

Supplementary Information

Medium-Throughput Evaluation of Quantum Geometry-Driven Topological Transports in Altermagnets

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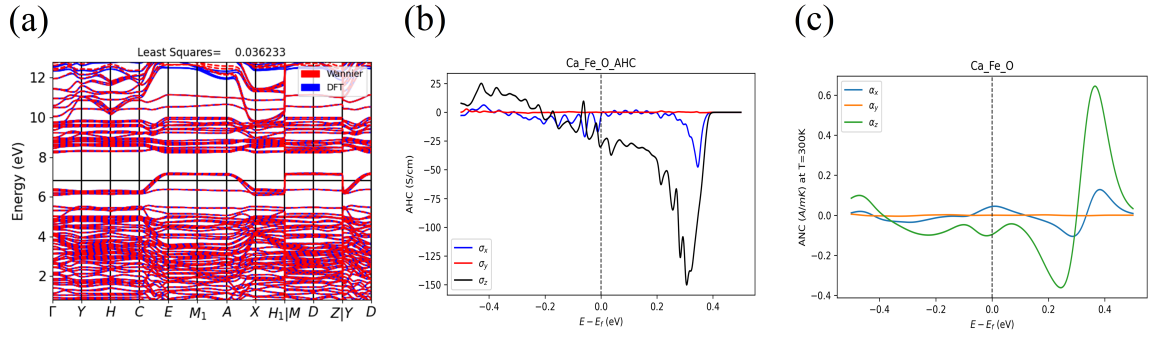


Figure S1: Wannier function, AHC and ANC of CaFe_5O_7 .

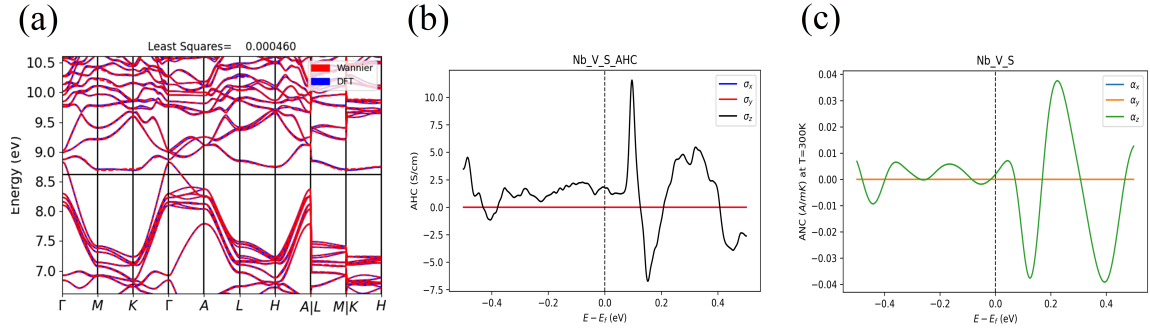


Figure S2: Wannier function, AHC and ANC of VNb_3S_6 .

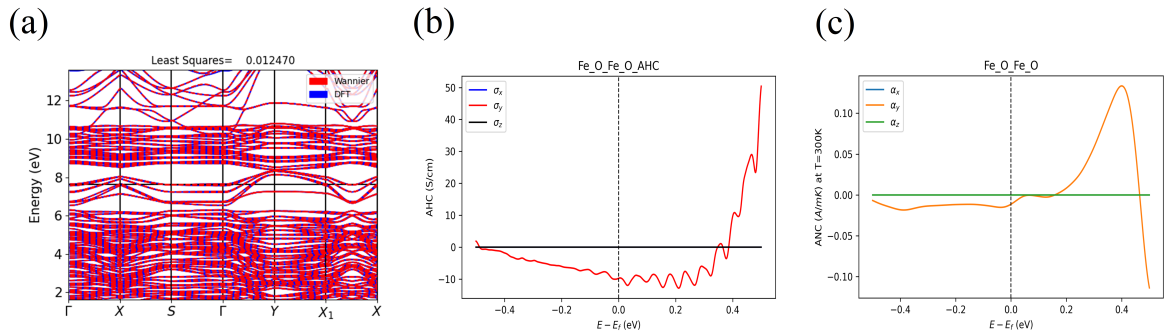


Figure S3: Wannier function, AHC and ANC of Fe_4O_5 .

1 Non-zero AHC, ANC and Wfs of metallic altermagnetic

2 K-mesh convergence test

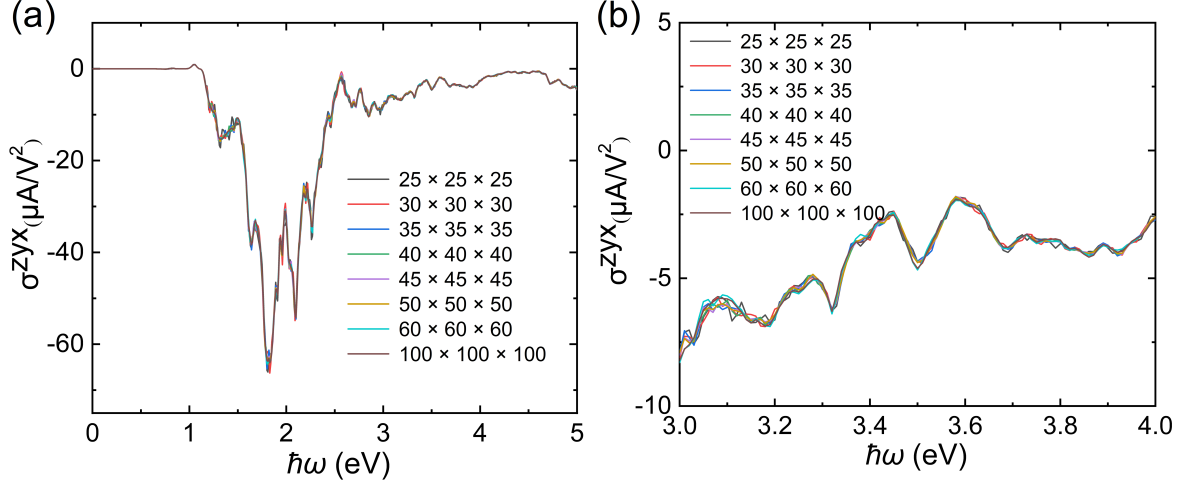
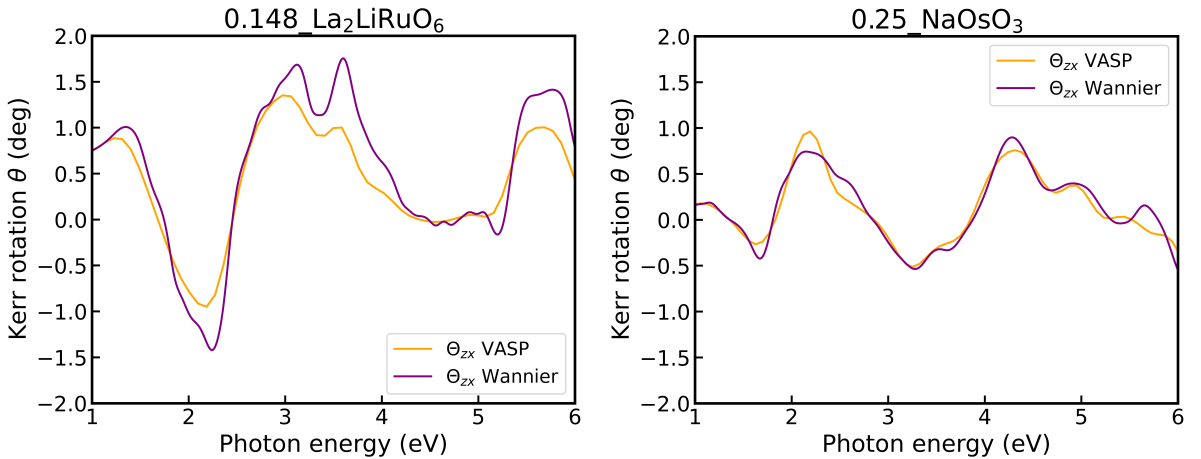
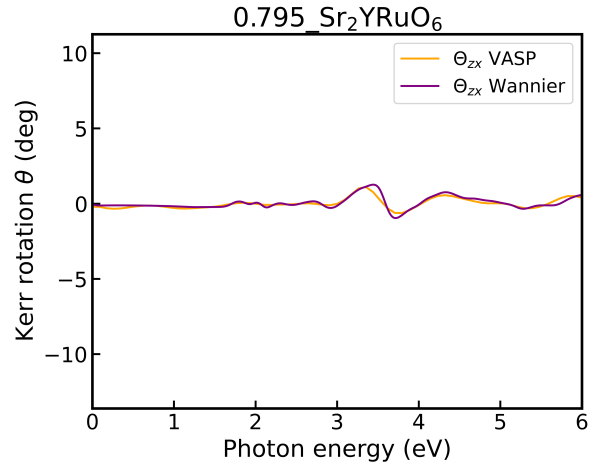
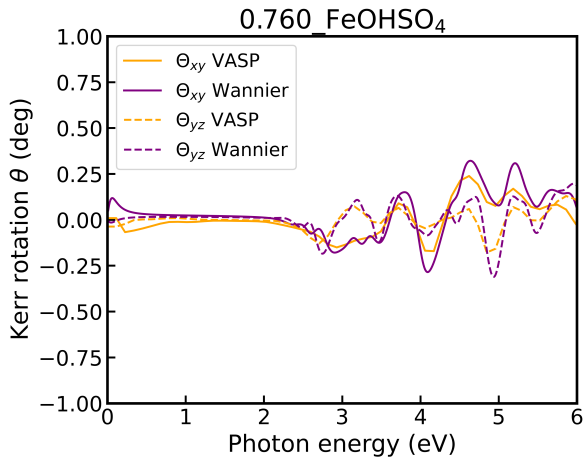
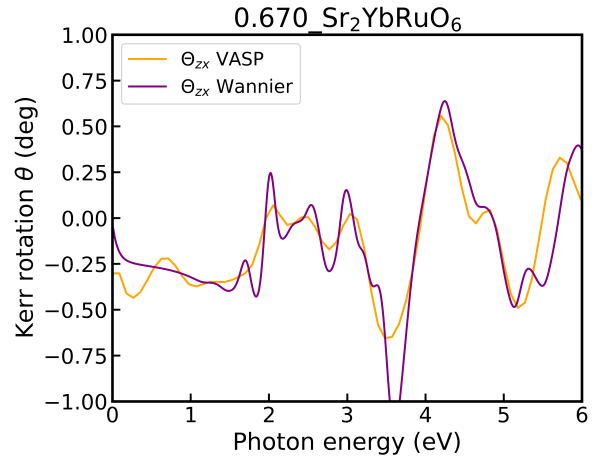
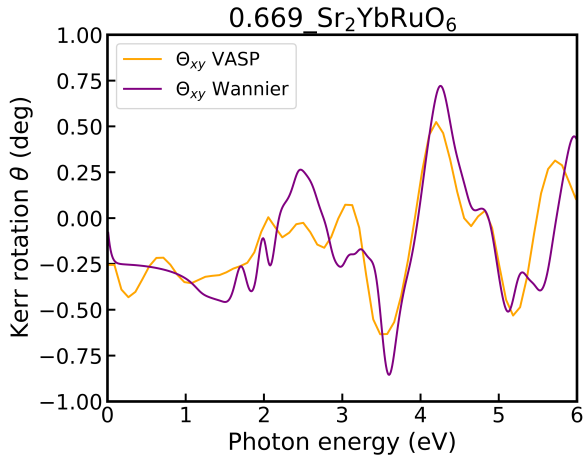
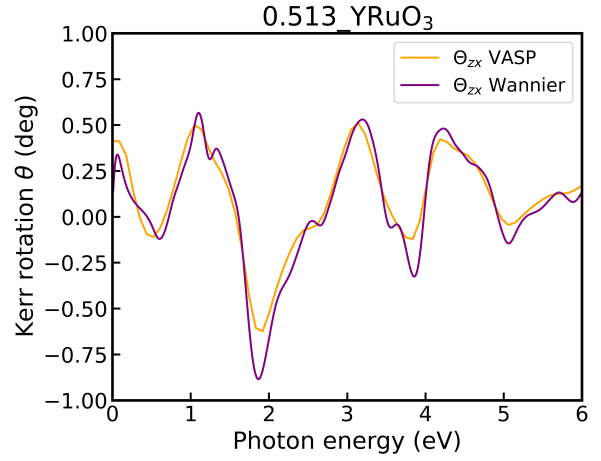
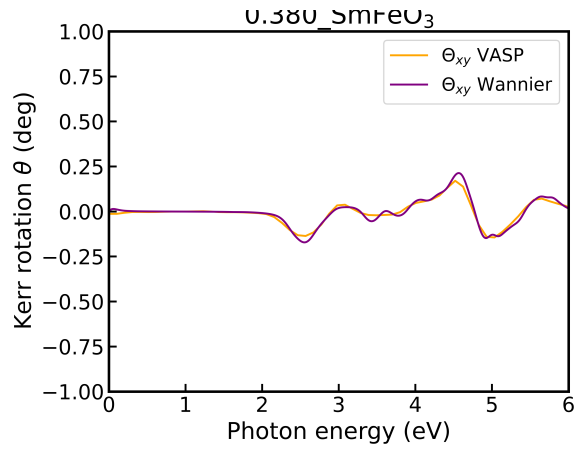


