Supplementary Information (SI)

Hidden Spin-Valley-Locking Extends Room Temperature Spin Lifetime in 2D Perovskite Semiconductors

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A. Supplementary Tables.

Table S1. Crystal structure refinement parameters for $(AzF_2)_2PbI_4$.

Temperature (K)	298
Space group	*Pc*
a (Å)	25.6055(5)
b (Å)	8.8128(10)
c (Å)	25.9344(4)
α (°)	90
β (°)	110.232(2)
γ (°)	90
Density (g/cm^3)	3.277
μ (mm^{-1})	15.984
F(000)	4704
2Θ range for data collection (°)	3.186 to 61.536
Index ranges	$-36 \le h \le 35$, $-12 \le k \le 11$, $-35 \le l \le 31$
Reflections collected	120068
Independent reflections	27188 [R_{int} = 0.0370, R_{sigma} = 0.0341]
Data/ restraints/ parameters	27188/9/19
Goodness-of-fit on F^2	1.024
Final R indexes [I>=2σ (I)]	R_1 = 0.0362, wR_2 = 0.0771
Final R indexes [all data]	R_1 = 0.0499, wR_2 = 0.0808
Largest diff. peak/hole (e Å^{-3})	1.85/-0.930
Flack parameter	0.005(4)

Table S2. Pb – I octahedra distances in $(AzF_2)_2PbI_4$ at room temperature. Atomic positions corresponding to the atom indices are provided in section D.5.

Label of Pb atoms	Label of I atoms	Distance (Angstrom)
Pb1	I9	3.2047
Pb1	I13	3.1963
Pb1	I15	3.1756
Pb1	I19	3.1506
Pb1	I21	3.2063
Pb1	I29	3.2613
Pb3	I9	3.2099
Pb3	I11	3.2079
Pb3	I21	3.203
Pb3	I23	3.1615
Pb3	I25	3.198
Pb5	I7	3.2062
Pb5	I12	3.2312
Pb5	I13	3.1643
Pb5	I15	3.182
Pb5	I17	3.2057
Pb5	I27	3.2303
Pb31	I37	3.2032
Pb31	I43	3.2121
Pb31	I47	3.2052
Pb31	I51	3.2018
Pb31	I53	3.1428
Pb31	I55	3.2357
Pb33	I39	3.2329
Pb33	I41	3.1622
Pb33	I43	3.2181
Pb33	I49	3.1733
Pb33	I51	3.2428
Pb33	I59	3.181
Pb35	I38	3.2198
Pb35	I41	3.1867
Pb35	I45	3.1962
Pb35	I48	3.2195
Pb35	I49	3.1553
Pb35	I57	3.2308

Table S3. Pb – I – Pb bond angles in $(AzF_2)_2PbI_4$ at 298 K. Atomic positions corresponding to the atomic indices are provided in section D.5.

Pb – I – Pb angle (°)	**Atom indices**
148.605	(1, 9, 3)
142.804	(1, 13, 5)
159.173	(4, 12, 5)
148.407	(33, 43, 31)
159.734	(36, 47, 31)
147.293	(3, 18, 6)
159.772	(3, 21, 1)
144.598	(5, 15, 1)
148.561	(31, 37, 36)
159.069	(31, 51, 33)
143.149	(33, 49, 35)
142.799	(35, 41, 33)

Table S4. Crystal structure refinement parameters for $(AzOH)_2PbI_4$.

Temperature (K)	298	100
Space group	$P2_1/m$	$P2_1/m$
a (Å)	6.41330(10)	6.3733(2)
b (Å)	20.5227(5)	20.3267(5)
c (Å)	6.47590(10)	6.4050(2)
α (°)	90	90
β (°)	90.096(2)	90.112(2)
γ (°)	90	90
Density (g/cm^3)	3.363	3.454
μ (mm^{-1})	17.130	17.596
F(000)	752.0	752.0
2Θ range for data collection (°)	3.97 to 61.784	4.008 to 62.266
Index ranges	$-9 \le h \le 7$, $-26 \le k \le 27$, $-9 \le l \le 8$	$-8 \le h \le 9$, $-28 \le k \le 27$, $-9 \le l \le 8$
Reflections collected	19326	12454
Independent reflections	2391 [R_{int} = 0.0327, R_{sigma} = 0.0198]	2306 [R_{int} = 0.0338, R_{sigma} = 0.0237]
Data/ restraints/ parameters	2391/0/105	2306/0/105
Goodness-of-fit on F^2	1.027	1.039
Final R indexes [I>=2σ (I)]	R_1 = 0.0185, wR_2 = 0.0353	R_1 = 0.0168, wR_2 = 0.0333
Final R indexes [all data]	R_1 = 0.0232, wR_2 = 0.0364	R_1 = 0.0184, wR_2 = 0.0337
Largest diff. peak/hole (e $Å^{-3}$)	0.71/-0.93	0.77/-1.05

Table S5. Comparison of non-covalent interactions in A_2PbI_4 (A = EOA, AzOH, AzF_2) structures at room temperature. For A=EOA and AzOH, the I labels correspond to the three closest iodine atoms to the ammonium nitrogen; For A=AzF_2, atomic positions corresponding to the iodine indices are provided in section D.5.

Structure	N-H···X Interaction	I labels	d_{H-X} Distance (Å)	N-H···X Angle (degree)
$(EOA)_2PbI_4$	N-H···I	I1	2.86	139.55
		I2	2.92	178.09
		I3	3.13	123.59
	N-H···O	--	2.23	138.93
$(AzOH)_2PbI_4$	N-H···I	I1	3.16	127.45
		I2	3.21	141.23
		I3	3.23	110.98
	N-H···O	--	2.12	147.37
$(AzF_2)_2PbI_4$	N-H···I	I1	2.85	142.62
		I2	3.14	135.65
		I3	3.17	110.08
		I4	2.95	142.64
		I5	2.96	136.11
		I6	3.08	125.42
		I7	3.11	133.35
		I8	2.82	154.55
		I9	3.96	141.00
		I10	3.08	124.99
		I11	2.73	154.71
		I12	2.77	148.87

Table S6. Crystal structure refinement parameters for $(AzOH)_2SnI_4$.

Temperature (K)	298	100
Space group	$P2_1/m$	$P2_1/m$
a (Å)	6.3796(2)	6.33480(10)
b (Å)	20.4457(5)	20.2446(5)
c (Å)	6.47180(10)	6.40680(10)
α (°)	90	90
β (°)	90.576(2)	90.622(2)
γ (°)	90	90
Density (g/cm^3)	3.047	3.131
μ (mm^{-1})	8.817	9.059
F(000)	688.0	688.0
2Θ range for data collection (°)	3.984 to 61.908	4.024 to 61.824
Index ranges	$-7 \le h \le 9$, $-28 \le k \le 25$, $-8 \le l \le 8$	$-8 \le h \le 8$, $-28 \le k \le 26$, $-8 \le l \le 8$
Reflections collected	18951	18600
Independent reflections	2422 [R_{int} = 0.0345, R_{sigma} = 0.0180]	2317 [R_{int} = 0.0361, R_{sigma} = 0.0191]
Data/ restraints/ parameters	2422/0/105	2317/0/105
Goodness-of-fit on F^2	1.042	1.087
Final R indexes [I>=2σ (I)]	R_1 = 0.0219, wR_2 = 0.0479	R_1 = 0.0187, wR_2 = 0.0417
Final R indexes [all data]	R_1 = 0.0268, wR_2 = 0.0496	R_1 = 0.0209, wR_2 = 0.0424
Largest diff. peak/hole (e $Å^{-3}$)	0.82/-0.66	1.03/-0.73

Table S7. Spin lifetime in bulk semiconductors at or near room temperature.

