Erratum: *Ab initio* study of subsurface diffusion of Cu on the H-passivated Si(001) surface [Phys. Rev. B 80, 155426 (2009)]

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We have realized that the energy zero used in presenting binding energies in our paper was incorrect. This makes the absolute magnitudes of the energies in Tables I–III incorrect, but the relative sizes are unchanged. We present the correct numbers below.

TABLE I. Total energy (ΔE) referred to the most stable position (T3) and binding energy (BE) in eV.

Adsorption site	ΔE (eV)	Binding energy (eV)
T3	0	−3.33
HSL2	0.03	−3.30
T2	0.05	−3.28
HSL	0.05	−3.28
HSL3	0.12	−3.21
T4	0.16	−3.18
C	0.24	−3.10
HSL4	0.29	−3.05
P	0.60	−2.73
A	0.69	−2.64
BD	0.83	−2.50

TABLE II. Energies of the different saddle points appearing in Figs. 3 and 4. First column indicates the saddle point as labeled in the Figs. 3 and 4, second column displays the energies in eV (calculated as a binding energy for Cu at that position), whereas third column shows which two adsorption sites are connected by each saddle point.

Saddle point	BE (eV)	Connecting
a	−2.02	P, P′
b	n/a	P, BD
c	−2.29	P, C
d	−2.64	C, C′
e	−3.03	C, HSL
f	−2.45	HSL, BD
g	n/a	HSL, HSL′
h	−3.11	HSL, T2
i	n/a	T2, T2′
j	−3.00	T2, HSL2
k	−3.10	T3, HSL2
l	−3.03	HSL3, T3
m	−2.97	T4, HSL3
n	n/a	T4, T4′
o	−2.90	HSL4, T4
p	n/a	HSL4, HSL4′

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TABLE III. Total energies and binding energies (ΔE) relative to the most stable position (T3) for the long, thin slab.

Adsorption site	ΔE (eV)	Binding energy (eV)
T3	0	−3.38
HSL2	0.02	−3.36
T2	0.04	−3.34
HSL	0.07	−3.31
HSL3	0.10	−3.28
T4	0.20	−3.18
C	0.21	−3.17
HSL4	0.24	−3.14
P	0.69	−2.69
A	0.69	−2.69
BD	0.81	−2.57
B	*xx*	*xx*