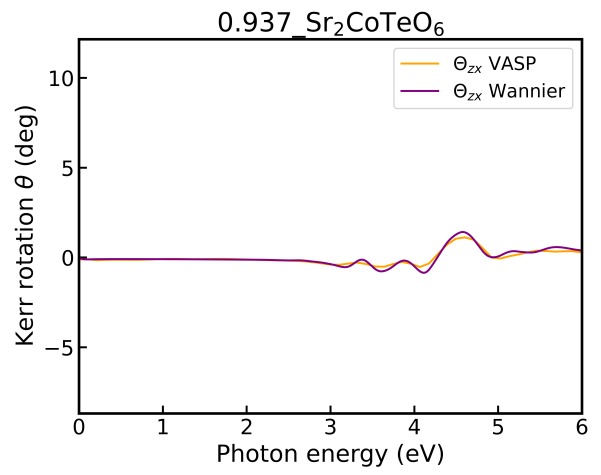
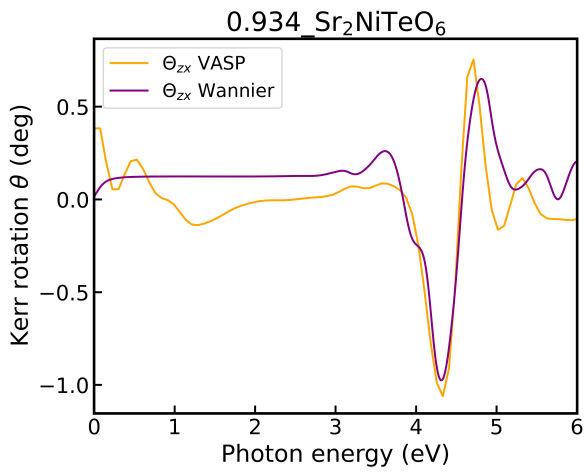
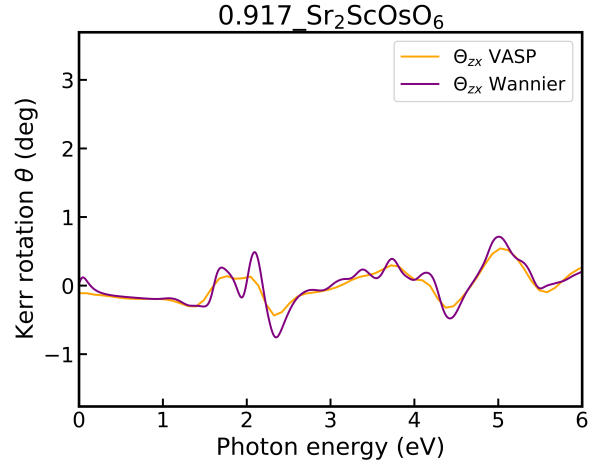
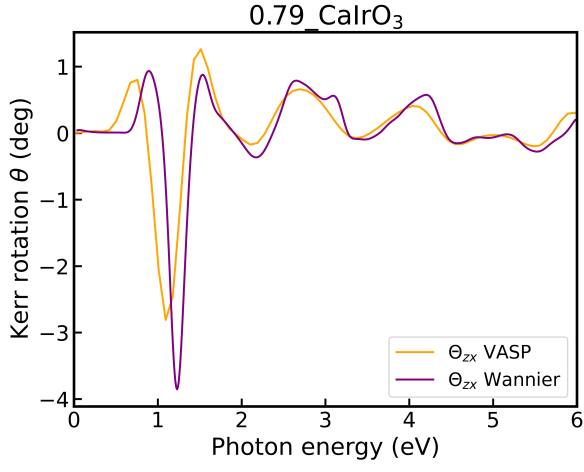
Figure S4: k -point convergence test of the shift current response σ^{zyx} in CuFeS₂. Different curves correspond to different k -point sampling densities. (a) Shift current spectrum over a broad photon energy range. (b) Enlarged view in the 3.0–4.0 eV region, demonstrating the convergence of the calculated response with increasing k -point density.

To assess convergence, we systematically increase the k -mesh density and monitor the change in shift current. As representative test case, we consider CuFeS₂, as shown in Fig. S4, once the k -mesh reaches $40 \times 40 \times 40$ k -mesh, the shift current curves are essentially converged.