Semiconductor	τ_s	Temperature (K)	Measurement method	Reference
GaAs	100 ps	300	Pump-probe optical spectroscopy	[1]
GaNAs	196 ps	300	Hanle fitting of PL with B_{ext} = 0.06 T	[2]
Cubic GaN	530 ps	300	Time resolved Kerr rotation at B_{ext} = 0.11 T	[3]
InSb (grown on GaAs)	2.5 ps	290	Circularly polarized pump-probe	[4]
$CsPbBr_3$	10 ps	300	Circularly-polarized photoinduced reflectivity at B_{ext} = 0.7 T	[5]
	3.7 ps	295	Circularly polarized pump-probe	[6]
$CsPbI_3$	1.3 ps			
$MAPbBr_3$	4.3 ps			
$MAPbI_3$	2.2 ps			

B. Supplementary Figures.

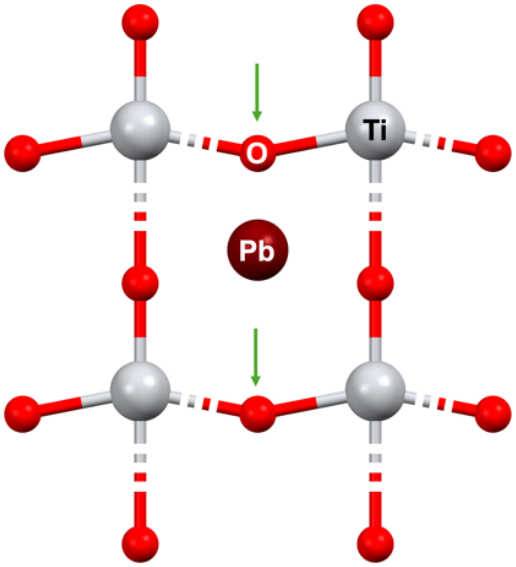

Figure S1. Polar distortions (green arrows show displacement of the Ti–O–Ti bond angle) in the tetragonal phase of $PbTiO_3$ (010 plane); the crystal structure is obtained from reference.[7]

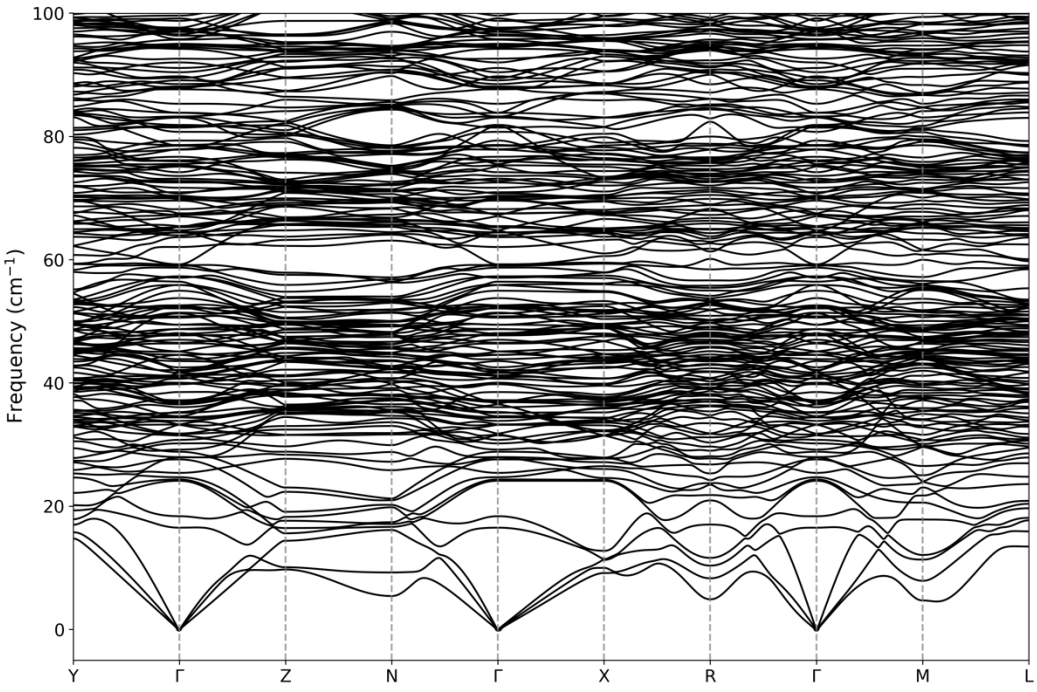

Figure S2. Simulated phonon band structure of $(AzOH)_2PbI_4$.

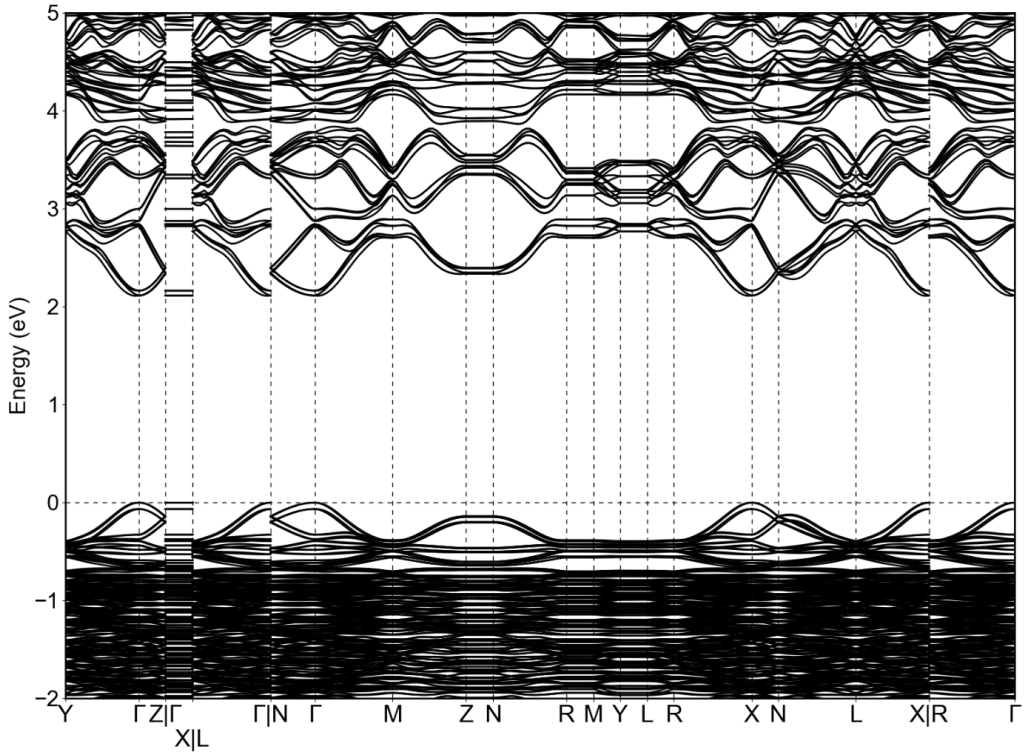

Figure S3. DFT-based HSE06 + SOC electronic band structure of $(AzF_2)_2PbI_4$.

