Erratum: Titration of Ce^{3+} Ions in the $\text{CeO}_2(111)$ Surface by Au Adatoms [Phys. Rev. Lett. 111, 206101 (2013)]

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Because of an error in some of the routines of VASP5.2.12 (“T point only” version, release 26May11) [1], the O defect formation energies in the subsurface position of the $\text{CeO}_2(111)$ surface had to be recalculated. For this purpose, VASP5.3.5 (release 31Mar14) was used. Results are shown in Table I. The adjustments of the previously published formation energies are within 0.07 eV. The conclusions of the Letter are not affected.

TABLE I. Structure and vacancy formation energy (E_{def}) with respect to $\frac{1}{2}\text{O}_2$ for different subsurface O vacancy/ Ce^{3+} configurations obtained with HSE.

Ce^{3+} configuration	$\text{Ce}^{3+} - \text{Ce}^{3+}$ distance [Å]	Ce^{3+} —defect distances [Å]	$E_{\text{def}}(\frac{1}{2}\text{O}_2)$ [eV]	
			High spin	Low spin
$b_1 - b_3$	7.67	4.41; 4.42	2.32	2.27
$a_1 - b_3$	6.77	2.33; 4.44	2.43	2.41
$b_3 - c_6$	6.65	4.41; 5.84	2.41	
$a_3 - b_3$	3.89	2.34; 4.43	2.50	2.54
$b_3 - d_3$	10.11	4.40; 7.94	2.47	
$c_5 - c_6$	3.88	5.84; 5.85	2.69	
$c_1 - c_6$	7.66	5.85; 5.84	2.66	
$a_1 - d_3$	7.63	2.35; 7.93	2.62	
$a_3 - c_5$	3.77	2.32; 5.86	2.63	
$a_1 - a_3$	4.08	2.37; 2.37	2.71	2.71

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[1] See www.vasp.at.