3 MOKE calculation using VASP and Wannier function







4 MOKE under different SOC strength

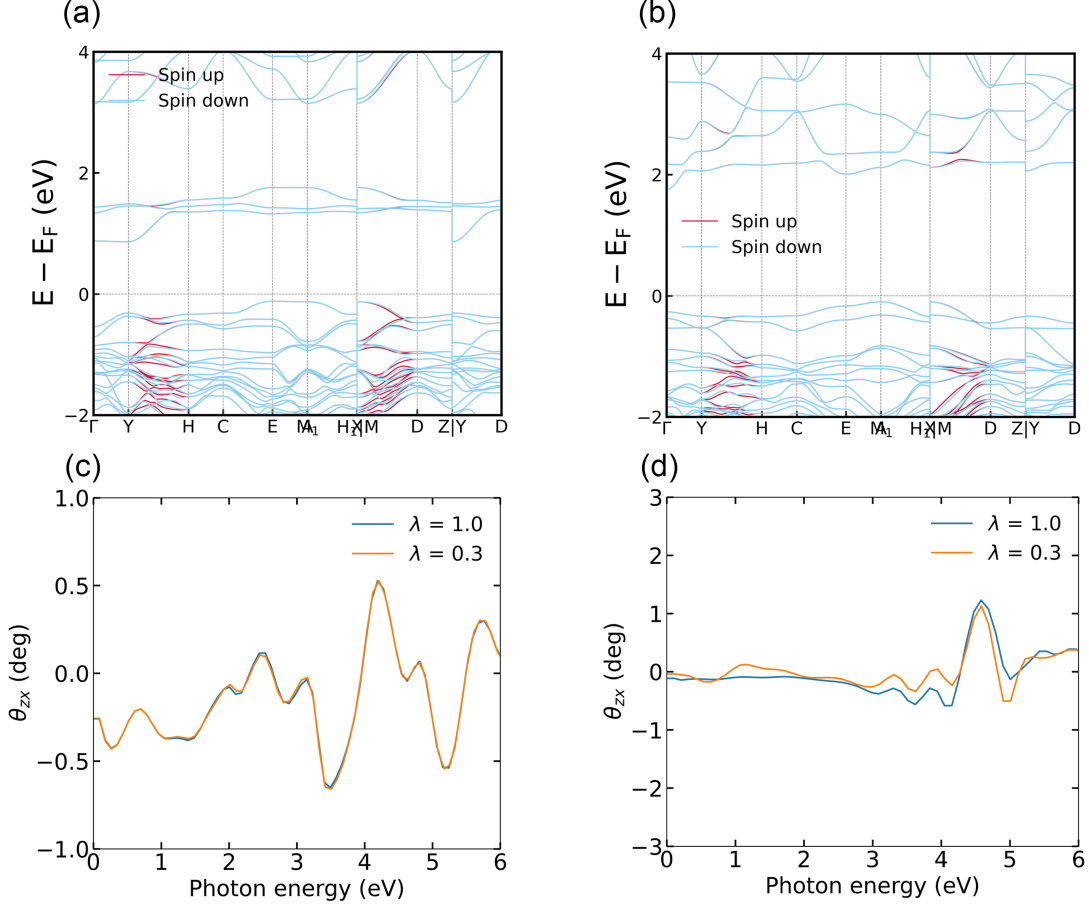


Figure S11: Spin-polarized band structure of (a) $0.670\text{-Sr}_2\text{YbRuO}_6$ and (b) $0.937\text{-Sr}_2\text{CoTeO}_6$, along with the Kerr rotation angle θ_{zx} ((c) for $0.670\text{-Sr}_2\text{YbRuO}_6$ and (d) $0.937\text{-Sr}_2\text{CoTeO}_6$) calculated using different SOC scaling factor λ of 1.0 and 0.3, respectively.

5 Shift current and Wfs of without inversion altermagnetic

Table S1: Lattice parameters of the two $\text{Co}_2\text{Mo}_3\text{O}_8$ crystal structures in MAGNDATA.

ID	Chemical formula	a (Å)	b (Å)	c (Å)	Band gap (eV)
0.332	$\text{Co}_2\text{Mo}_3\text{O}_8$	5.7670	5.7670	9.9160	1.63
0.338	$\text{Co}_2\text{Mo}_3\text{O}_8$	5.7658	5.7658	9.9053	1.70

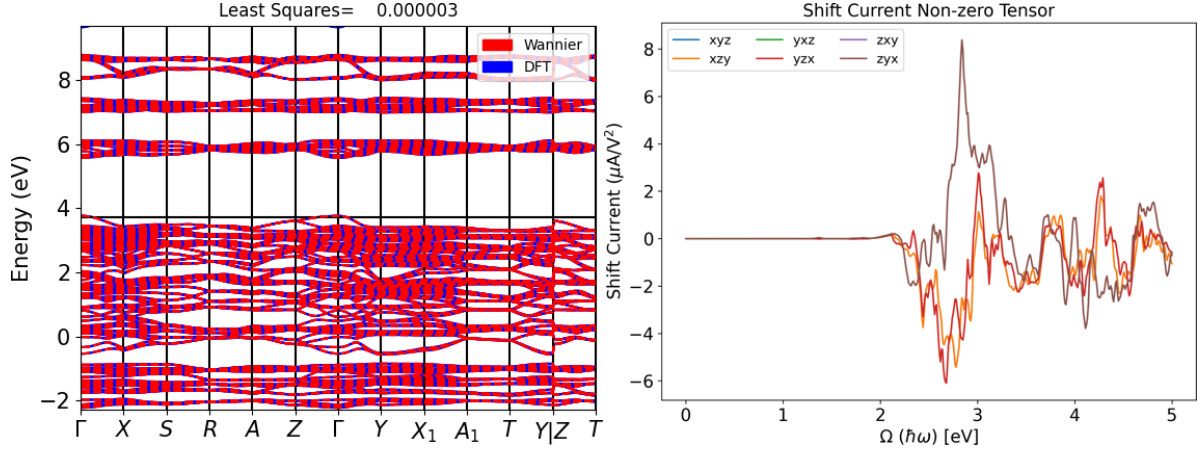


Figure S12: Wannier functions and shift current response of SrMnO_3 . The nonzero tensor components are $\sigma^{xyz} = \sigma^{xzy}$, $\sigma^{yxz} = \sigma^{yzx}$, and $\sigma^{zxy} = \sigma^{zyx}$.

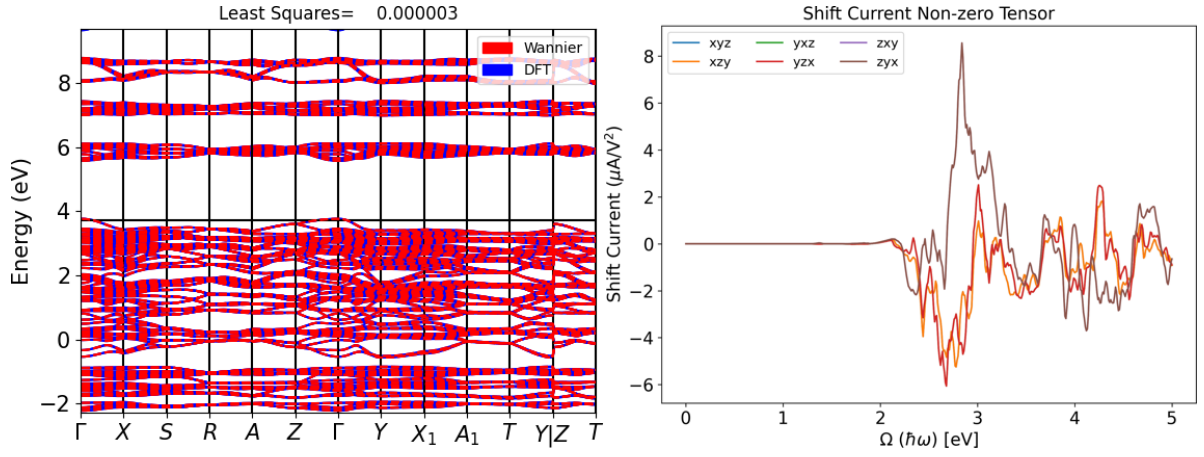


Figure S13: Wannier function and shift current response of SrMnO_3 . The nonzero tensor components are $\sigma^{xyz} = \sigma^{xzy}$, $\sigma^{yxz} = \sigma^{yzx}$, and $\sigma^{zxy} = \sigma^{zyx}$.

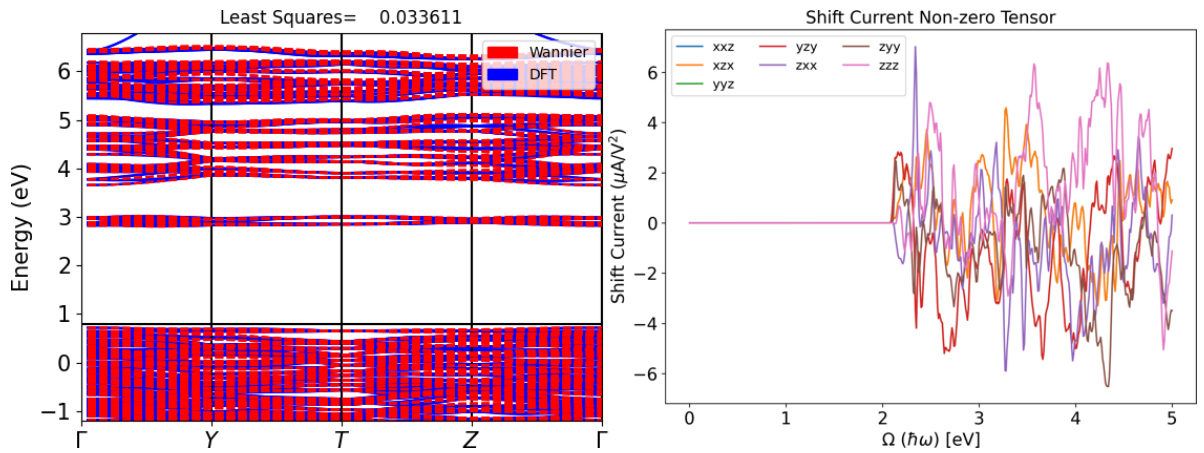


Figure S14: Wannier function and shift current response of $\text{Cu}_2\text{V}_2\text{O}_7$. The nonzero tensor components are $\sigma^{xxz} = \sigma^{xzx}$, $\sigma^{yyz} = \sigma^{yzy}$, σ^{zxx} , σ^{zxy} and σ^{zyy} .