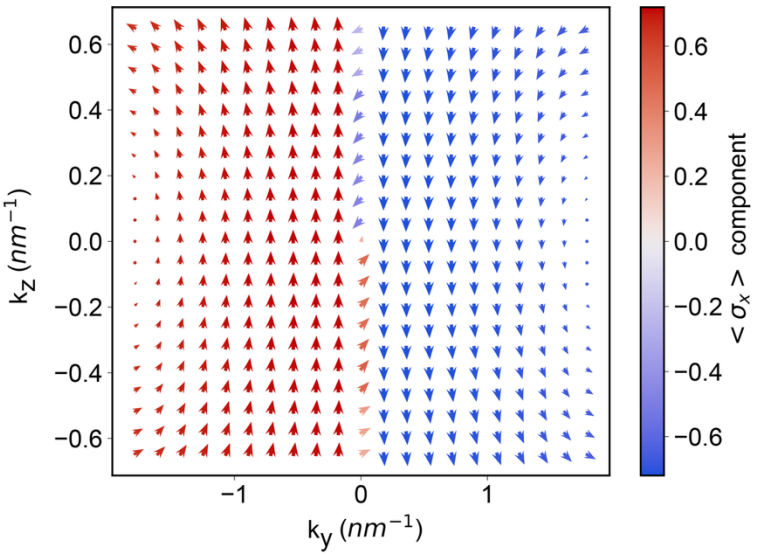

Figure S4. Two-dimensional spin texture plot of $(AzF_2)_2PbI_4$ for the conduction band minima on the k_y-k_z plane (parallel to the Pb – I layer), simulated with DFT (PBE + SOC).

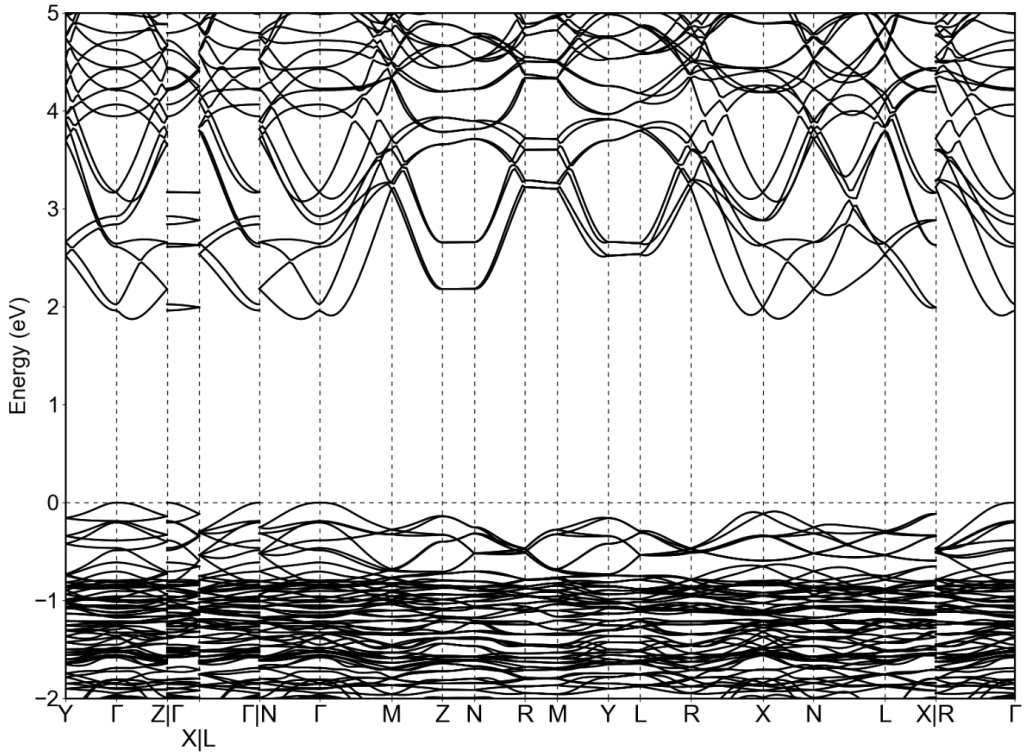

Figure S5. DFT-based HSE06 + SOC electronic band structure of $(AzOH)_2PbI_4$.

