Erratum: Electronic structure of layered quaternary chalcogenide materials for band-gap engineering: The example of $\text{Cs}_2\text{M}^{\text{II}}\text{M}_3^{\text{IV}}\text{Q}_8$ [Phys. Rev. B **93**, 165205 (2016)]

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In band-structure plots such as the one shown in the figure here, the energies corresponding to a particular set of $\mathbf{k}$ points along specific lines in the three-dimensional first Brillouin zone are obtained and the dispersion relations $E(\mathbf{k})$ of each band are then represented in a two-dimensional figure, where the distances between consecutive $\mathbf{k}$ points provide the scaling along the x axis. The electronic band structures shown in Fig. 7 of our original paper were plotted using fractional coordinates to calculate the distances between two consecutive $\mathbf{k}$ points, instead of Cartesian coordinates in the reciprocal space, and hence the differences among the a_0 , b_0 , and c_0 lattice parameters (orthorhombic unit cell) are not properly taken into account. Therefore, due to the use of incorrect coordinates, the curvature of the bands is not correctly represented because of the wrong scaling in the distance between the $\mathbf{k}$ points. The differences between the corrected figure, shown here, and the original figure are minor, which can be related to the orthogonality of the reciprocal space basis vectors for the orthorhombic lattice. The same mistake affected the band-structure plots shown in the Supplemental Material of the original paper, and corrected figures are provided in a new Supplemental Material. The discussion and conclusions of the paper are not affected by the present problem.

FIG. 7. DFT-PBE band structures of the $\text{Cs}_2\text{CdGe}_3\text{Q}_8$ compounds for $\text{Q} = \text{S}, \text{Se}, \text{and Te}$ in the orthorhombic crystal structure. The top of the valence band is shifted to zero energy.