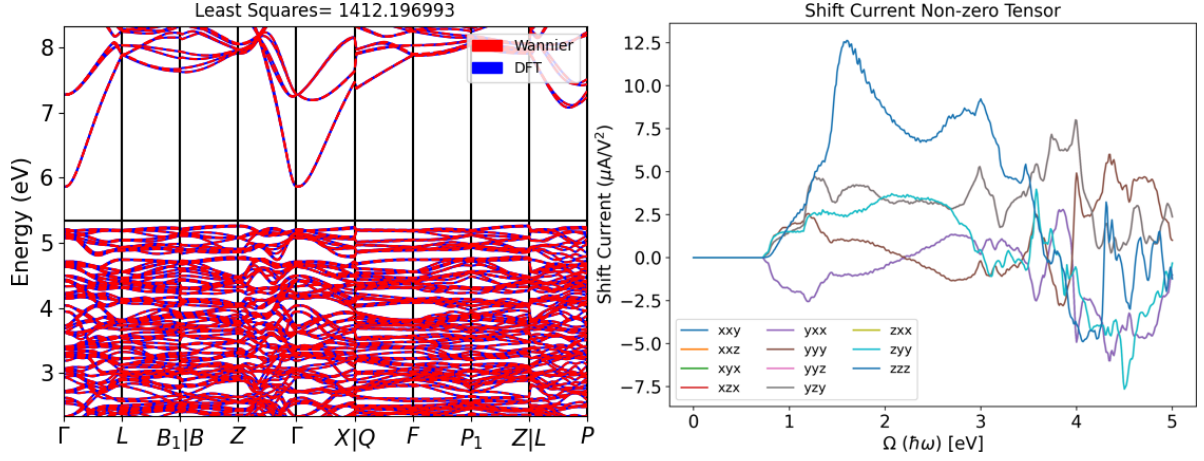


Figure S15: Wannier function and shift current response of PbNiO_3 . The nonzero tensor components are $\sigma^{xxy} = \sigma^{xyx} = \sigma^{yxx} = \sigma^{yyy}$, $\sigma^{xxz} = \sigma^{xzx} = \sigma^{yyz} = \sigma^{yzy}$, $\sigma^{zxx} = \sigma^{zzy}$, σ^{zzz}

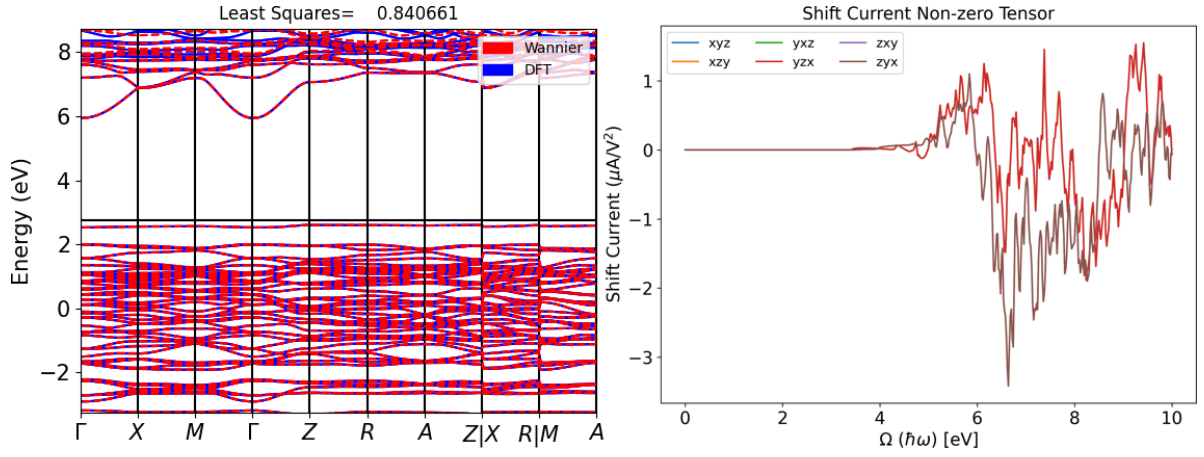


Figure S16: Wannier function and shift current response of $\text{Ba}_2\text{MnSi}_2\text{O}_7$. The nonzero tensor components are $\sigma^{xyz} = \sigma^{xzy} = \sigma^{yxz} = \sigma^{yzx}$, $\sigma^{zxy} = \sigma^{zyx}$

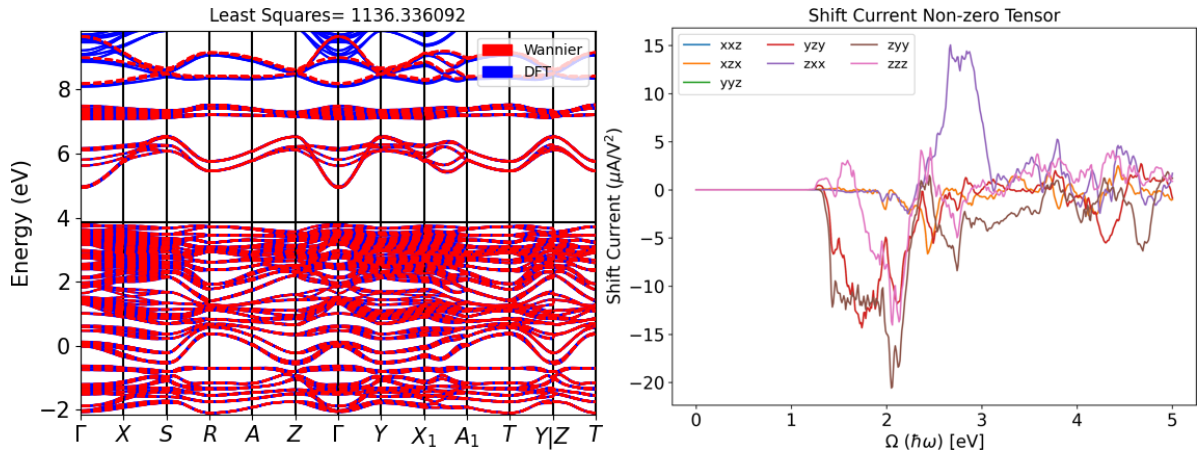


Figure S17: Wannier function and shift current response of $\text{Ca}_3\text{Mn}_2\text{O}_7$. The nonzero tensor components are $\sigma^{xxz} = \sigma^{xzx}$, $\sigma^{yyz} = \sigma^{yzy}$, σ^{zxx} , σ^{zxy} , and σ^{zzz} .

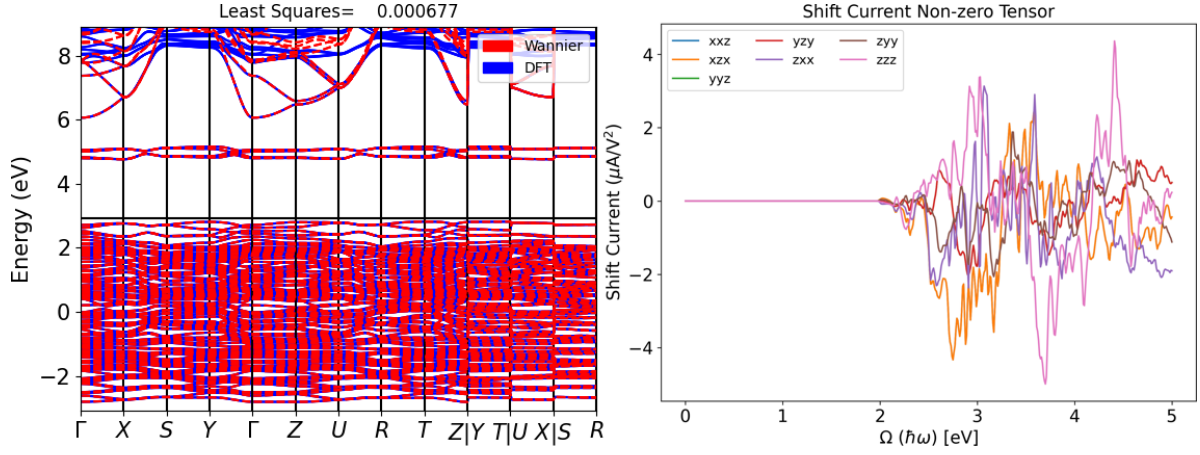


Figure S18: Wannier function and shift current response of $\text{Y}_2\text{Cu}_2\text{O}_5$. The nonzero tensor components are $\sigma^{xxz} = \sigma^{xzx}$, $\sigma^{yyz} = \sigma^{yzy}$, σ^{zxx} , σ^{zzy} , and σ^{zzz} .

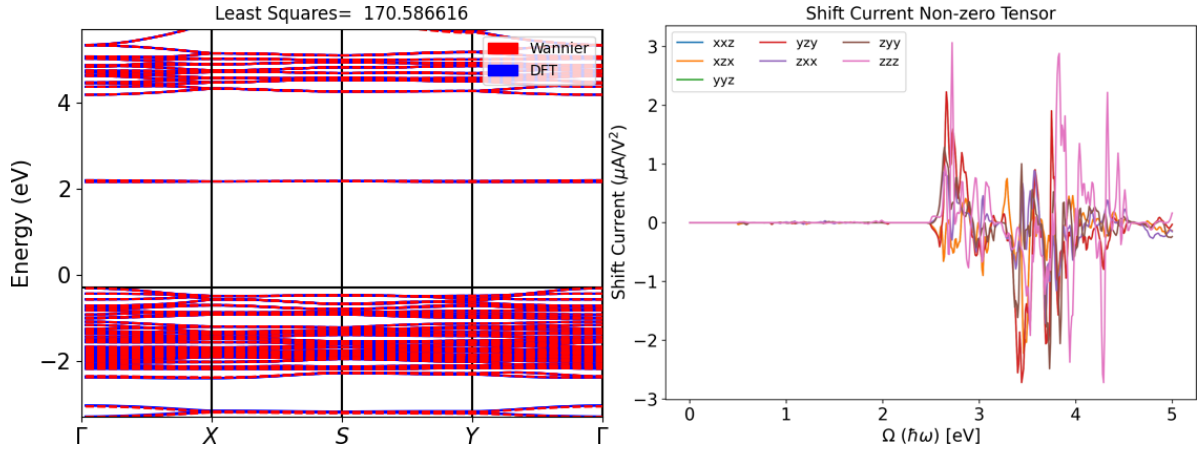


Figure S19: Wannier function and shift current response of $\text{C}(\text{ND}_2)_3]\text{Cu}(\text{DCOO})_3$. The nonzero tensor components are $\sigma^{xxz} = \sigma^{xzx}$, $\sigma^{yyz} = \sigma^{yzy}$, σ^{zxx} , σ^{zzy} , and σ^{zzz} .