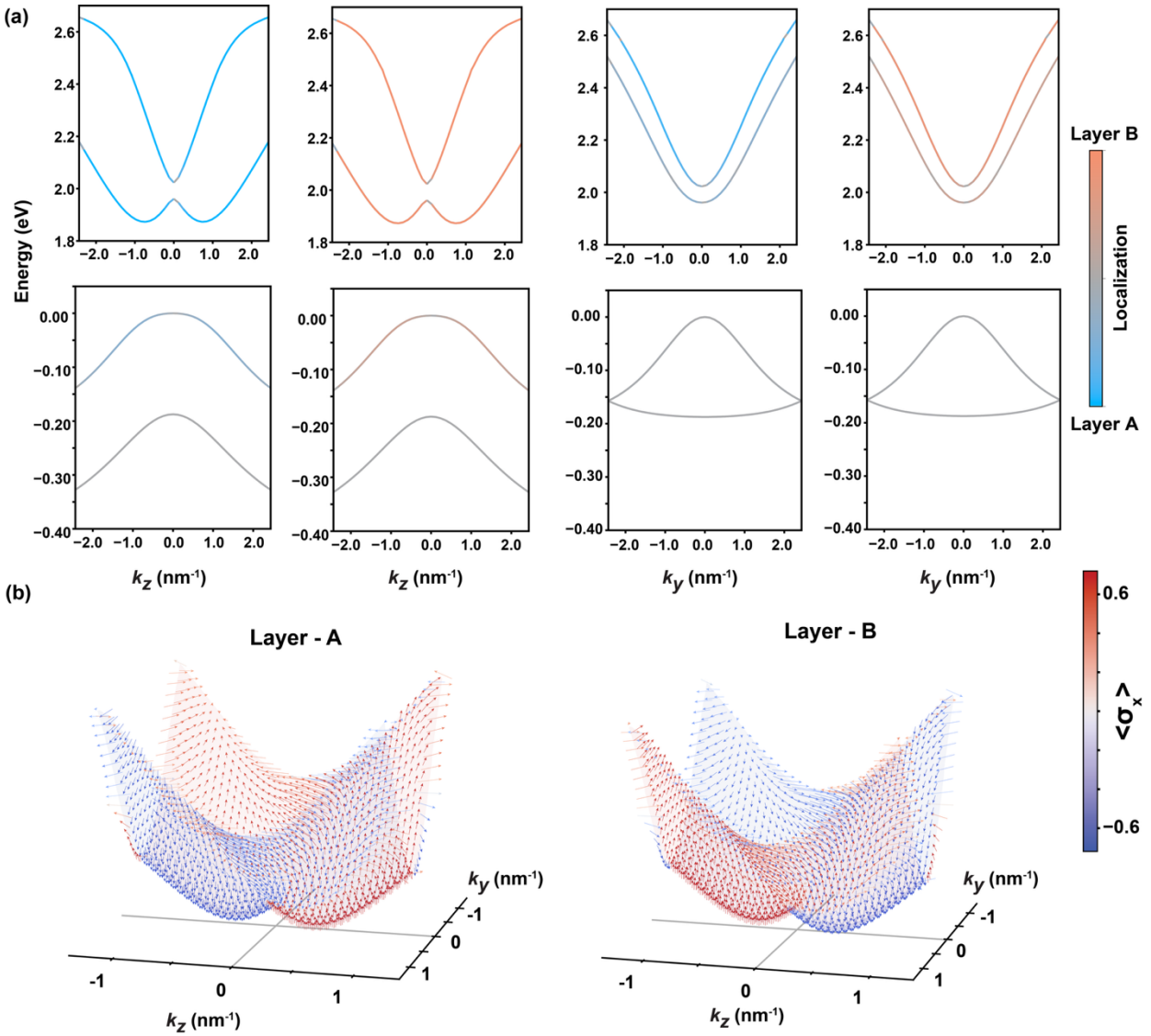

Figure S6. (a) Localization of the DFT (HSE06 + SOC)-derived electronic bands on two Pb – I layers and at the conduction (top panels) and valence (bottom panels) band edges in $(AzOH)_2PbI_4$, calculated using Mulliken analysis, following the method described in reference[8] ; (b) spin textures of the spin valleys at the conduction band minima on the $k_y - k_z$ plane in $(AzOH)_2PbI_4$, calculated using DFT (PBE + SOC); the left panel is reproduced in Figure 3c in the main text.

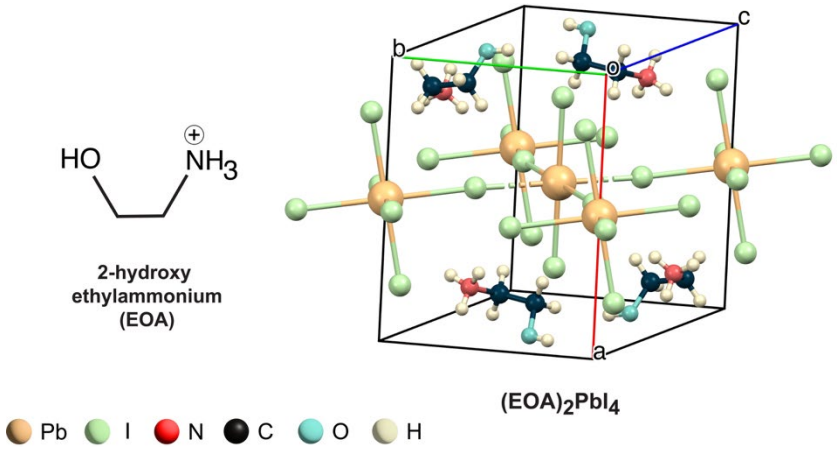

Figure S7. Schematic of the molecular structure of EOA (left) and the crystal structure of $(EOA)_2PbI_4$ (right) at room temperature. The crystal structure is obtained from reference[9].

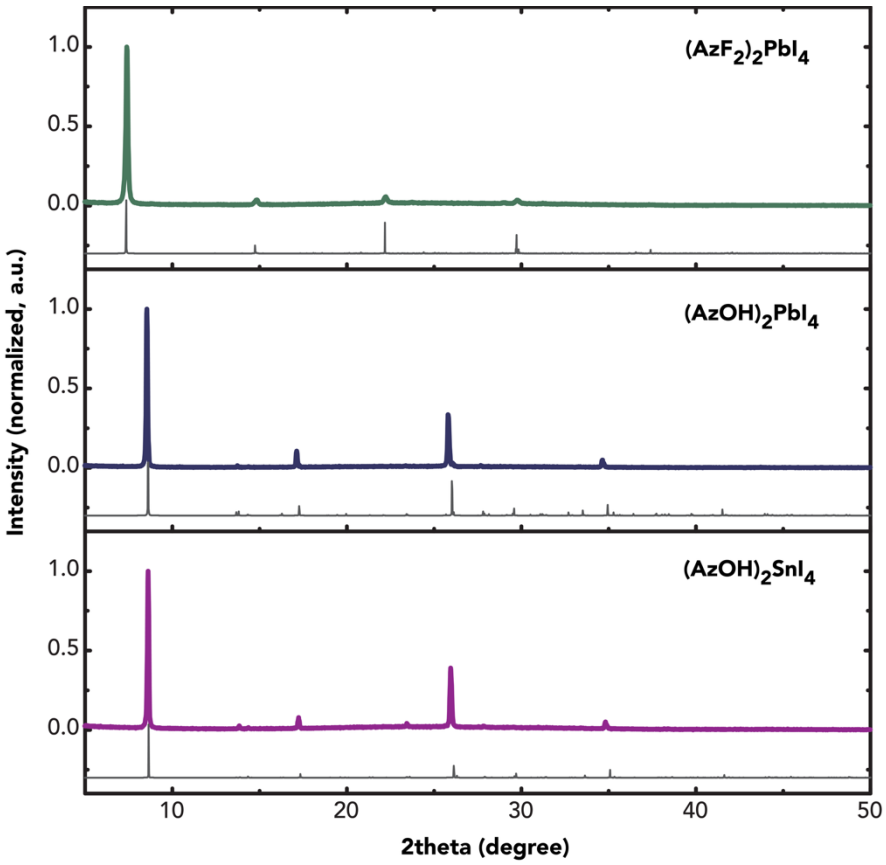

Figure S8. Powder X-ray diffraction (PXRD) profiles of 2D perovskite films with the azetidinium-based cations; the colored lines represent the experimental measurements at room temperature, while the grey lines are simulated from the corresponding room temperature single-crystal X-ray diffraction-derived structure with 50% orientational preference for the crystallographic directions (*100* for $(AzF_2)_2PbI_4$ or *010* for $(AzOH)_2PbI_4$ and $(AzOH)_2SnI_4$) perpendicular to the 2D Pb-I layers.

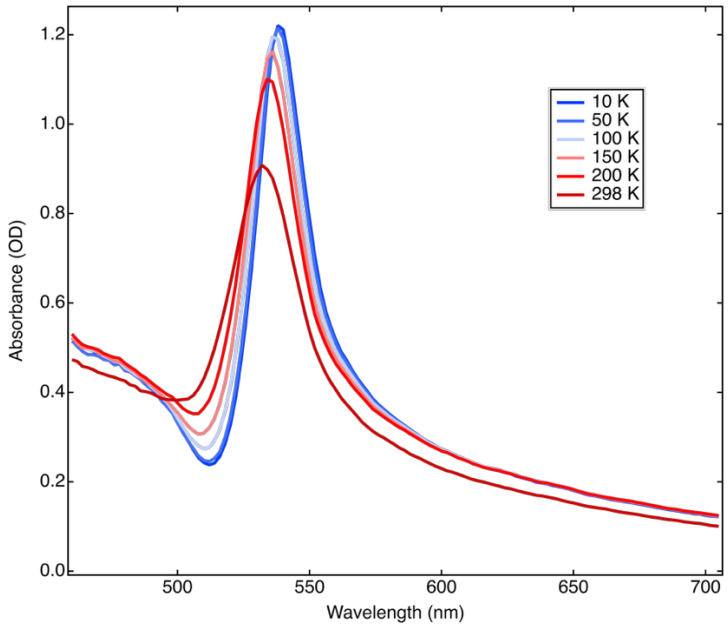

Figure S9. Temperature-dependent UV-vis spectra for $(AzOH)_2PbI_4$ thin films.

