Erratum: First-principles study of the phonon replicas in the photoluminescence spectrum of 4H-SiC [Phys. Rev. B **101**, 045203 (2020)]

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An inconsistency in the symmetry labeling of phonons and energy bands in the original paper was brought to our attention by Professor R. P. Devaty and W. M. Klahold (Department of Physics and Astronomy, University of Pittsburgh). Although the symmetry labeling of electronic energy bands was consistent with Ivanov *et al.* [1], in the phonon labeling, the mirror planes σ_v and $\sigma_{v'}$ had inadvertently been interchanged, which interchanges M_2 and M_4 irreducible representations. σ_v and $\sigma_{v'}$ can be distinguished, regardless of the choice of the Cartesian axes choice, by $\sigma_{v'}$ being an ordinary mirror plane and σ_v being a glide mirror plane with translation by $\mathbf{c}/2$. Since, in the paper, we had chosen M_4 to correspond to x and M_2 to y , the σ_v plane is the yz plane and $\sigma_{v'}$ is the xz plane.

Hence, the following changes need to be made in the paper. (1) At the end of Sec. III A in the sentence, “They define the symmetry labeling: M_1 and M_2 states are even under σ_v on the xz plane whereas M_3 and M_4 are odd,” xz should be replaced by yz . (2) In Fig. 2, σ_v and $\sigma_{v'}$ must be interchanged. (3) To be consistent with this figure, Eq. (9) should be corrected to

$$\mathbf{a}_1 = a \left(\frac{\sqrt{3}}{2}, -\frac{1}{2}, 0 \right), \quad \mathbf{a}_2 = a(0, 1, 0), \quad \mathbf{a}_3 = c(0, 0, 1).$$

(4) In Tables III and V, the labels M_2 and M_4 should be interchanged so that there are four M_2 and eight M_4 phonon modes.

Note however, that the symmetry labeling of the electron energy bands in Table II is correct. Thus, the conduction-band minimum, indeed, has symmetry M_4 . The discussion on p. 6 in Sec. III E also stays correct. Since the experimental spectra for $\mathbf{E} \parallel \mathbf{c}$ correspond to M_1 and M_3 modes, and for $\mathbf{E} \perp \mathbf{c}$ corresponding to M_2 and M_4 , the interpretation of the spectra remains unchanged.

Apart from this symmetry labeling issue, we also wish to correct here the reported quasiparticle-self-consistent *GW* or *QSGW* (G stands for the Green’s function and W for the screened Coulomb interaction) band structure results of Table II [2,3]. The main conclusion drawn from this calculation was that the phonon-replica spectra are insensitive to the band-gap correction of the *GW* method compared to density functional theory (DFT) in the local density approximation (LDA). Both these calculations used the same relaxed crystal structure. However, although adequate for the purposes of the paper, it turns out that some small splittings in the band structure are very sensitive to the crystal structure and to convergence parameters of the *QSGW* calculation. In particular, the crystal-field splitting, i.e., the splitting between the topmost Γ_5 valence-band maximum and the next Γ_1 band below was given in Table II to be only 4 meV, which was inconsistent with previous calculations in literature [4,5] and with the DFT results in Table II.

Repeating this calculation with experimental lattice constants as quoted in Ref. [5], $a = 3.073 \text{ \AA}$, $c/a = 3.271$, and relaxing all atomic positions until the forces were smaller than $2 \text{ meV}/a_0$ with a_0 as the Bohr radius using the all-electron full-potential linearized muffin-tin orbital method using the *questaal* codes available in Ref. [6] and fully described in Ref. [7], we obtain a crystal-field splitting of 46.2 meV in the generalized gradient approximation (GGA) to DFT [8], consistent with the DFT results listed in the paper obtained from the *ABINIT* code and within 0.03 eV of previous DFT calculations [4,5]. The crystal structure obtained in this way gives reduced coordinates in very close agreement with those of Käckel *et al.* [9] and Bauer *et al.* [10]. The only parameters in the structure not specified by symmetry are the reduced coordinates in the $\mathbf{c}$ direction, which, are for Si_2 (cubic site) $\frac{1}{4} + \delta$ for C_1 (hexagonal site) $\frac{3}{16} + \epsilon_1$, and for C_2 (cubic site) $\frac{7}{16} + \epsilon_2$ when the hexagonal site Si_1 is chosen at the origin. Our values for these parameters are $\delta = -0.6 \times 10^{-4}$, $\epsilon_1 = 5.8 \times 10^{-4}$, and $\epsilon_2 = -0.7 \times 10^{-4}$, whereas those of Käckel *et al.* [9] are $\delta = -2.1 \times 10^{-4}$, $\epsilon_1 = 4.810^{-4}$, and $\epsilon_2 = -2.3 \times 10^{-4}$ and those of Bauer *et al.* [10] are $\delta = -0.2 \times 10^{-4}$, $\epsilon_1 = 6.0 \times 10^{-4}$, and $\epsilon_2 = -0.8 \times 10^{-4}$. These are there shown to be in excellent agreement with high-precision measurements of the structure [10,11]. This also implies an axial bond length for the hexagonal site of 1.890 Å, slightly higher than for the cubic site 1.885 Å, in excellent agreement with experiment.