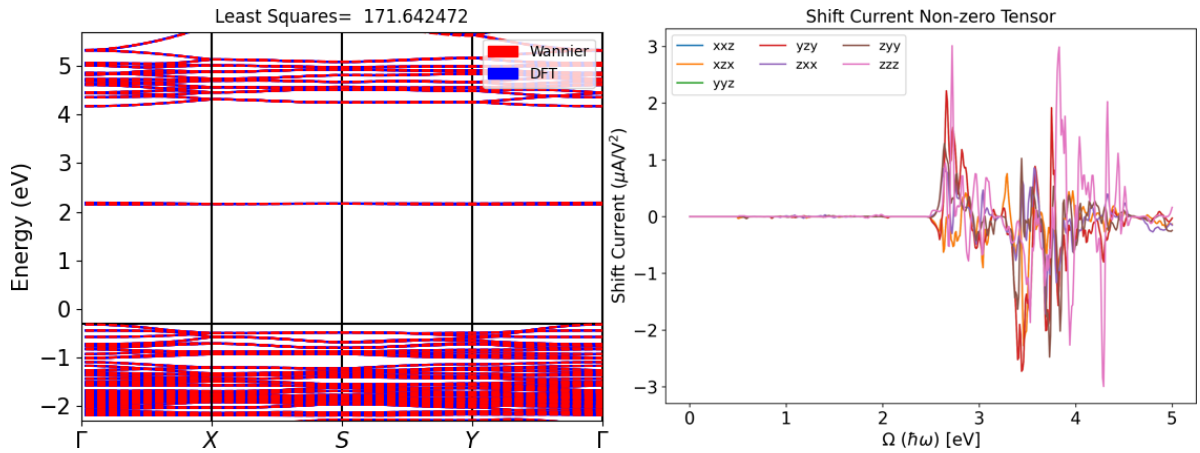


Figure S20: Wannier function and shift current response of $\text{C}(\text{ND}_2)_3]\text{Cu}(\text{DCOO})_3$. The nonzero tensor components are $\sigma^{xxz} = \sigma^{xzx}$, $\sigma^{yyz} = \sigma^{yzy}$, σ^{zxx} , σ^{zzy} , and σ^{zzz} .

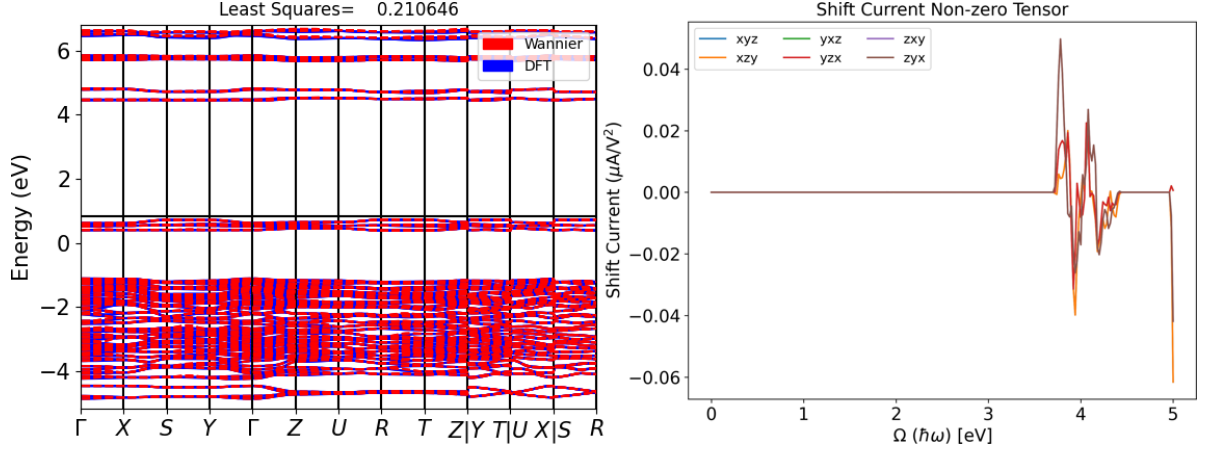


Figure S21: Wannier function and shift current response of BaCrF_5 . The nonzero tensor components are $\sigma^{xyz} = \sigma^{xzy}$, $\sigma^{yxz} = \sigma^{yzx}$, and $\sigma^{zxy} = \sigma^{zyx}$

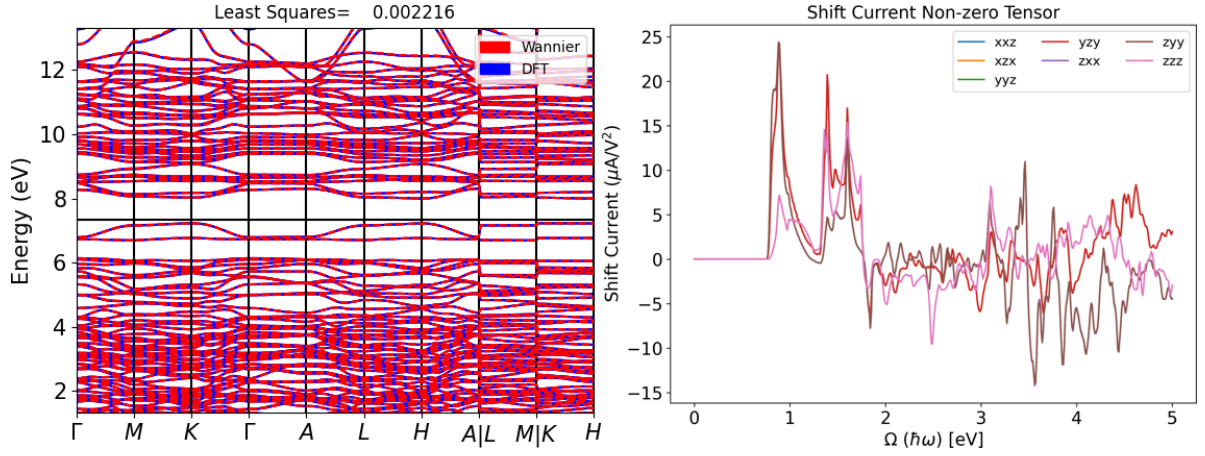


Figure S22: Wannier function and shift current response of $\text{Fe}_2\text{MO}_3\text{O}_8$. The nonzero tensor components are $\sigma^{xxz} = \sigma^{xzx} = \sigma^{yyz} = \sigma^{yzy}$, $\sigma^{zxx} = \sigma^{zyy}$, and σ^{zzz} .

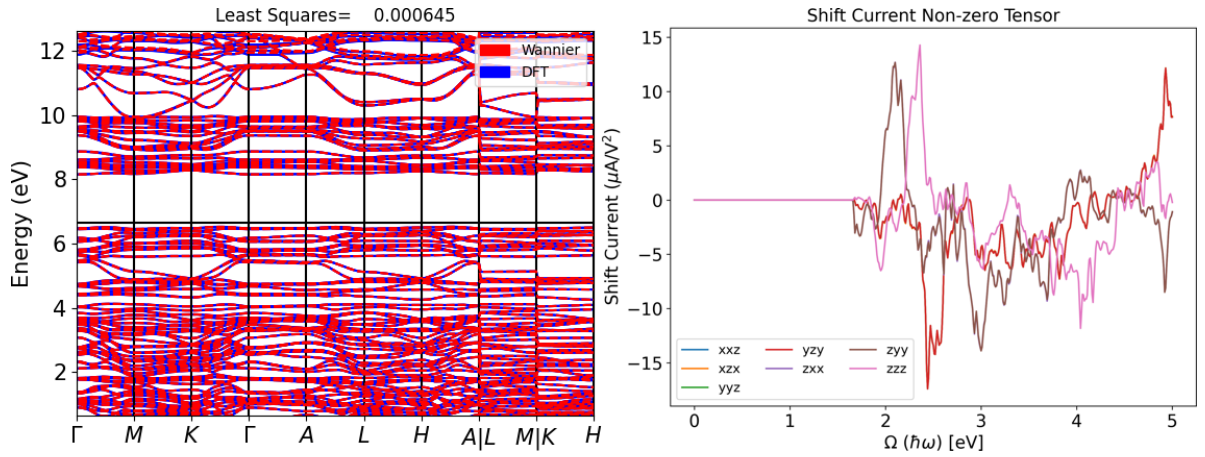


Figure S23: Wannier function and shift current response of $\text{Co}_2\text{MO}_3\text{O}_8$. The nonzero tensor components are $\sigma^{xxz} = \sigma^{xzx} = \sigma^{yyz} = \sigma^{yzy}$, $\sigma^{zxx} = \sigma^{zyy}$, and σ^{zzz} .

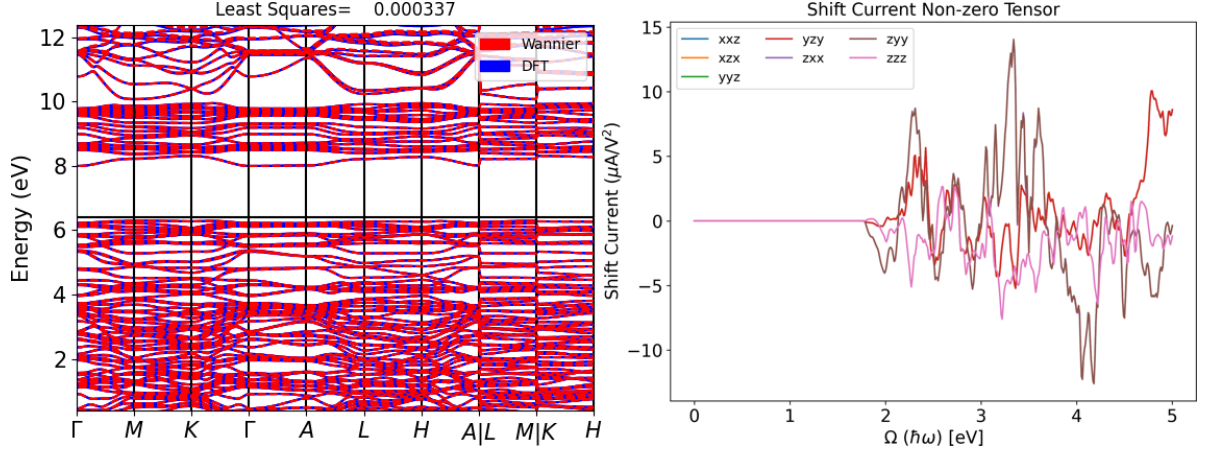


Figure S24: Wannier function and shift current response of $\text{Co}_2\text{MO}_3\text{O}_8$. The nonzero tensor components are $\sigma^{xxz} = \sigma^{xzx} = \sigma^{yyz} = \sigma^{yzy}$, $\sigma^{zxx} = \sigma^{zzy}$, and σ^{zzz} .