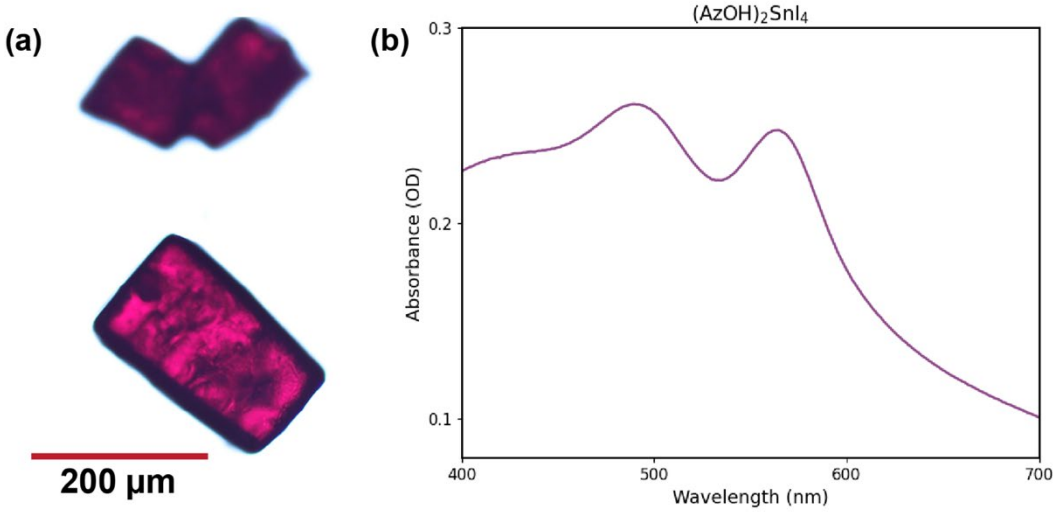

Figure S10. (a) Photograph of $(AzOH)_2SnI_4$ crystals and (b) UV-vis absorption spectrum of $(AzOH)_2SnI_4$ thin film at room temperature.

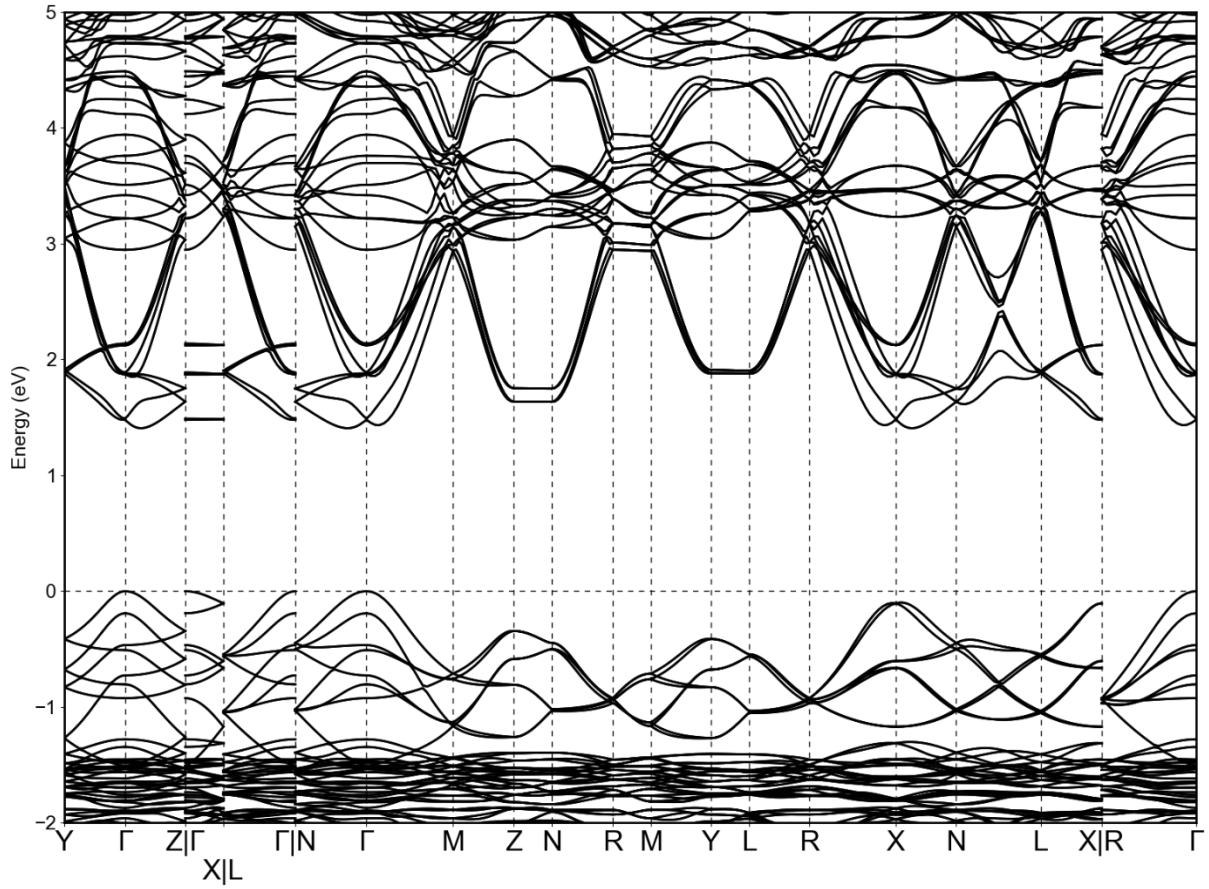

Figure S11. DFT-based HSE06 + SOC electronic band structure of $(AzOH)_2SnI_4$.

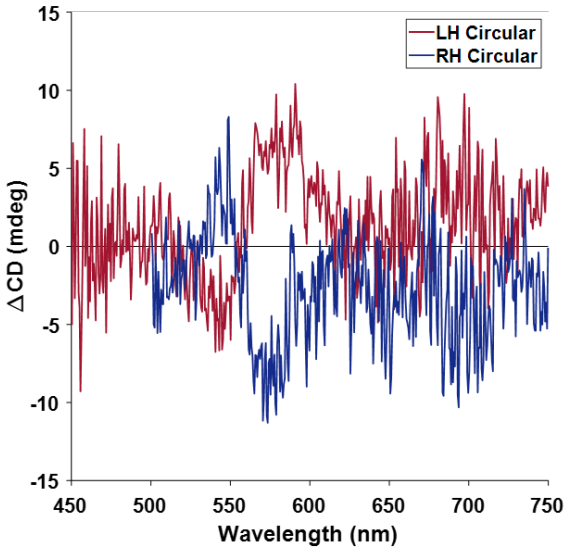

Figure S12. Comparison of TRCD response of $(AzOH)_2SnI_4$ film at 290 K on left and right circularly polarized excitation (400 nm) and different probe wavelengths.

