Supporting Information

Bloch-type magnetic skyrmions in two-dimensional lattice

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**Note 1**: Calculation details of magnetic parameters in spin Hamiltonian

The magnetic parameters are obtained from DFT calculations. The DMI vector $D_{ij}$ for the nearest-neighboring Mn atoms can be expressed as $D_{ij} = d_\parallel u_{ij} + d_\perp z$ with $u_{ij}$ representing the unit vector pointing from site $i$ to $j$ and $z$ being the out-of-plane unit vector. To obtain the in-plane component $d_\parallel$, the left- and right-hand spin-spiral configurations are considered, as shown in Fig. 2(a). The energy of two spin configurations represented by $E_L$ and $E_R$ can be written as:

$$E_L = E_0 - \frac{3}{2}d_\parallel |S|^2 \times 4$$
$$E_R = E_0 + \frac{3}{2}d_\parallel |S|^2 \times 4$$

As a result, the in-plane component $d_\parallel$ can be obtained by

$$d_\parallel = \frac{E_R - E_L}{12}.$$

To obtain $J$, $\lambda$ and $K_{MCA}$, we consider four different spin configurations as displayed in Fig. S4. The energy of these different spin configurations can be written as:

$$E_1 = E_0 - 6J|S|^2$$
$$E_2 = E_0 + 2J|S|^2$$
$$E_3 = E_0 - 6J|S|^2 - 6\lambda|S|^2 - 2K_{MCA}|S|^2$$
$$E_4 = E_0 + 2J|S|^2 + 2\lambda|S|^2 - 2K_{MCA}|S|^2$$

Here, $E_1$, $E_2$, $E_3$ and $E_4$ represents the energy of x-FM, x-AFM, z-FM, and z-AFM configurations, respectively. Based on the above formula, magnetic parameters $J$, $\lambda$ and $K_{MCA}$ can be obtained.
Fig. S1. Phonon spectra of monolayer (a) MnInP$_2$Te$_6$ and (b) MnTlP$_2$Te$_6$. It can be seen that only a tiny negative frequency is observed around the $\Gamma$ point, suggesting the dynamic stability of monolayer MnXP$_2$Te$_6$.

Fig. S2. Variations of total energies with time during the Ab initio molecular dynamics simulations for monolayer (a) MnInP$_2$Te$_6$ and (b) MnTlP$_2$Te$_6$ at 300 K and the corresponding snapshots taken from the end of the simulations. The slight free-energy fluctuations and well-defined structures indicate the thermal stability of monolayer MnXP$_2$Te$_6$.

Fig. S3. Spin charge densities of monolayer (a) MnInP$_2$Te$_6$ and (b) MnTlP$_2$Te$_6$. 
Fig. S4. Four different magnetic configurations used to obtain the magnetic parameters $J$, $\lambda$, and $K_{MCA}$ in monolayer MnXP$_2$Te$_6$.

Fig. S5. Average magnetization ($M$) per formula as a function of temperature ($T$) of monolayer (a) MnInP$_2$Te$_6$ and (b) MnTlP$_2$Te$_6$ from Monte-Carlo simulations.

Fig. S6. Spin-polarized band structures of monolayer (a) MnInP$_2$Te$_6$ and (b) MnTlP$_2$Te$_6$ with SOC. The red and blue lines in (a, b) correspond to spin-up and spin-down states, respectively. The Fermi level is set to 0 eV.
Fig. S7. Spin texture of monolayer MnTlP$_2$Te$_6$ under in-plane magnetic field of 19 mT. It is superimposed by in-plane cycloidal structure and small out-of-plane waved spin pattern.

![Image](image_url)

Fig. S8. Magnetic anisotropy energy (MAE) per unit cell of monolayer MnXP$_2$Te$_6$ as a function of strain. MAE is defined as the energy difference between the systems with magnetization axis along in-plane ($E_{\text{in-plane}}$) and out-of-plane ($E_{\text{out-of-plane}}$) directions.

![Image](image_url)

Table S1. Lattice constant $a$ (Å), magnetic parameters [exchange coupling $J$ (in meV), anisotropic symmetric exchange $\lambda$ (in meV), magnetocrystalline anisotropy $K_{MCA}$ (in meV), magnetic shape anisotropy $K_{MSA}$ (in meV), single ion anisotropy $K$ (in meV), in-plane DMI $d_{\parallel}$ (in meV)] and magnetic moment $m$ ($\mu_B$) on Mn atom for monolayer MnXP$_2$Te$_6$.

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<thead>
<tr>
<th></th>
<th>$a$</th>
<th>$J$</th>
<th>$\lambda$</th>
<th>$K_{MCA}$</th>
<th>$K_{MSA}$</th>
<th>$K$</th>
<th>$d_{\parallel}$</th>
<th>$m$</th>
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<tbody>
<tr>
<td>MnInP$_2$Te$_6$</td>
<td>7.13</td>
<td>10.108</td>
<td>-0.048</td>
<td>1.015</td>
<td>-0.026</td>
<td>0.989</td>
<td>2.873</td>
<td>4.191</td>
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<td>MnTlP$_2$Te$_6$</td>
<td>7.20</td>
<td>18.168</td>
<td>-0.955</td>
<td>-0.064</td>
<td>-0.025</td>
<td>-0.089</td>
<td>5.791</td>
<td>4.173</td>
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Table S2. Lattice constants $a$ (Å), magnetic parameters [exchange coupling $J$ (in meV), anisotropic symmetric exchange $\lambda$ (in meV), magnetocrystalline anisotropy $K_{MCA}$ (in meV), magnetic shape anisotropy $K_{MSA}$ (in meV), single ion anisotropy $K$ (in meV), in-plane DMI $d_{\parallel}$ (in meV)] and
magnetic moments $m$ ($\mu_B$) on Mn atom for monolayer MnInP$_2$Te$_6$ under various strains.

<table>
<thead>
<tr>
<th>MnInP$_2$Te$_6$</th>
<th>$a$</th>
<th>$J$</th>
<th>$\lambda$</th>
<th>$K_{MCA}$</th>
<th>$K_{MSA}$</th>
<th>$K$</th>
<th>$d_\parallel$</th>
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<td>2.873</td>
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Table S3. Lattice constants $a$ (Å), magnetic parameters [exchange coupling $J$ (in meV), anisotropic symmetric exchange $\lambda$ (in meV), magnetocrystalline anisotropy $K_{MCA}$ (in meV), magnetic shape anisotropy $K_{MSA}$ (in meV), single ion anisotropy $K$ (in meV), in-plane DMI $d_\parallel$ (in meV)] and magnetic moments $m$ ($\mu_B$) on Mn atom for monolayer MnTlP$_2$Te$_6$ under various strains.

<table>
<thead>
<tr>
<th>MnTlP$_2$Te$_6$</th>
<th>$a$</th>
<th>$J$</th>
<th>$\lambda$</th>
<th>$K_{MCA}$</th>
<th>$K_{MSA}$</th>
<th>$K$</th>
<th>$d_\parallel$</th>
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<td>-0.064</td>
<td>-0.025</td>
<td>-0.089</td>
<td>5.791</td>
<td>4.173</td>
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<tr>
<td>1%</td>
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