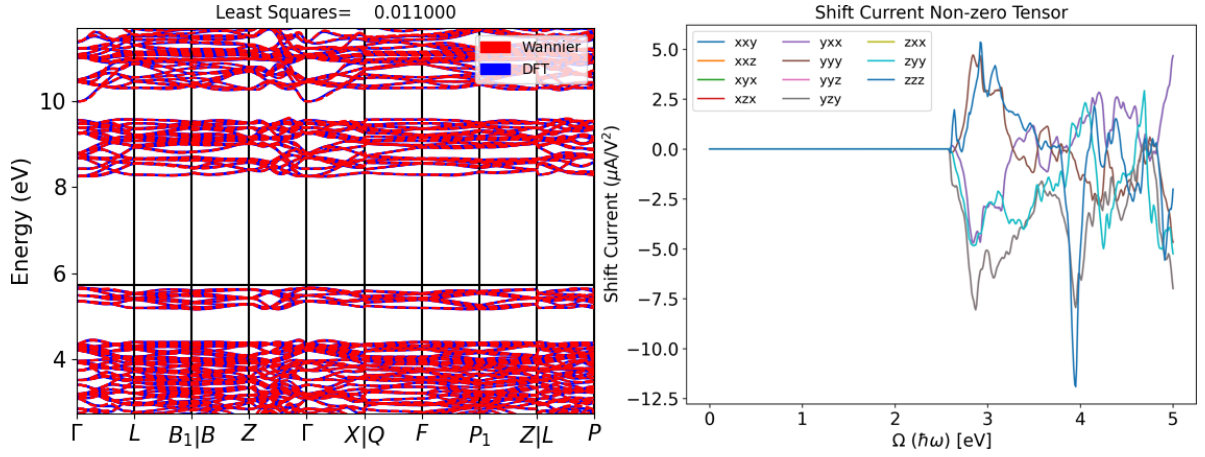


Figure S25: Wannier function and shift current response of MnTiO_3 . The nonzero tensor components are $\sigma^{xxy} = \sigma^{xyx} = \sigma^{yxx} = \sigma^{yyy}$, $\sigma^{xxz} = \sigma^{xzx} = \sigma^{yyz} = \sigma^{yzy}$, $\sigma^{zxx} = \sigma^{zzy}$, σ^{zzz} .

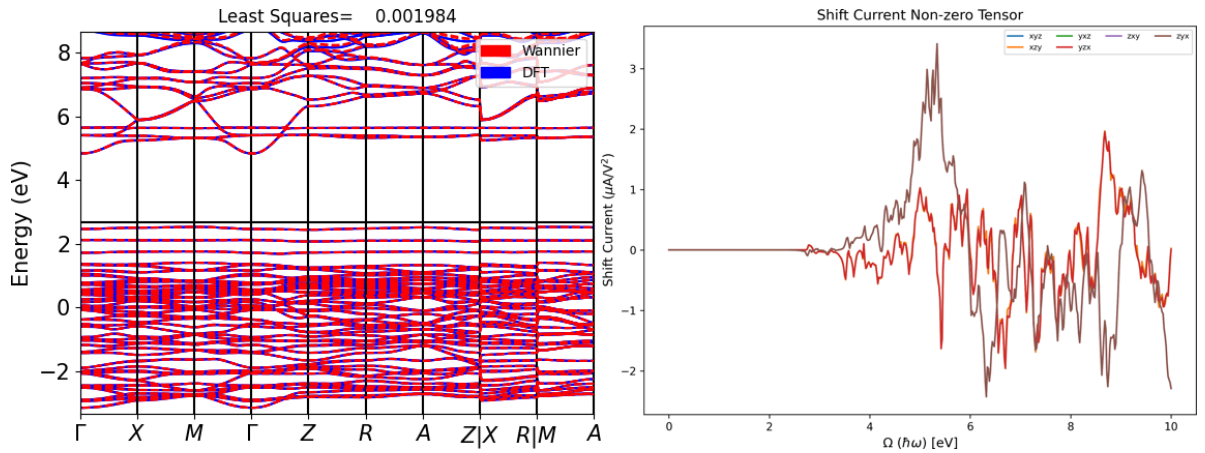


Figure S26: Wannier function and shift current response of $\text{Ba}_2\text{CoGe}_2\text{O}_7$. The nonzero tensor components are $\sigma^{xyz} = \sigma^{xzy} = \sigma^{yxz} = \sigma^{yzx}$, $\sigma^{zxy} = \sigma^{zyx}$.

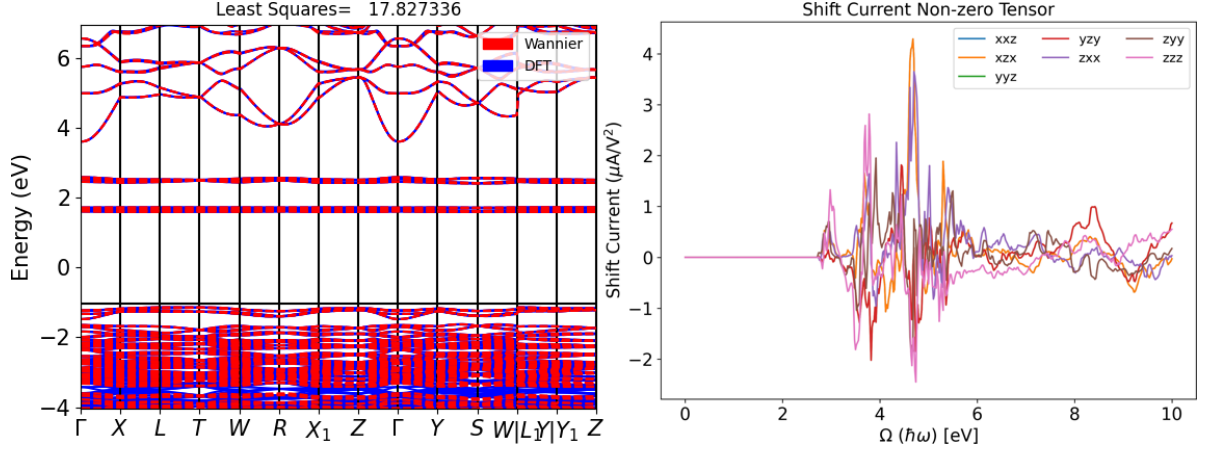


Figure S27: Wannier function and shift current response of $\text{ZnFeF}_5(\text{H}_2\text{O})_2$. The nonzero tensor components are $\sigma^{xxz} = \sigma^{xzx}$, $\sigma^{yyz} = \sigma^{yzy}$, σ^{zxx} , σ^{zzy} , and σ^{zzz} .

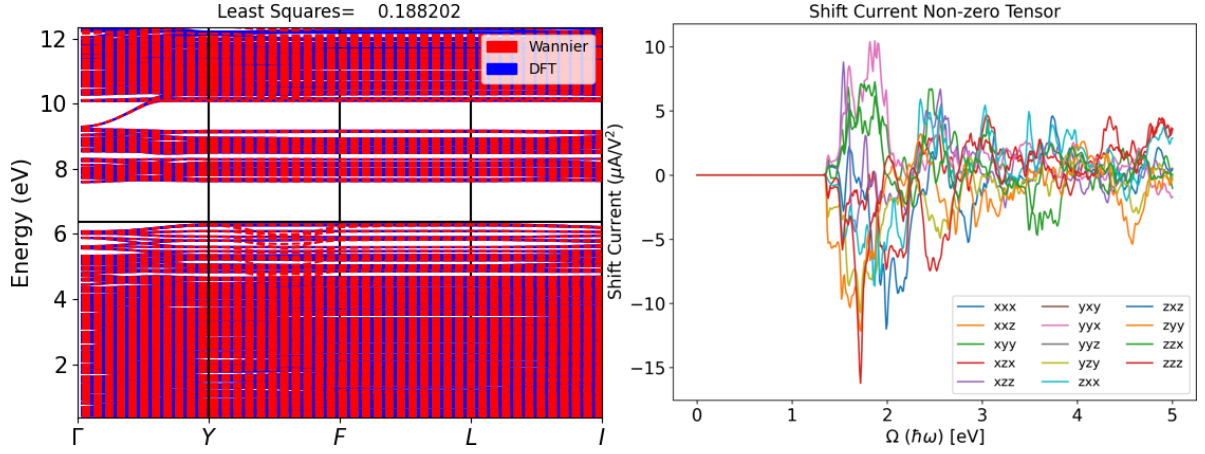


Figure S28: Wannier function and shift current response of $\text{Mn}_4\text{Nb}_2\text{O}_9$. The nonzero tensor components are σ^{xxx} , $\sigma^{xxz} = \sigma^{xzx}$, σ^{xyy} , σ^{xzz} , $\sigma^{yxy} = \sigma{yyx}$, $\sigma^{yyz} = \sigma^{yzy}$, σ^{zxx} , $\sigma^{zxy} = \sigma^{zyx}$, σ^{zyy} , and σ^{zzz} .

