Erratum: Atomistic simulations of copper oxidation and Cu/Cu₂O interfaces using charge-optimized many-body potentials [Phys. Rev. B **84**, 125308 (2011)]

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We have identified some errors in our original paper on Cu/Cu₂O charge-optimized many-body (COMB) potentials:

First, there was an error in our reporting of the atomic-specific and interaction-dependent parameters for COMB2011. The corrected values are given in Tables I–III below and correspond to Tables I, II(b), and III in the published paper. These corrected parameters lead to the predicted properties of Cu and Cu₂O that are given in Tables IV and VII in the published paper.

Second, in Table VII of the published paper, the shear modulus predicted by COMB2011 is 38 GPa rather than 8.27 GPa.

Third, on p. 15, in the last paragraph of Sec. II E, the word COMB2011 in the sentence, “Considering the computational efficiency of the COMB2011 potential presented in this work,” should be COMB2010 (instead of 2011).

Fourth, the Greek symbol “ ζ ” in the exponential term in Eq. (35) should be “ ξ ”.

TABLE I. Atomic and electrostatic potential parameters.

	COMB2010		COMB2011	
	Cu	O	Cu	O
χ (eV q^{-1})	0	5.634 414	3.768 251	4.700 782
J (eV q^{-2})	4.321 185	6.064 346	2.966 470	5.064 537
K (eV q^{-3})	0	4.511 4270	0.515 044	2.756 183
L (eV q^{-4})	0	1.330 079	0.257 522	0.992 188
ξ ($\text{\AA}^{-1}$)	0.454 784	2.243 072	1.540 170	3.000 115
$Z(q)$	0	0	0.211 810	0.030 538
P ($\text{\AA}^3$)	0	0	0.335 000	0.325 274
P_1^J ($\text{\AA}^2 q^{-1}$)	−0.274 649	−3.922 011	0.199 423	−0.503 453
P_2^J ($\text{\AA}^4 q^{-2}$)	0.725 710	0.971 086	0.466 738	1.124 890
D_u ($\text{\AA}$)	−0.161 007	−0.001 120	−0.413 129	−1.628 757
D_l ($\text{\AA}$)	0.167 765	0.001 480	0.686 816	0.270 362
$Q_u(q)$	2	5.504 600	2	6
$Q_l(q)$	−6	−1.834 900	−6	−2
CN	0	0	2.2	4.2
γ_{Coord}	0	0	0.250 000	0.249 569
E_{Coord} (eV)	0	0	0.732 288	1.821 557

TABLE II. Bond-dependent potential parameters for COMB2011.

	Cu-Cu	O-O	Cu-O	O-Cu
A (eV)	712.3527	3523.3586	601.2823	601.2823
B (eV)	102.8261	204.6259	101.2525	101.2525
λ ($\text{\AA}^{-1}$)	2.712 035	5.516 839	3.159 474	3.159 474
α ($\text{\AA}^{-1}$)	1.467 089	2.527 568	1.442 101	1.442 101
β	0.231 055	2	0.231 055	2
η	1	1	1	1
m	1	1	1	1
c	0	6.600	1.328 406	1.433 090
d	1	1	1	1
h	0	−0.229 00	−0.354 592	0.427 488
n_B	10	10	10	10
R_s ($\text{\AA}$)	3.2	2.2	2.2	2.2
S_s ($\text{\AA}$)	3.6	2.8	2.6	2.6

TABLE III. Coefficients for charge-independent bond angle energy functions.

	Cu-Cu-Cu	O-O-O	Cu-O-Cu	O-Cu-O
K_{LP}^1 (eV)	0.073 078	0.000 000	0.507 861	0.099 696
K_{LP}^2 (eV)	0.000 000	0.000 000	0.507 861	0.000 000
K_{LP}^3 (eV)	0.019 678	0.000 000	0.000 000	0.162 259

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