C. Supplementary Note. Origin of Symmetry Transfer in $(AzOH)_2PbI_4$.

$(AzOH)_2PbI_4$, and $(EOA)_2PbI_4$ crystallize in the centrosymmetric $P2_1/m$ and $P2_1/a$ space groups, respectively. While the octahedra, Pb–I layer, and unit cell individually exhibit inversion symmetry in $(EOA)_2PbI_4$, the former two structural units lose their inversion centers in $(AzOH)_2PbI_4$, leading to the observed hidden spin polarization in the DFT simulations. The contrast in the symmetry of the Pb-I layers originates from the differences in the N-H···I and N-H···O interactions between the organic and inorganic sublattices (dashed lines in Extended Data Figure 3a-b; Table S5 provides the corresponding distances). The intermolecular interactions provide rigidity and restrict the A-cation motion within the assessed range of 100 - 298 K,[9,10] inducing phase stability for $(AzOH)_2PbI_4$ in the same temperature window (Table S4 shows slight deviations in the lattice parameters). A crucial difference between EOA and AzOH is the number of hydrogen atoms in the ammonium group—i.e., *three* different N-H···I interactions of similar strengths (based on H-I distances and N-H···I angles) in $(EOA)_2PbI_4$ for each A-cation. In contrast, the secondary ammonium group in AzOH includes only *two* hydrogen atoms, reducing the number of possible N-H···I interactions in the structure to two (Extended Data Figure 3b). The AzOH cation also introduces symmetry-breaking for these interactions (red dashed lines in Extended Data Figure 3b point to longer H-I distances of >3 Å; see Table S5 for distances and angles), indicating the distinctive nature of the two hydrogen atoms in AzOH. The above analysis indicates that, at the organic-inorganic interface, the molecular asymmetry of AzOH extends to the observed local symmetry breaking in $(AzOH)_2PbI_4$ through noncovalent interactions, seemingly pointing to a broader pattern of the previously explored *chirality transfer* phenomenon in 2DHPs.[11]

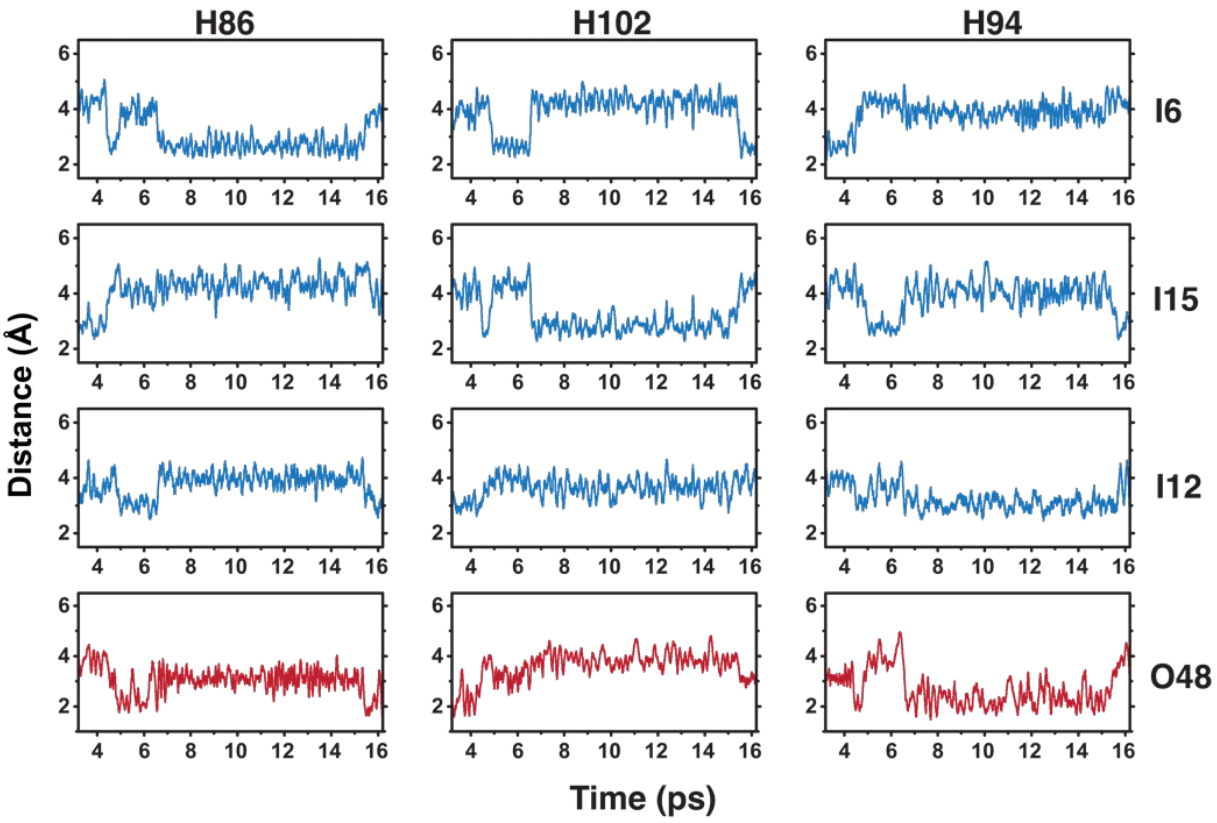

Figure S13. Evolution of interatomic distances involving the EOA-NH_3^+ group that contributes to non-covalent interactions in $(EOA)_2PbI_4$, simulated using AIMD at 300 K; the hydrogen, oxygen, and iodine indices correspond to those of an ammonium group, and the iodine and oxygen atoms closest to it in the static structure, respectively.