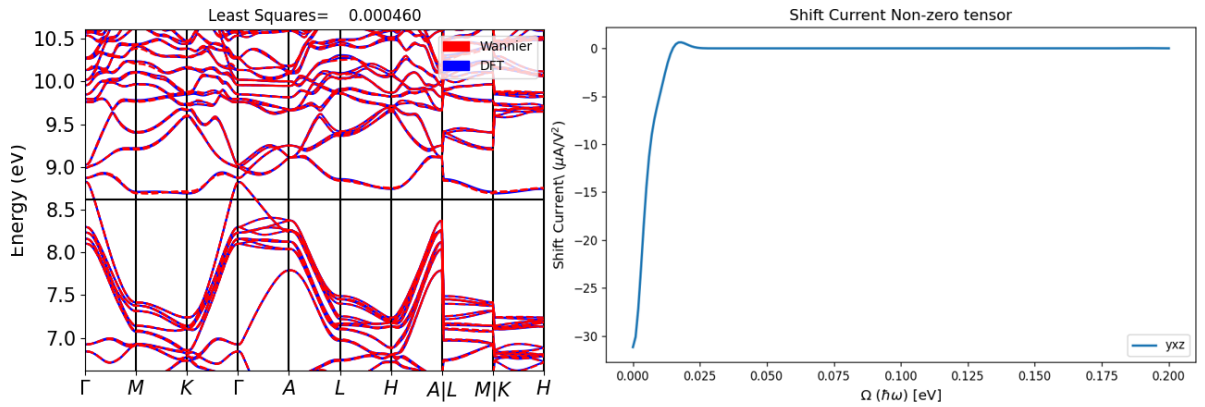


Figure S29: Wannier function and shift current response of VNb_3S_6 .

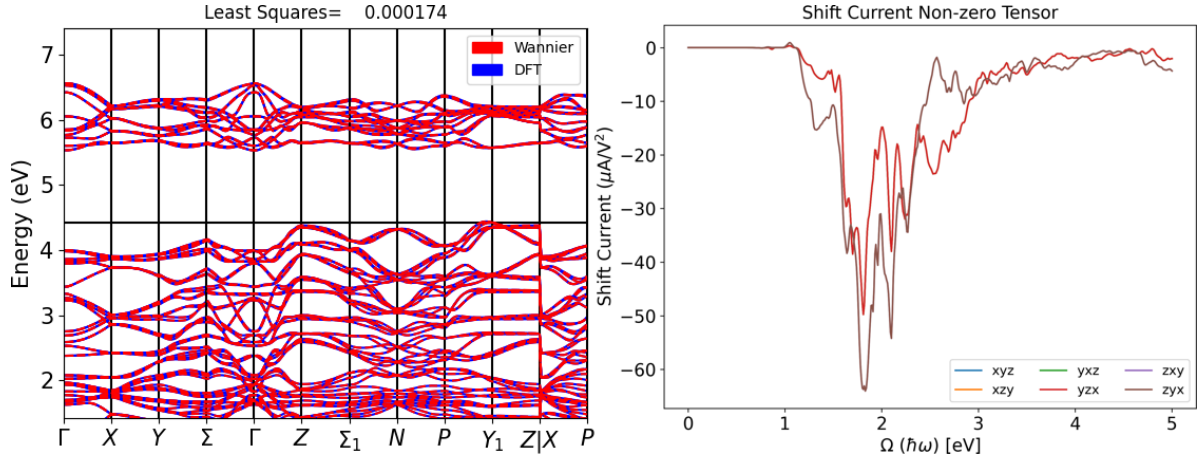


Figure S30: Wannier function and shift current response of CuFeS₂. The nonzero tensor components are $\sigma^{xyz} = \sigma^{xzy} = \sigma^{yxz} = \sigma^{yzx}$, $\sigma^{zxy} = \sigma^{zyx}$

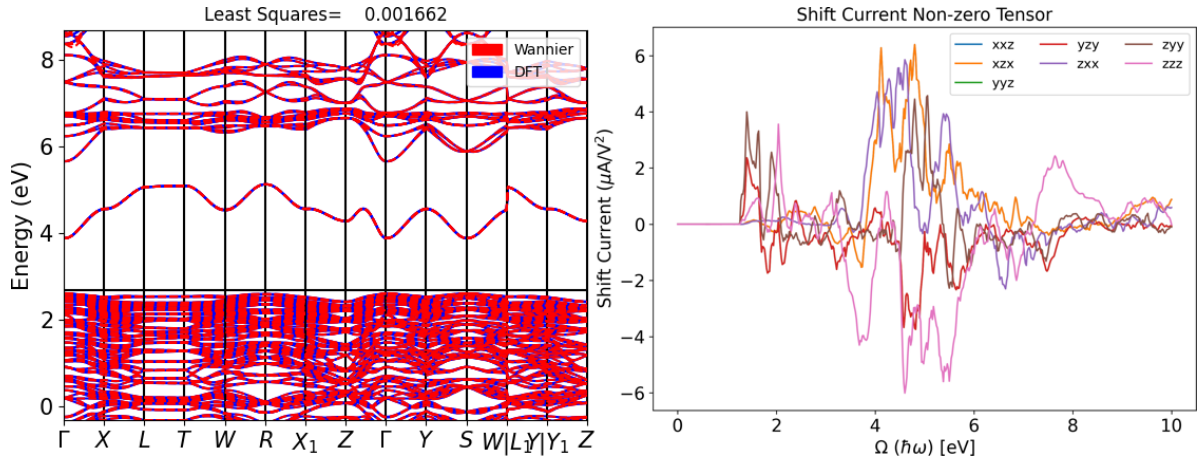


Figure S31: Wannier function and shift current response of Sr₂MnGaO₅. The nonzero tensor components are $\sigma^{xxz} = \sigma^{xzx}$, $\sigma^{yyz} = \sigma^{yzx}$, σ^{zxx} , σ^{zyy} , and σ^{zzz} .

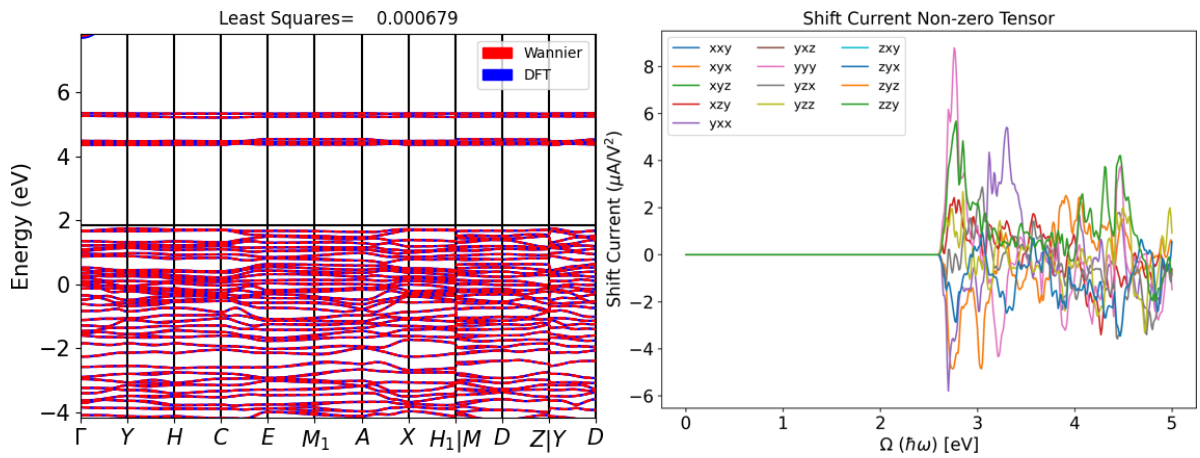


Figure S32: Wannier function and shift current response of LiFeP₂O₇. The nonzero tensor components are $\sigma^{xxy} = \sigma^{xyx}$, $\sigma^{xyx} = \sigma^{xzy}$, $\sigma^{yxz} = \sigma^{yzx}$, $\sigma^{yxx} = \sigma^{yzy}$, $\sigma^{yzz} = \sigma^{zyx}$, $\sigma^{zyx} = \sigma^{zyx}$, $\sigma^{zyx} = \sigma^{zyx}$, and $\sigma^{zyx} = \sigma^{zyx}$.

6 Additional Computational Details

6.1 Hubbard U parameters

To account for the on-site Coulomb interactions of localized d and f electrons, we employed the DFT+ U method within the Dudarev scheme. The effective Hubbard parameters ($U_{\text{eff}} = U - J$) used in this work are summarized below. For transition-metal elements, we adopted element-specific U values in the range of 2–6 eV, depending on the degree of electron localization. In particular, $U = 3$ –4 eV was used for $3d$ elements such as V, Cr, Mn, Fe, Co, and Ni, while larger values ($U = 6$ eV) were assigned to rare-earth and actinide elements to properly describe their strongly localized f electrons. For elements with more delocalized electronic states (e.g., Zn, Cd, Hg), $U = 0$ eV was used. The complete list of U values employed in this work is given in Table S2.

Table S2: Hubbard U parameters (in eV) used in the DFT+ U calculations.

Element	U	Element	U	Element	U	Element	U
Sc	2	Ti	4	V	3	Cr	3
Mn	4	Fe	4	Co	3	Ni	6
Cu	6	Zn	0	Y	2	Zr	3
Nb	2	Mo	3	Tc	2	Ru	2
Rh	2	Pd	3	Ag	3	Cd	0
Hf	3	Ta	2	W	2	Re	2
Os	2	Ir	2	Pt	3	Au	3
Hg	0	La	6	Ce	6	Pr	6
Nd	6	Pm	6	Sm	6	Eu	6
Gd	6	Tb	6	Dy	6	Ho	6
Er	6	Tm	6	Yb	6	Lu	6
Ac	6	Th	6	Pa	6	U	6
Np	6	Pu	6	Am	6	Cm	6
Bk	6	Cf	6	Es	6	Fm	6
Md	6	No	6	Lr	6		

7 Calculations Table

Material ID in the MAGNDATA database (ID), chemical formula (Compound), atomic index in the crystal structure (Atom_index), magnetic element in the crystal structure (Element), Hubbard U parameter used in the DFT calculations on the magnetic element(U), and magnetic moment (M_{out}), together with the corresponding experimental input magnetic moment (M_{in}).

