Erratum: Electronic and optical properties of two-dimensional InSe from a DFT-parametrized tight-binding model [Phys. Rev. B **94**, 245431 (2016)]

S. J. Magorrian, V. Zólyomi, and V. I. Fal'ko
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I. SPIN-ORBIT COUPLING

In the published paper we analyzed selection rules and the polarization of photons for optical interband transitions neglecting spin-orbit coupling (SOC). In the absence of SOC the electron-spin orientation is preserved in the transition between the valence and the conduction bands (v and c , respectively). Emission of in-plane polarized light therefore requires a difference in orbital angular momentum $\Delta L_z = \pm 1$ between the initial and the final states, which is impossible between c and v since they are nondegenerate at the Γ point in InSe. Atomic SOC, $\mathbf{L} \cdot \mathbf{s}$, opens a spin-flip channel for the interband optical transitions, allowing angular momentum ± 1 to be transferred to the photon by an electron spin flip. The interaction with in-plane $\sigma^\pm$ -polarized light can be described using $\delta H = \frac{e}{cm_e} \lambda_{\text{SO}} (s^+ \mathbf{A}^- + s^- \mathbf{A}^+)$, applied to Eq. (28), where $\mathbf{A}^\pm = A(\hat{\mathbf{x}} \pm i\hat{\mathbf{y}})/\sqrt{2}$ corresponds to $\sigma^\pm$ -polarized light, and $s^{+(-)}$ is the spin angular momentum raising (lowering) operator.

We evaluated the coupling constant $\lambda_{\text{SO}}^{cv} \simeq 0.55 \hbar/\text{\AA}$ in the monolayer for the $c \rightarrow v$ transition across the principal band gap by examining the changes in the DFT bands at Γ induced by SOC due to the admixture of $p_{x,y}$ orbitals to the p_z -dominated valence band. λ_{SO}^{cv} has a nonzero value due to the opposite symmetry of c - and v -band states under σ_h reflection in the monolayer, so the coupling δH is invariant with respect to the symmetry group D_{3h} of the crystal. In the stoichiometric monolayer In_2Se_2 this gives an absorption coefficient of 2.8% for in-plane polarized light incident perpendicular to the two-dimensional crystal. In few-layer InSe the effect of SOC on the band-edge states is weaker than in the monolayer, so λ_{SO}^{cv} and the absorption coefficient for the spin-flip transition will be smaller than in the monolayer.

II. CORRECTION TO EQ. (28)

The off-diagonal matrix elements between H_c and H_{v_1} in Eq. (28) arising from the coupling of the transition between these bands to in-plane polarized light should read $\frac{\beta_N e}{cm_e} A$ since β_N has units of $\hbar/\text{\AA}$, in contrast to the matrix element between c and v where we use the linearity in $\mathbf{k}$ to express the matrix element with α_N as a dimensionless constant.

III. CORRECTION TO EQ. (31)

The effective masses given in Eq. (31) are hole effective masses and are therefore $m = -0.31$ and $m' = -0.45$ in band v_1 and $m = -0.30$ and $m' = -0.45$ in band v_2 in units of m_e .

IV. CORRECTIONS TO APPENDIX A

In Appendix A Sec. 2b (M - X off-diagonal elements) the matrix element $H_{M_{py}, X_{py}}^{(\pm)}$ should be

$$H_{M_{py}, X_{py}}^{(\pm)} = f_1 (T_\pi^{(1)} \pm T_\pi'^{(2)}) - \frac{f_5 a^2}{12} \left[\frac{T_\pi^{(1)} + T_\sigma^{(1)}}{L_1^2} \pm \frac{T_\pi'^{(2)} + T_\sigma'^{(2)}}{L_2^2} \right] + f_{12} T_\pi^{(3)} - \left[\frac{f_{16} a^2}{3 L_4^2} (T_\pi^{(3)} + T_\sigma^{(3)}) \right]$$

(note the division by 3 in the final term). In the first six equations of Appendix A Sec. 2c (M - M , X - X off-diagonal elements) $T_{sp}^{(3)}$ should be replaced by $T_{sp}'^{(3)}$, $T_\pi^{(3)}$ by $T_\pi'^{(3)}$, and $T_\sigma^{(3)}$ by $T_\sigma'^{(3)}$. $H_{M_{px}, M_{py}}^{(\pm)}$ should be corrected further to read

$$H_{M_{px}, M_{py}}^{(\pm)} = -\frac{f_9 \sqrt{3}}{4} \left[T_\pi^{(2M)} + T_\sigma^{(2M)} \pm \frac{a^2}{L_3^2} (T_\pi'^{(3)} + T_\sigma'^{(3)}) \right],$$

and $H_{M_{py}, M_{pz}}^{(\pm)}$ should read

$$H_{M_{py}, M_{pz}}^{(\pm)} = \mp \frac{f_{11} \sqrt{3} d_{MM} a}{2 L_3^2} [T_\pi'^{(3)} + T_\sigma'^{(3)}].$$

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