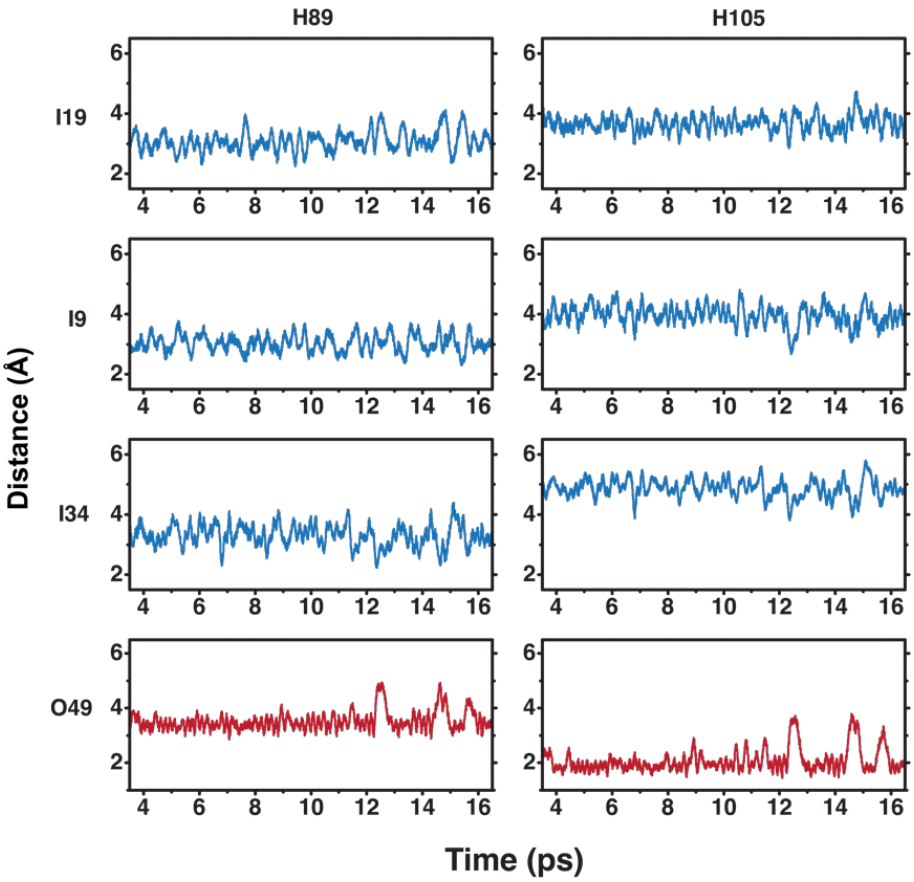

Figure S14. Evolution of interatomic distances involving the AzOH-NH_2^+ group that contribute to non-covalent interactions in $(AzOH)_2PbI_4$, simulated using AIMD at 300 K; the hydrogen, oxygen, and iodine indices correspond to those of an ammonium group, and the iodine and oxygen atoms closest to it in the static structure, respectively.

The structural origin of the symmetry transfer, which ultimately results in the spin-valley formation, can further be understood by considering the limited dynamics of the nonprimary ammonium group. Extended Data Figure 3e shows the dynamics of H-I distances between three hydrogen atoms (labeled H1, H2, H3 in Extended Data Figure 3c) of EOA-NH_3^+ and one iodine from the Pb-I layer (labeled I1 in Extended Data Figure 3a), simulated using ab initio molecular dynamics (AIMD; see Supporting Methods for details). For different hydrogen atoms, the individual distances each fall into the expected range of N-H···I interactions at different times (Figure S13 shows the interaction dynamics from Extended Data Figure 3e). The periodic

switching of the hydrogen atom indices indicates that the C-N bond can undergo discrete (stepwise) rotations at room temperature, breaking and reforming N-H···I and N-H···O non-covalent interactions over different periods. Extended Data Figure 3f shows the dynamic changes in the AIMD simulations to the H-I distances involving AzOH-NH_2^+ and I1, which has the shortest distance in the static structure. The evolution of the H1-I1 distance indicates that it is the primary contributing factor towards the N-H···I1 interactions throughout the probed simulation time. However, in contrast to $(EOA)_2PbI_4$, the fluctuation of the H–I distance is larger in $(AzOH)_2PbI_4$; consequently, the standard deviation of the H–I distance is also larger by ~0.1 Å, consistent with a weaker H-bonding interaction in $(AzOH)_2PbI_4$. Also, unlike EOA, the hydrogen atom indices do not switch for a specific type of interaction (see Figure S14), indicating that the two hydrogen atoms in the AzOH -NH_2^+- group cannot rotate as readily, due to the restricted rotation of the C-N bonds (Extended Data Figure 3d).

The dynamics of the octahedral distortion parameters (bond distance variance, λ_{oct} , and bond angle variance, σ_{oct}^2) for the Pb-I octahedra in $(EOA)_2PbI_4$ and $(AzOH)_2PbI_4$ can be used to track the resultant structural asymmetry. The distortion parameters are defined as follows:[12]

$\lambda_{oct} = \frac{1}{6}\sum_{i=1}^{6}\left(\frac{d_i}{d_0}\right)^2$; d_i: Pb – I distances in the distorted octahedron, and d_0: Pb – I distance in an ideal octahedron of the same volume.

$\sigma_{oct}^2 = \frac{1}{11}\sum_{i=1}^{12}(\alpha_i - 90)^2$; α_i: I – Pb – I angles in the distorted octahedron (following Robinson et al.'s approach of using the unbiased estimator[13]).

In the static room temperature structure, $(AzOH)_2PbI_4$ provides larger λ_{oct} and σ_{oct}^2 values, compared to $(EOA)_2PbI_4$. This difference remains well maintained throughout the probed time

window (Extended Data Figure 3g), indicating that the octahedra in $(AzOH)_2PbI_4$ remain anisotropically distorted over time. The structural anisotropy of the Pb–I layers is also reflected in the distributions of Pb–I–Pb angles from the AIMD simulation (Extended Data Figure 3h). Gaussian fitting of the distributions suggests the existence of one Pb–I–Pb angle in $(EOA)_2PbI_4$, while two such angles exist in $(AzOH)_2PbI_4$. Thus, the interaction asymmetry and restricted dynamics lead to the observed dissymmetry for the Pb–I bond lengths in $(AzOH)_2PbI_4$ compared to $(EOA)_2PbI_4$.

Like $(AzOH)_2PbI_4$, $(AzF_2)_2PbI_4$ possesses a secondary ammonium group and inversion asymmetric Pb–I layers. However, the difference in the distortion patterns of their respective inorganic layers highlights the crucial role that the intermolecular interactions play. Specifically, the N-H···O non-covalent interactions in $(AzOH)_2PbI_4$ allow for an inversion-symmetric relationship between the two AzOH cations separating the Pb–I layers (see Figure 2c) and induce rigidity within the organic sublattice. The N-H···I interactions then imprint polar distortions in the Pb–I layers, while still maintaining overall inversion symmetry in the unit cell, leading to the HSP with the layer-dependent spin valleys. In contrast, analogous N-H···F non-covalent interactions are absent in the SCXRD-derived structure of $(AzF_2)_2PbI_4$ (Extended Data Figure 1), presumably allowing some flexibility for the AzF_2 cations to assume three distinct configurations relative to the Pb–I layer, and ultimately to a reduced degree of polar displacements within the inorganic sublattice and near absence of spin valleys.