Using this same structure, the *QSGW* calculations are now performed using a double *spdf-spd* basis set with smoothed Hankel function energies κ^2 and smoothing radii R_{sm} , optimized for *GW* calculations, approximating the self-energy matrix Σ above a cutoff energy of 2.5 Ry by its diagonal average value calculated up to 3 Ry and using a $6 \times 6 \times 2$ $\mathbf{k}$ -point set. In contrast, the calculation in the original paper used a $4 \times 4 \times 2$ set, a cutoff of only 2 Ry, and only the *spd-spd* basis set, even though the

TABLE I. Corrected 0.8Σ QSGW energy levels at Γ and M (in eV) with symmetry labels.

QSGW	Sym	QSGW	Sym
-16.251	Γ_1	-12.684	M_1
-15.051	Γ_4	-12.110	M_4
-14.940	Γ_4	-11.910	M_4
-12.517	Γ_1	-11.127	M_1
-9.150	Γ_1	-9.064	M_4
-4.762	Γ_4	-8.787	M_1
-4.668	Γ_4	-7.483	M_1
-1.317	Γ_5	-7.087	M_4
		-5.293	M_1
-0.818	Γ_6	-4.406	M_4
		-3.567	M_2
-0.638	Γ_6	-2.657	M_3
		-2.556	M_3
-0.045	Γ_1	-2.441	M_4
0.000	Γ_5	-1.705	M_1
		-1.233	M_2
6.276	Γ_1	3.133	M_4
6.901	Γ_4	3.286	M_1
7.506	Γ_4	5.335	M_4
7.550	Γ_1	5.885	M_1
8.278	Γ_5	6.497	M_4
		6.984	M_1
8.297	Γ_6	8.476	M_2
		8.914	M_1
8.744	Γ_1	10.187	M_4
9.411	Γ_5	11.681	M_4
		11.829	M_1
9.710	Γ_6	11.870	M_3
		11.970	M_3
10.293	Γ_4	13.294	M_4
10.987	Γ_4	13.440	M_1
12.305	Γ_1	15.612	M_2
13.661	Γ_5	15.693	M_4
		16.342	M_1
14.529	Γ_6	16.784	M_1
		18.364	M_1
15.565	Γ_4	18.433	M_4
16.050	Γ_1	18.685	M_2
17.315	Γ_6	19.121	M_3
		19.274	M_3

text of the original paper stated the basis set used was *spdf-spd*. The gap, as usual in QSGW, is, then, slightly overestimated at 3.35 eV because of the underestimate of the screening of W by neglecting electron-hole interaction diagrams. As explained in Bhandari *et al.* [12], this can usually be remedied by applying only 80% of the self-energy correction to the exchange-correlation energy $\Sigma - v_{xc}^{LDA}$. In this 0.8Σ approach, the gap becomes 3.13 eV. Both full QSGW and 0.8Σ are within ~ 0.1 eV from the experimental value of 3.26 eV. The crystal-field splitting, Γ_5 - Γ_1 becomes 44.9 meV in 0.8Σ and 42.2 meV in full QSGW. Thus, we conclude that the crystal-field splitting is 43.5 ± 1.5 meV. This is slightly reduced from the GGA calculation because the lowest conduction band at Γ has the same symmetry as the crystal-field splitoff band (Γ_1) and their interaction is, thus, reduced by the GW increase in gap.

To compare this value with experiment, we add that the inclusion of spin-orbit coupling splits the Γ_5 into Γ_9 and Γ_7 , and Γ_1 becomes Γ_7 in the double group notation. We find a splitting of the Γ_9 - Γ_{7+} of 8.2 meV and Γ_9 - Γ_{7-} of 49.0 meV, where $\Gamma_{7\pm}$ are the upper and lower Γ_7 levels. Using the theory of invariants [13] for hexagonal crystals, one can describe this in terms of

$$\begin{aligned}\Gamma_9 &= \Delta_1 + \Delta_2, \\ \Gamma_{7\pm} &= \frac{\Delta_1 - \Delta_2}{2} \pm \sqrt{\left(\frac{\Delta_1 - \Delta_2}{2}\right)^2 + 2\Delta_3^2}.\end{aligned}\quad (1)$$

In the present case, and using the 0.8Σ results we find $\Delta_3 \approx 0$, $\Delta_2 = 4.1$, and $\Delta_1 = 44.9$ meV.

Another splitting of interest to optical absorption spectra is the splitting between the lowest conduction-band M_4 and the second conduction-band M_1 . We, here, find a value of 152.4 meV without and 151.0 meV including spin-orbit coupling. This value has been measured by ballistic electron emission microscopy (BEEM) by Im *et al.* [14] to be 0.14 eV and by differential absorption spectroscopy 144 ± 2 meV [15], recently revised to be 136 ± 3 meV [16].

The QSGW levels in Table II in the original paper differ from our new calculation by ~ 0.2 eV but since even the difference between QSGW and LDA bands did not significantly change the relevant results in Fig. 6, this will not change any major conclusions of the paper. For completeness, we, here, provide corrected values for the Γ - and M -point energy band levels in the 0.8Σ QSGW approximation in Table I.

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