Erratum: Band offsets between $ZnGeN_2$, GaN, ZnO, and $ZnSnN_2$ and their potential impact for solar cells [Phys. Rev. B 88, 075302 (2013)]

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The band offsets in this paper included a GW correction, Δ_{GW}, describing the shift of the valence band maximum relative to the average electrostatic potential arising from the quasiparticle self-consistent (QS) GW self-energy shift. Since that work was published, we have found that this quantity requires a higher level of convergence in terms of basis set than the band gaps. In particular, in our previous work [1], we found an anomalous behavior for $ZnSnN_2$, in which the shift was positive, 0.20 eV, while for the other materials it was negative as one expects. Performing better converged calculations (in particular, using at least an $spdf$-spd basis set, and further checking with an $spdfg$-spd+floating orbitals on empty sites) we find that the values of Δ_{GW} in Table II should be replaced by -0.4 ± 0.1 eV for GaN, -0.5 ± 0.1 for $ZnGeN_2$, -0.3 ± 0.1 eV for $ZnSnN_2$, and -1.5 ± 0.1 eV for ZnO. These are 0.8Σ values, meaning that the self-energy as calculated is reduced by a factor 0.8 to take into account the underscreening by the random phase approximation in calculating the screened Coulomb interaction W. This implies that there is almost no change in this shift between $ZnSnN_2$ and GaN or $ZnGeN_2$ to within an accuracy of 0.1 eV. Thus, this correction only is important for the cases involving ZnO.

We have recalculated the resulting changes in Tables III and IV and Fig. 4 in the paper, which should be replaced by the following.

TABLE III. Dipole potentials and valence band offsets in each direction from eight-layer supercell (units in eV). (Values in parentheses are obtained from 12-layer supercell.)

	$GaN/ZnGeN_2$	$ZnO/ZnGeN_2$	$GaN/ZnSnN_2$
$\Delta E_v^0(GW)$	0.00	3.95	1.22
$\Delta_s^{[100]}$	0.15	0.25	0.24
$\Delta_s^{[010]}$	0.19	0.29	0.33
$\Delta_s^{[001]}$	0.14	0.21	0.34
$V_D^{[100]}$	1.15(1.29)	−2.21	0.18
$V_D^{[010]}$	1.04(1.17)	−2.10	0.18
$V_D^{[001]}$	1.10(1.24)	−2.43	0.23
$\bar{V}_D$	1.10(1.23)	−2.25	0.20
$\Delta E_v^{[100]}$	1.30(1.44)	1.99	1.64
$\Delta E_v^{[010]}$	1.23(1.36)	2.14	1.73
$\Delta E_v^{[001]}$	1.24(1.38)	1.73	1.79

TABLE IV. Natural valence and conduction band offsets, gap differences, and effective interface gaps of type-II heterostructures (in units of eV).

	ΔE_v^{nat}	ΔE_c^{nat}	ΔE_g	$\Delta E_g^{i,av}$
$GaN/ZnGeN_2$	1.1	1.0	−0.1	2.4
$GaN/ZnSnN_2$	1.4	−0.3	−1.7	
ZnO/GaN	0.6	0.7	0.1	2.8
$ZnO/ZnGeN_2$	1.7	1.7	0.0	1.8
$ZnO/ZnSnN_2$	2.0	0.4	−1.6	1.4
$ZnGeN_2/ZnSnN_2$	0.3	−1.3	−1.6	

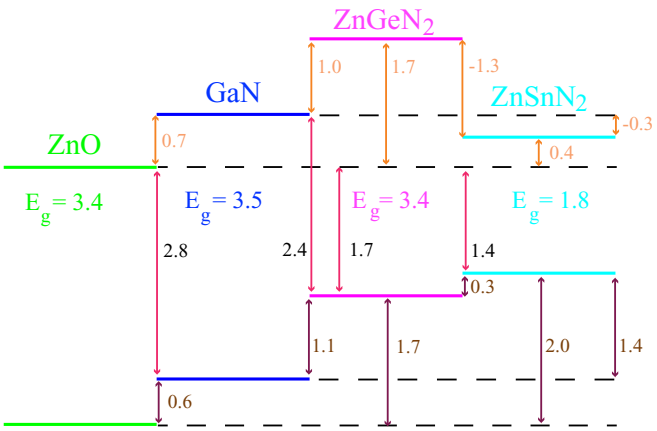

FIG. 4. Natural band-offset alignment of ZnO, GaN, $ZnGeN_2$, and $ZnSnN_2$ and their effective interface gaps (in eV).

[1] A. Punya, W. R. L. Lambrecht, and M. van Schilfgaarde, Phys. Rev. B **84**, 165204 (2011).