D. Supplementary Data: Atomic positions used in DFT calculations.

1. DFT- relaxed $(EOA)_2PbI_4$

lattice_vector 20.4144879999999986 0.0000000000000000 0.0000000000000000
lattice_vector 0.0000048684297949 8.9980799999986836 0.0000000000000000

lattice_vector -1.6027149812312760 -0.0000003818359338 8.8004686038243261
atom 4.3021832621060483 4.4990038167560291 4.4003575084726165 Pb
atom 14.5094272621060476 4.4990038167560291 4.4003575084726165 Pb
atom 5.1038129626236381 8.9980530057495187 0.0002112112464918 Pb
atom 15.3110569626236384 8.9980530057495187 0.0002112112464918 Pb
atom 7.4101296614588241 4.1435256414834170 5.0178687894657603 I
atom 17.6173736614588208 4.1435256414834170 5.0178687894657603 I
atom 1.1942629270435432 4.8545629747597134 3.7825910138899599 I
atom 11.4015069270435436 4.8545629747597134 3.7825910138899599 I
atom 0.3927301664025372 8.6425655041627198 8.1827901139277088 I
atom 10.5999741664025358 8.6425655041627198 8.1827901139277088 I
atom 8.2118885841730744 0.3555051159207930 0.6176608889594103 I
atom 18.4191325841730738 0.3555051159207930 0.6176608889594103 I
atom 3.7578828426979847 1.7392206239288222 6.0641212999000196 I
atom 13.9651268426979840 1.7392206239288222 6.0641212999000196 I
atom 4.8466650479971607 7.2586160460724001 2.7363825057987206 I
atom 15.0539090479971609 7.2586160460724001 2.7363825057987206 I
atom 4.0452325193840046 6.2383685543465646 7.1368016175515647 I
atom 14.2524765193840040 6.2383685543465646 7.1368016175515647 I
atom 4.5592032617939724 2.7595041079674032 1.6638693970506502 I
atom 14.7664472617939708 2.7595041079674032 1.6638693970506502 I
atom 7.4264855427189795 0.2958386310497960 5.6049920523699024 C
atom 17.6337295427189780 0.2958386310497960 5.6049920523699024 C
atom 1.1780563580690513 8.7022679813548631 3.1954325491114051 C
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2. DFT- relaxed $(AzOH)_2PbI_4$

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3. DFT- relaxed $(AzOH)_2SnI_4$

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atom	6.22877315	7.07685825	13.49797649	F
atom	10.86373160	1.71211382	1.39173384	F

5. Pb and I atom indices of $(AzF_2)_2PbI_4$ (as used in Tables S2, S3 and S5 and derived from the reported CIF)

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17.3088423	2.081495232	0.467460908	Pb2
11.14836076	2.229726528	16.72590215	Pb3
15.63270767	6.583073472	4.558778054	Pb4
14.04651555	2.305604736	8.684649833	Pb5
9.562168644	6.507195264	20.85177392	Pb6
16.98433156	2.717603136	9.900875558	I7
12.49998465	6.095196864	22.06799965	I8
12.1860411	8.345545344	15.32838627	I9
16.67038801	0.467254656	3.161262181	I10
10.02577793	0.3503088	19.0707503	I11
14.51012484	8.4624912	6.903626209	I12
13.39367911	0.809279424	11.39524174	I13
8.9093322	8.003520576	23.56236583	I14
13.44721462	5.166327744	9.942487122	I15
8.962867711	3.646472256	22.10961121	I16
14.61345164	3.883095936	5.952157105	I17
10.12910473	4.929704064	18.1192812	I18
9.911931842	7.099062912	11.49087533	I19
5.427584933	1.713737088	23.65799942	I20
12.29238448	4.104473472	14.39443783	I21
16.77673138	4.708326528	2.227313736	I22
13.78776468	2.617577856	18.42248593	I23
18.27211159	6.195222144	6.255361838	I24
8.471319466	1.84363776	15.01958466	I25
12.95566638	6.96916224	2.852460572	I26
10.9434599	1.85333184	7.909117344	I27
6.459112991	6.95946816	20.07624143	I28
15.98357883	6.28044192	13.30742696	I29
20.46792574	2.53235808	1.14030287	I30
1.352356999	2.204610048	8.735995097	Pb31

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-1.759219249	2.302344	16.6838039	Pb35
2.72512766	6.510456	4.516679805	Pb36
1.476742194	4.900004928	7.009723531	I37
-3.007604715	3.912795072	19.17684762	I38
-3.229951402	7.112899008	11.9094244	I39
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-1.444049147	5.191972992	15.3777848	I41
3.040297763	3.620827008	3.210660705	I42
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2.617429751	6.323800896	14.37059026	I59
7.10177666	2.488999104	2.203466173	I60

Supplementary References

1 Malinowski, A. *et al.* Spin relaxation in GaAs/$Al_xGa_{1-x}As$ quantum wells. *Phys. Rev. B* **62**, 13034-13039 (2000). https://doi.org/10.1103/PhysRevB.62.13034

2 Huang, Y. *et al.* Room-temperature electron spin polarization exceeding 90% in an opto-spintronic semiconductor nanostructure via remote spin filtering. *Nat. Photon.* **15**, 475-482 (2021). https://doi.org/10.1038/s41566-021-00786-y

3 Buß, J. H. *et al.* Long room-temperature electron spin lifetimes in highly doped cubic GaN. *Appl. Phys. Lett.* **97**, 062101 (2010). https://doi.org/10.1063/1.3478838

4 Litvinenko, K. L. *et al.* Spin lifetime in high quality InSb epitaxial layers grown on GaAs. *J. Appl. Phys.* **101**, 083105 (2007). https://doi.org/10.1063/1.2719017

5 Xu, J. *et al.* How spin relaxes and dephases in bulk halide perovskites. *Nat. Commun.* **15**, 188 (2024). https://doi.org/10.1038/s41467-023-42835-w

6 Zhou, M., Sarmiento, J. S., Fei, C., Zhang, X. & Wang, H. Effect of composition on the spin relaxation of lead halide perovskites. *J. Phys. Chem. Lett.* **11**, 1502-1507 (2020). https://doi.org/10.1021/acs.jpclett.0c00004

7 Dataset: mp-20459, Materials data on $TiPbO_3$ by Materials Project. https://doi.org/10.17188/1195590

8 Chakraborty, R., Sercel, P. C., Qin, X., Mitzi, D. B. & Blum, V. Design of two-dimensional hybrid perovskites with giant spin splitting and persistent spin textures. *J. Am. Chem. Soc.* **146**, 34811-34821 (2024). https://doi.org/10.1021/jacs.4c13597

9 Mercier, N., Poiroux, S., Riou, A. & Batail, P. Unique hydrogen bonding correlating with a reduced band gap and phase transition in the hybrid perovskites $(HO(CH_2)_2NH_3)_2PbX_4$ (X = I, Br). *Inorg. Chem.* **43**, 8361-8366 (2004). https://doi.org/10.1021/ic048814u

10 Chakraborty, R., Sheikh, T. & Nag, A. Iodine–Iodine Interactions Suppressing phase transitions of 2D layered hybrid $(I\text{-}(CH_2)_n\text{-}NH_3)_2PbI_4$ (n = 2–6) perovskites. *Chem. Mater.* **34**, 288-296 (2021). https://doi.org/10.1021/acs.chemmater.1c03492

11 Jana, M. K. *et al.* Organic-to-inorganic structural chirality transfer in a 2D hybrid perovskite and impact on Rashba-Dresselhaus spin-orbit coupling. *Nat. Commun.* **11**, 4699 (2020). https://doi.org/10.1038/s41467-020-18485-7

12 Jana, M. K., Xie, Y. & Mitzi, D. B. Impact of structural distortions on the optoelectronic and spin-related properties of two-dimensional hybrid perovskites in *Hybrid Organic Inorganic Perovskites*. World Scientific 1-61 (2022). https://doi.org/10.1142/9789811242014_0001

13 Robinson, K., Gibbs, G. V. & Ribbe, P. H. Quadratic elongation: A quantitative measure of distortion in coordination polyhedra. *Science* **172**, 567-570 (1971). https://doi.org/doi:10.1126/science.172.3983.567