# Electronic Supplementary Information for "Topological bands in $PdSe_2$ pentagonal monolayer"

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## A. Topological invariant extraction from the symmetry indicators of space group #14

In this section we follow Ref. [1] applying the expressions for the particular case of 2D space group (SG) #14. The Smith normal form presented in main text can be decomposed as

$$\Delta = L \cdot EBR \cdot R. \tag{S.1}$$

Here $EBR$ is the matrix of the elementary band representations (EBR). L and R are unimodular matrices that can be obtained from the numerical computation of $\Delta$. Choosing a particular ordering of the irreducible representations (IR) in the EBR we have the $EBR'$ matrix

$$EBR' = \begin{bmatrix} 2 & 2 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 2 & 2 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}. \tag{S.2}$$

This particular choice renders all the elements in the $\Delta$ matrix positive. Next a general band representation is defined by a vector $B$ that comprises the multiplicities of the IR of the set of bands of interest, such that

$$B = \begin{bmatrix} n_{\Gamma_3\Gamma_4} \\ n_{D_3} \\ n_{\Gamma_5\Gamma_6} \\ n_{D_4} \\ n_{D_5} \\ n_{D_6} \\ n_{Z_2} \\ n_{B_2} \end{bmatrix}. \tag{S.3}$$

The topological information of the bands is encoded in the vector (eq.(6) in [1])

$$C = L \cdot B. \tag{S.4}$$

In the case of SG #14, for the particular $EBR'$ matrix presented above we obtain for the L matrix

$$L = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & -2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 & -1 & 0 & 1 & 0 \end{bmatrix}. \tag{S.5}$$

Thereby, the C vector is given by

$$C = \begin{bmatrix} n_{D_5} \\ n_{D_3} \\ n_{\Gamma_5\Gamma_6} \\ -n_{D_3} + n_{D_4} \\ n_{\Gamma_3\Gamma_4} - 2n_{D_3} + n_{\Gamma_5\Gamma_6} - 2n_{D_5} \\ -n_{D_5} + n_{D_6} \\ -n_{D_3} - n_{D_5} \\ -n_{D_3} - n_{D_5} \end{bmatrix}. \tag{S.6}$$

Additionally we set $r$ as the range of the $EBR'$ matrix, that is $r = 3$. The component $C_r$ of vector $C$ yields the definition of the topological index as stated by eq. (8) in [1]. For our case this results in the relation

$$\mathbb{Z}_2 = n_{\Gamma_5\Gamma_6} \pmod 2, \tag{S.7}$$

which defines the topological invariant only in terms of the multiplicities of the $\Gamma$ point IR (An equivalent result holds for the other IR, $\Gamma_3\Gamma_4$, by choosing

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a different ordering in the EBR matrix). A complementary result: using the components $C_i$ and imposing the condition $C_i = 0$ for $i > r$ allows to construct the compatibility relations for the particular band representation.

## B. Spin Hall conductivity formula

The optical spin Hall conductivity, is calculated with the Kubo-Greenwood formula [2]

$$\sigma^{\gamma}_{\alpha\beta}(\omega) = \frac{\hbar}{V_c N_{\mathbf{k}}} \sum_{\mathbf{k}} \sum_{n} f_{n\mathbf{k}} \sum_{m \neq n} \frac{\mathrm{Im}\left[\langle n\mathbf{k}| \hat{j}^{\gamma}_{\alpha} |m\mathbf{k}\rangle \langle m\mathbf{k}| - e\hat{v}_{\beta} |n\mathbf{k}\rangle\right]}{(\epsilon_{n\mathbf{k}} - \epsilon_{m\mathbf{k}})^2 - (\hbar\omega - i\eta)^2}. \tag{S.8}$$

Here $\hat{j}^{\gamma}_{\alpha} = \frac{1}{2}\{\hat{s}_{\gamma}, \hat{v}_{\alpha}\}$ is the spin current operator with the spin operator $\hat{s}_{\gamma}$ defined as $\hat{s}_{\gamma} = \frac{\hbar}{2}\hat{\sigma}_{\gamma}$ with $\hat{\sigma}_{\gamma}$ as Pauli matrices. Indices $\alpha$, $\beta$ represent Cartesian coordinates and $\gamma$ appoints for the direction of spin (typically $z$-direction). $V_c$ is the cell volume and $N_k$ is the number of sampled points in reciprocal space. Finally, $f_{n\mathbf{k}}$ denotes the Fermi-Dirac distribution and $\hbar\omega$ corresponds to the external perturbation frequency. The static case is calculated by taking the limit $\omega \to 0$ in the above formula.

