# Supporting Information for "Hidden Zeeman-type spin polarization in bulk crystals"

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## I. DETAILS OF FIRST-PRINCIPLES CALCULATIONS

Our first-principle calculations were performed by using Vienna *ab-initio* simulation package (VASP)[1,2] within the framework of the projector augmented wave (PAW) method[3]. The generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE)[4] realization was employed for the exchange-correlation potential. The structures were fully optimized until the energy and force converged to less than $10^{-5}$ eV and $10^{-2}$ eV/$\mathring{A}$, respectively. The plane-wave energy cutoff was set to be 350 and 520 eV for $WSe_2$ and $BaBi_4O_7$, respectively. Van der Waals interaction is considered by using the approach of Dion et al[5] in the structural optimization of $WSe_2$. The Brillouin zone (BZ) integration was carried out on a Γ-centered Monkhorst-Pack grid with sizes of 21×21×5 and 9×9×7 for $WSe_2$ and $BaBi_4O_7$, respectively. The optimized lattice constants are $a = b = 3.297$, $c = 13.095$ $\mathring{A}$ for $WSe_2$ and $a = b = 7.818$, $c = 13.574$ $\mathring{A}$ for $BaBi_4O_7$. The spin polarization was evaluated by summing the projection of the calculated wavefunction $|\psi_k\rangle$ on the spin and orbital basis of each atomic site $|C_{i,l,m,\eta}|^2 = \langle\psi_k|(\frac{\hbar}{2}\sigma_\eta \otimes |l,m\rangle_{ii}\langle l,m|)|\psi_k\rangle$ in a given sector.

## II. HIDDEN ZEEMAN-TYPE SPIN POLARIZATION FOR $WSe_2$

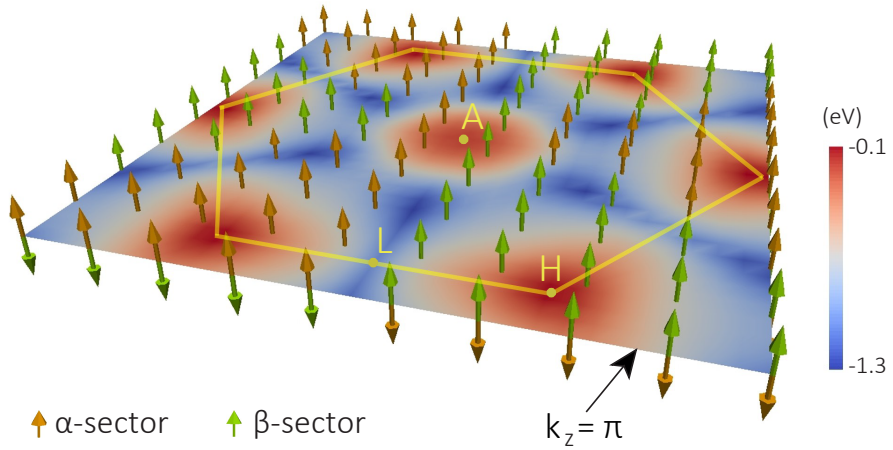


FIG. 1: The calculated local spin polarization for the highest occupied valence band in $WSe_2$ at $k_z = \pi$. One observes that the twofold degenerate band states on the whole BZ plane have opposite spin polarizations pointing exactly to the $\pm z$-direction and remain independent of the momentum, demonstrating a hidden Zeeman-type spin polarization as proposed in the main text.

## III. BAND STRUCTURE WITHOUT CONSIDERING SOC FOR $BaBi_4O_7$

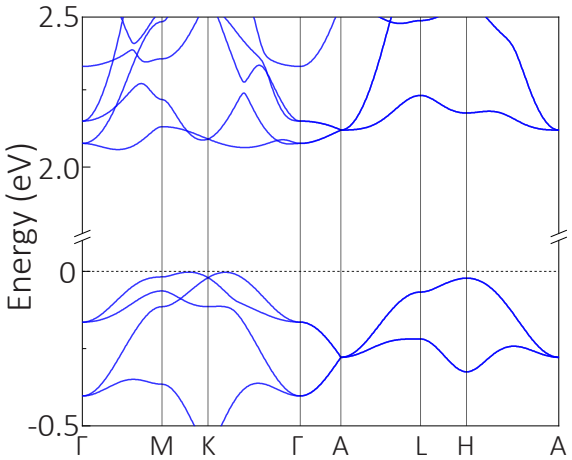


FIG. 2: The calculated band structure of $BaBi_4O_7$ in the absence of SOC.

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