Ab-initio electronic and structural properties of the clean and hydrogen saturated β-SiC(100)(3×2) surfaces

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Erratum

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In a paper published last year [1] we presented theoretical calculations which were compared, among others, with the experimental results by D'angelo *et al* [2]. In doing this, we calculated the values obtained by those authors for three different distances, referred to in our paper as d_1, d_4 and d_5. The data we used was taken from table 2 of their paper. As a result of a misinterpretation, we could not obtain adequate values for the distances we referred to as d_2 and d_3. In fact, the value of 3.48 Å presented by D'angelo *et al* [2] refers to the displacement between dimers and not the long and short distances (d_2 and d_3) of the Si–Si dimers as we wrongly interpreted. Had we correctly interpreted the data in [2], distances d_2 and d_3 would have been correctly obtained. This error appears both in the text and table 1 of our paper. The table containing the corrected data is given below. Although these errors do not affect the main

Table 1. Structural parameters corresponding to the ones shown in figure 1 for the three explored systems: *clean*, *hydrogenated* and *saturated*. A comparison with two previous works is also shown.

	d_1(Å)	d_2(Å)	d_3(Å)	d_4(Å)	d_5(Å)	Θ(deg)
A (This work—*clean*)	2.36	2.48	2.51	2.52	3.60	5.38
B (Lu *et al* [3]—*clean*)	2.24	2.37	2.38	2.41	3.43[a]	12.8
C (D'angelo *et al* [2]—*clean*)	2.78	2.41	2.27	2.38	3.43	5.34
D (Tejeda *et al* [4]—*clean*	2.54	1.83	2.40	2.43	3.41	5.5
E (This work—*hydrogenated*)	2.44	2.56	2.56	2.52	3.61	
F (This work—*saturated*)	2.35	2.52	2.52	3.24	3.26	
Theo.–theo.: ratio (A/B)	1.053	1.046	1.055	1.046	1.049	0.420
Theo.–exp.: atio (A/C)	0.849	0.713	0.721	1.059	1.049	1.007
Theo.–exp: ratio (A/D)	0.929	1.355	1.046	1.037	1.056	0.978

[a] Value indirected determined from the reference data.

conclusions of the paper we feel that it is our obligation to register the error and apologize for any inconvenience this may have caused.

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