## C. Additional figures

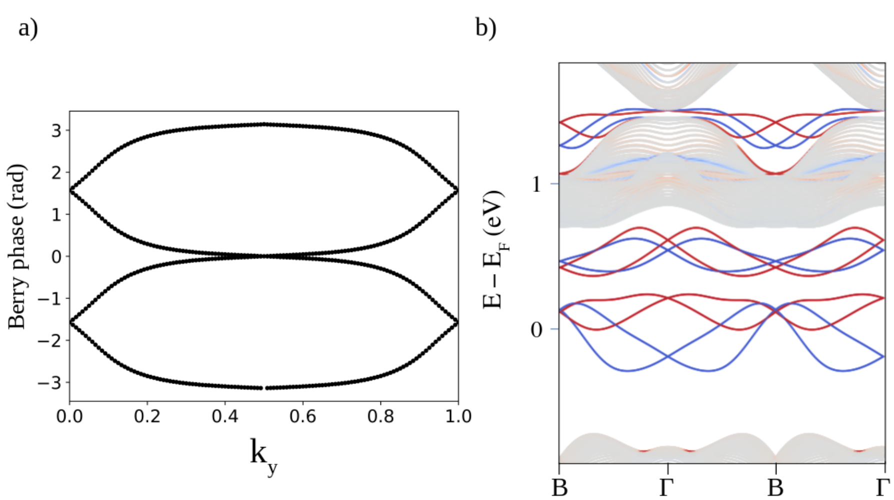


Figure S.1: a) Evolution of the Wannier charge center (Wilson loop) along the $k_y$ direction. b) Energy dispersion of the ribbons for the Wannier interpolated 12B model for a cut along the $y$ direction in real space. Red-colored and blue-colored bands represent states that are localized at the upper and lower edges of the ribbon, respectively.

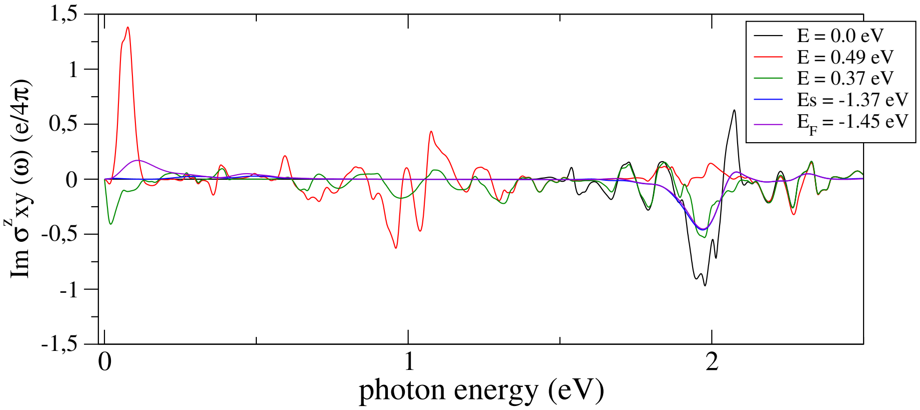


Figure S.2: Imaginary part of the spin Hall conductivity $\sigma^z_{xy}$ as a function of external photon energy for different values of the chemical potential.

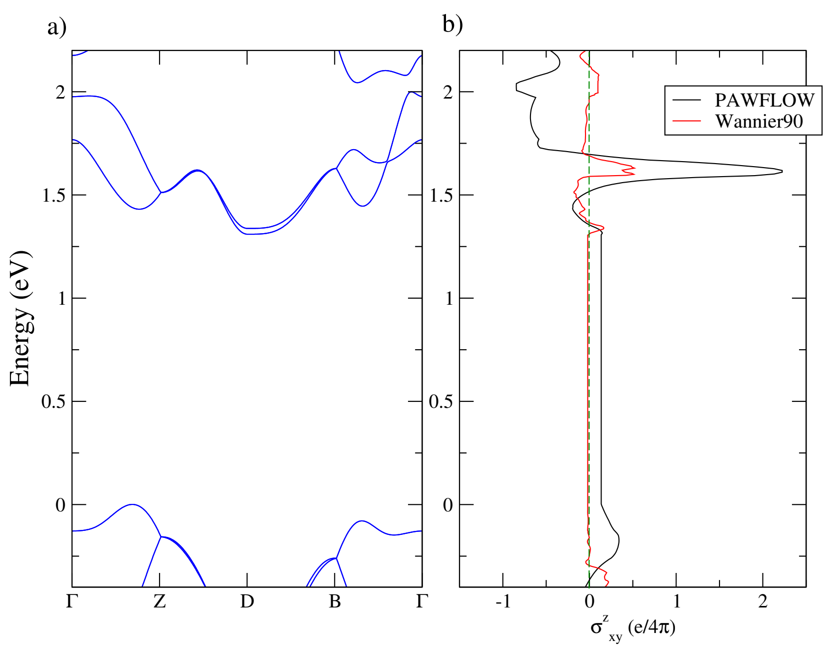


Figure S.3: a) Electronic bands of monolayer $PdSe_2$ from the PAWFLOW code. b) Static spin Hall conductivity $\sigma^z_{xy}$ as a function of the Fermi level for two different codes.

# References

[1] Luis Elcoro, Zhida Song, and B. Andrei Bernevig. Application of induction procedure and Smith decomposition in calculation and topological classification of electronic band structures in the 230 space groups. *Phys. Rev. B*, 102:035110, Jul 2020.

[2] Junfeng Qiao, Jiaqi Zhou, Zhe Yuan, and Weisheng Zhao. Calculation of intrinsic spin Hall conductivity by Wannier interpolation. *Phys. Rev. B*, 98:214402, Dec 2018.