

CORRECTION

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Correction: Theoretical studies on the mechanism of oxygen reduction reaction on clean and O-substituted Ta₃N₅(100) surfaces

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Correction for 'Theoretical studies on the mechanism of oxygen reduction reaction on clean and O-substituted Ta₃N₅(100) surfaces' by Eriko Watanabe *et al.*, *Catal. Sci. Technol.*, 2015, DOI: 10.1039/c5cy00088b.

The authors apologise for a mistake in the layout of Table 1. The corrected Table 1 is presented below.

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Table 1 (a) Calculated adsorption energy for Pauling-type or Griffiths-type O₂ adsorption. The 'site' column shows the positions of O₂ adsorption shown in Fig. 1(d). The middle column, 'style', shows adsorption type; G means Griffiths-type structure and P means Pauling-type structure. (b) Calculated adsorption energy for Yeager-type structure together with the adsorbed Ta-Ta length in the middle column

(a)		
Clean surface		
Site	Style	E_{ad} (eV)
A	G	0.00
B	G	-0.04
O1-substituted surface		
Site	Style	E_{ad} (eV)
A	G	-0.99
B	P	-0.55
C	P	-0.55
E	G	-0.95
F	G	-1.02
O2-substituted surface		
Site	Style	E_{ad} (eV)
A	G	-1.83
B	P	-0.82
C	P	-0.71
D	G	-1.71
E	G	-1.55
F	G	-1.67
(b)		
Clean surface		
Site	$d_{\text{Ta-Ta}}$ (Å)	E_{ad} (eV)
A-B	4.06	0.00
A-C	4.03	-0.04
B-D	3.38	-0.06
C-D	3.19	0.05
O1-substituted surface		
Site	$d_{\text{Ta-Ta}}$ (Å)	E_{ad} (eV)
B-D	3.56	-0.85
C-D	3.37	-0.71
D-E	4.04	-0.54
D-F	3.95	-0.63
E-F	4.04	-0.67
A-E	3.38	-0.87
A-B	4.04	-0.66
A-C	4.07	-0.55
B-F	3.27	-0.93
B-C	4.20	-0.54
C-E	3.31	-0.82
O2-substituted surface		
Site	$d_{\text{Ta-Ta}}$ (Å)	E_{ad} (eV)
B-D	3.64	-2.00
C-D	3.35	-1.71
D-E	4.00	-0.69
D-F	3.89	-0.70
E-F	4.03	-1.06
A-E	3.34	-1.35
A-B	3.99	-0.52
A-C	4.06	-0.56
B-F	3.23	-1.43
B-C	4.17	-1.03
C-E	3.36	-1.48
A-F	3.32	-1.58

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

