaces with respective terminations (term.), slab thickness in layers of formula units without terminal F-deficit (L_{MF_3}), nominal surface net charge (q_{surf}) in e, surface energies of relaxed (E_{surf}) and unrelaxed slabs ($E_{surf}^{unrel.}$) in J m⁻², as well as the relaxed surface metal coordination number (CN_{surf}). The lowest surface energies per (*hkl*) cut are highlighted in bold. For these, also the abundance obtained by the Wulff plot ($\%_{surf}$) is given.

<i>(hkl)</i>	term.	q_{surf}	L_{MF_3}		CN_{surf}		E_{surf} ($E_{surf}^{unrel.}$)		$\%_{surf}$	
			YF ₃	HoF ₃	YF ₃	HoF ₃	YF ₃	HoF ₃	YF ₃	HoF ₃
(100)	1	0	20	24	5,9		1.61 (2.87)	0.93 (1.48)	7%	25%
	2	0	22	26	6,9		1.03 (2.02)	0.58 (0.96)		
	3	+1	20	24	5,8		1.24 (1.61)	0.62 (0.68)		
	4	+2	22	26	4,7		1.79 (2.14)	0.87 (0.90)		
(010)	1	0	10	12	8,8		0.58 (0.84)	0.47 (0.49)	26%	34%
	2	+2	10	12	6,6		1.80 (2.05)	1.52 (1.52)		
(001)	1	0	20	24	5,8,8,9		1.23 (2.45)	1.37 (2.25)	10%	6%
	2	0	22	26	6,7,8,9		0.58 (1.39)	0.67 (1.16)		
	3	+2	22	26	4,5,8,9		1.27 (1.70)	1.23 (1.29)		
(110)	1	0	20	24	6,8,8		1.01 (1.80)	0.99 (1.59)	5%	0%
	2	0	22	26	6,8,8		1.00 (2.41)	1.00 (2.18)		
	3	+2	22	26	4,6,9	4,6,8	1.42 (1.73)	2.09 (1.36)		
(101)	1	0	20	24	6,7,8,8		0.82 (1.48)	0.89 (1.33)	20%	14%
	2	0	20	24	6,6,8,8		0.82 (3.34)	0.88 (3.17)		
	3	+1	20	24	6,7,8,8		0.76 (1.16)	0.69 (0.89)		
	4	+1	22	26	5,6,7,9	5,6,8,8	1.07 (2.10)	1.03 (1.70)		
	5	+2	20	24	4,5,8,8	5,6,8,8	0.98 (1.39)	0.99 (0.99)		
(011)	1	0	10	12	7,7,9,9		0.78 (1.30)	0.81 (1.14)	22%	13%
	2	0	10	12	6,6,8,8		0.61 (1.32)	0.68 (1.15)		
	3	+2	10	12	4,4,8,8		1.25 (1.68)	1.35 (1.38)		
(111)	1	0	20	24	6,7,7,8	7,7,8,8	1.02 (3.46)	0.87 (3.29)	10%	7%
	2	+1	20	24	5,6,8,8		0.83 (1.30)	0.82 (1.04)		
	3	+1	22	26	6,6,7,9		1.05 (1.70)	0.75 (1.11)		
	4	+2	20	24	5,5,7,7		0.93 (1.22)	0.95 (1.13)		



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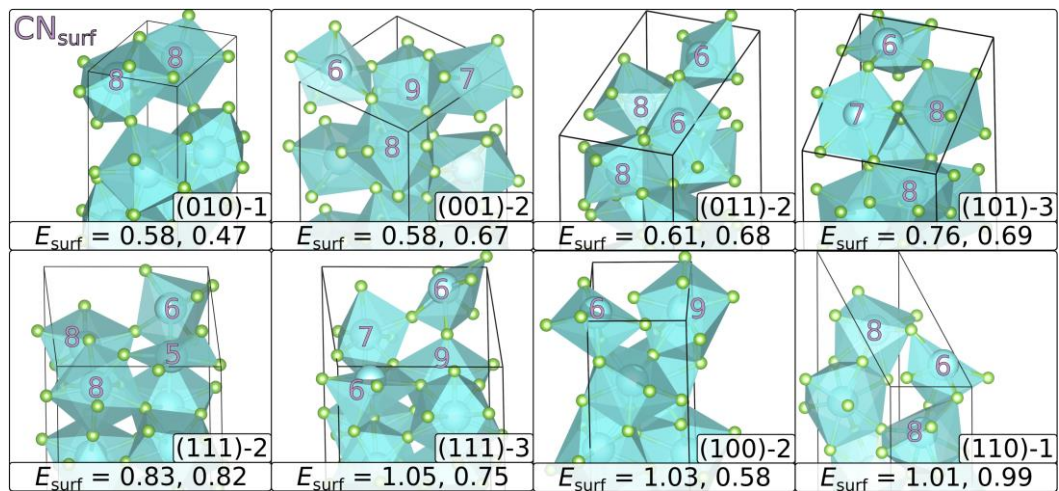


Figure 2. Most stable terminations of the relaxed surface structures: the coordination number of the surface metals (CN_{surf}) and the surface energies in J m^{-2} (E_{surf}) are given. The first entry corresponds to YF_3 and the second to HoF_3 . The mean of both values corresponds to the given order from top left to bottom right. Each (hkl) slab is rotated in a way to show the surface coordination best. For (111), two surfaces are given, as (111)-2 is preferred by YF_3 and (111)-3 by HoF_3 .

Reference

- Anders, J.; Limberg, N.; Paulus, B. First Principle Surface Analysis of YF_3 and Isostructural HoF_3 . *Materials* **2022**, *15*, 6048. [[CrossRef](#)] [[PubMed](#)]

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