Erratum: Quantum-continuum calculation of the surface states and electrical response of silicon in solution [Phys. Rev. B **95**, 205308 (2017)]

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We correct an error in Sec. II C of our original paper, appearing in Eqs. (21) and (22) which leads to errors in the reported results in Sec. IV. All of the trends shown remain the same, and the conclusions drawn from the paper remain valid.

Equations (21) and (22) should read

$$\bar{\varphi}_0 = \bar{\varphi}(z_c) - k_B T - \frac{\epsilon_0}{2\mathcal{N}} \left(\frac{d\bar{\varphi}}{dz}(z_c) \right)^2 \quad (21)$$

and

$$\bar{\varphi}_0 = \bar{\varphi}(z_c) + k_B T + \frac{\epsilon_0}{2\mathcal{P}} \left(\frac{d\bar{\varphi}}{dz}(z_c) \right)^2. \quad (22)$$

This removes an unphysical interaction between different dielectric constants at the boundary of Regions I and II and brings the physical picture more in line with the one shown in Fig. 3 of the original paper. Figure 1 here illustrates this difference.

TABLE I. Fitted surface-state properties for the ten surface configurations tested. The percentage of the total potential drop that takes place within Region I, the bulk of the semiconductor, is represented by γ_I (%). The capacitance of the surface state, assuming a metal-like distribution, is represented as C_{II} .

	γ_I (%)	C_{II} ($\mu\text{F cm}^{-2}$)
Si + O*	3.27	32.3
Si + O* + H*	7.59	55.7
Si + 2O*	2.74	29.7
Si + 2O* + H	7.79	32.2
Si + 4O* + H*	8.26	18.7
Rutile (110)	9.21	3.70
Cristobalite (100)	1.40	36.6
Cristobalite (110)	55.0	3.39
Quartz (1000)	2.98	20.0
Quartz (11 $\bar{2}$ 0)	19.1	69.5

FIG. 1. A cutoff value is selected within the material, and to the left of the cutoff a Mott-Schottky distribution is used. (a) How the potential would be distributed before this correction assuming an instantaneous transition between the dielectric constant of Region II and Region I, causing a reduction in the slope of a factor $1/\epsilon_I$. (b) How the potential is distributed after this correction with the macroscopic potential following a smooth curve.

This results in new charge-voltage curves as shown below in Fig. 2 here. Finally, this results in new and more reasonable values for the fit of the model using a semiconductor and metal capacitance in series. These results are shown in Table I.

FIG. 2. (a) The total charge versus voltage curves for Si (110) structures. (b) The total charge versus potential curves for SiO_2 structures. The lines correspond to the fitted trends of an empirical model that consists of an ideal Mott-Schottky semiconductor in series with a linear capacitor representing the surface states.