ID	Compound	MSG	Element	Wyckoff	U (eV)	M_x^{in}	M_y^{in}	M_z^{in}	M_x^{out}	M_y^{out}	M_z^{out}
0.1	LaMnO ₃	62.448	Mn	4b	4	3.87	0.00	0.00	3.83	0.01	0.04
0.1018	SrMnO ₃	20.34	Mn	8c	4	2.27	0.00	0.00	2.95	0.00	0.01
0.1019	SrMnO ₃	20.34	Mn	8c	4	0.00	2.27	0.00	0.00	2.95	0.00
0.105	ErVO ₃	14.75	Er	4e	6	0.00	0.00	8.20	0.00	0.12	2.85
			V	2d	3	0.00	0.00	1.47	0.00	0.00	1.79
0.112	FeBO ₃	15.89	Fe	6c	4	4.70	0.00	0.00	4.24	0.02	0.00
0.113	NiCO ₃	15.85	Ni	6c	6	1.00	2.00	0.00	0.82	1.60	0.00
0.114	CoCO ₃	15.85	Co	6c	3	1.00	2.00	0.00	1.22	2.42	0.00
0.115	MnCO ₃	15.85	Mn	6c	4	1.00	2.00	0.00	2.08	4.15	0.00
0.116	FeCO ₃	167.103	Fe	6b	4	0.00	0.00	1.00	0.00	0.00	3.71
0.118	Ba ₅ Co ₅ ClO ₁₃	194.268	Co1	4e	3	0.00	0.00	-0.61	0.00	0.00	-0.34
			Co2	4f	3	0.00	0.00	2.21	0.00	0.00	2.82
			Co3	2a	3	0.00	0.00	0.35	0.00	0.00	0.84
0.128	FeSO ₄ F	15.89	Fe	4d	4	0.00	4.32	0.00	0.00	4.30	0.00
0.13	Ca ₃ Co _{2-x} Mn _x O ₆	161.19	Mn	6a	4	0.00	0.00	1.93	0.00	0.00	3.00
			Co	6a	3	0.00	0.00	0.66	0.00	0.00	2.64
0.131	Mn(N(CN ₂)) ₂	58.398	Mn	2a	4	5.01	0.00	0.00	4.60	0.00	0.00
0.137	Cu ₂ V ₂ O ₇	43.227	Cu	16b	6	0.93	0.00	0.00	0.72	-0.01	0.00
0.148	La ₂ LiRuO ₆	14.75	Ru	2c	2	1.70	0.00	1.40	1.55	0.10	1.27
0.15	MnF ₂	136.499	Mn	2a	4	0.00	0.00	4.60	0.00	0.00	4.67
0.178	CoF ₂	136.499	Co	2a	3	0.00	0.00	2.60	0.00	0.00	2.76
0.189	CeMn ₂ Ge ₄ O ₁₂	125.367	Mn	4f	4	0.00	0.00	4.61	0.00	0.00	4.40
0.21	PbNiO ₃	161.69	Ni	6a	6	0.00	0.00	1.69	0.00	0.00	1.75
0.229	Ba ₂ MnSi ₂ O ₇	113.267	Mn	2a	4	0.00	0.00	4.10	0.00	0.00	4.58
0.23	Ca ₃ Mn ₂ O ₇	36.174	Mn	8b	4	2.67	0.00	0.00	2.96	-0.03	0.00
0.239	Ca ₃ LiRuO ₆	15.89	Ru	6d	2	2.80	0.00	0.00	1.98	0.03	0.00
0.241	Y ₂ Cu ₂ O ₅	33.144	Cu	4a	6	0.00	-1.10	0.00	-0.01	-0.66	0.00
0.25	NaOsO ₃	62.448	Os	4b	2	0.00	0.00	1.00	-0.11	-0.07	1.76
0.254	C(ND ₂) ₃ Cu(DCOO) ₃	33.144	Cu	4a	6	0.00	0.63	0.00	-0.01	0.74	0.00
0.255	C(ND ₂) ₃ Cu(DCOO) ₃	33.148	Cu	4a	6	0.63	0.00	0.00	0.74	-0.01	0.00
0.256	C(ND ₂) ₃ Mn(DCOO) ₃	52.310	Mn	4d	4	0.00	5.04	0.00	0.00	4.64	0.00
0.257	C(ND ₂) ₃ Co(DCOO) ₃	52.312	Co	4d	4	0.00	0.00	2.97	0.00	0.03	2.73
0.260	CuFePO ₅	62.441	Cu	4a	6	0.00	0.95	0.00	0.02	0.70	0.03
			Fe	4c	4	0.00	4.28	0.00	0.00	4.22	0.00
0.261	NiFePO ₅	62.441	Ni	4a	6	0.00	2.03	0.00	0.00	1.77	0.00
			Fe	4c	4	0.00	4.09	0.00	0.00	4.21	0.00
0.263	Fe ₂ PO ₅	62.441	Fe1	4a	4	0.00	3.89	0.00	-0.04	3.70	-0.02
			Fe2	4c	4	0.00	-4.22	0.00	0.00	-4.21	0.00
0.3	Ca ₃ LiOsO ₆	15.89	Os	6c	2	2.20	0.00	0.00	2.13	-0.04	0.00
0.301	Sr ₂ CoTeO ₆	14.75	Co	2d	3	0.93	0.00	1.88	1.89	0.04	1.89
0.303	BaCrF ₅	19.27	Cr	4a	3	0.00	0.00	1.00	0.00	-0.01	2.88
0.307	ScCrO ₃	62.441	Cr	4b	3	0.00	2.70	0.00	-0.02	2.83	0.03
0.308	InCrO ₃	62.441	Cr	4b	3	0.00	2.50	0.00	-0.01	2.88	0.02
0.309	TlCrO ₃	62.441	Cr	4b	3	0.00	2.46	0.00	-0.00	2.87	0.00
0.315	ZrMn ₂ Ge ₄ O ₁₂	125.367	Mn	4f	4	0.00	0.00	4.68	0.00	0.00	4.63
0.323	LaCrO ₃	62.441	Cr	4b	3	2.51	0.00	0.00	2.83	-0.02	0.02

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ID	Compound	MSG	Element	Wyckoff	U	M_x^{in}	M_y^{in}	M_z^{in}	M_x^{out}	M_y^{out}	M_z^{out}
0.329	RbMnF ₄	2.4	Mn1	1a	4	1.97	1.97	1.03	2.52	2.51	1.32
			Mn2	1e	4	-1.97	-1.97	-1.03	-2.52	-2.52	-1.31
			Mn3	1d	4	1.97	1.97	1.03	2.54	2.55	1.33
			Mn4	1c	4	-1.97	-1.97	-1.03	-2.55	-2.55	-1.32
0.331	Fe ₂ Mo ₃ O ₃	186.205	Fe1	2b	4	0.00	0.00	4.60	0.00	0.00	3.64
			Fe2	2b	4	0.00	0.00	4.60	0.00	0.00	3.74
0.332	Co ₂ Mo ₃ O ₃	186.205	Co1	2b	3	0.00	0.00	3.30	0.00	0.00	2.57
			Co2	2b	3	0.00	0.00	3.30	0.00	0.00	2.67
0.334	CoF ₃	167.103	Co	6b	3	0.00	0.00	3.21	0.00	0.00	3.18
0.335	FeF ₃	15.89	Fe	6d	4	2.60	0.00	0.00	4.33	-0.01	0.00
0.336	NdFeO ₃	62.448	Fe	4b	4	3.84	0.00	0.00	4.12	0.00	0.00
0.338	Co ₂ Mo ₃ O ₃	186.205	Co1	2b	3	0.00	0.00	3.44	0.00	0.00	2.64
			Co2	2b	3	0.00	0.00	3.35	0.00	0.00	2.67
0.351	TbFeO ₃	62.448	Fe	4b	4	4.80	0.00	0.00	4.13	0.00	0.00
0.354	TbCrO ₃	62.446	Cr	4b	3	0.00	0.00	2.55	0.05	0.03	2.83
0.358	CaFe ₅ O ₇	11.54	Fe1	4f	4	0.00	-3.80	0.00	0.00	-3.90	-0.15
			Fe2	4f	4	0.00	3.90	0.00	-0.03	3.96	0.06
			Fe3	2a	4	0.00	3.50	0.00	-0.03	3.64	0.21
0.361	Sr ₃ LiRuO ₆	15.89	Ru	6d	2	2.03	0.00	0.00	2.00	-0.01	0.00
0.379	SmFeO ₃	62.446	Fe	4b	4	0.00	0.00	3.69	0.00	0.00	4.12
0.380	SmFeO ₃	62.448	Fe	4b	4	2.80	0.00	0.00	4.10	0.00	0.00
0.392	Fe ₃ (PO ₄) ₂ (OH) ₂	14.75	Fe1	2a	4	1.50	0.00	4.80	1.12	0.02	3.61
			Fe2	4e	4	1.50	0.00	4.80	1.27	0.01	4.06
0.402	Sr ₄ Fe ₄ O ₁₁	65.486	Fe1	4i	4	0.00	0.00	0.00	0.03	0.04	0.01
			Fe2	4f	4	0.00	3.52	0.00	-0.03	4.07	-0.02
0.404	Sr ₃ NaRuO ₆	15.89	Ru	6d	2	1.00	0.00	0.00	2.01	-0.01	0.00
0.405	CsNaCoF ₄	82.41	Co1	4f	3	0.00	0.00	3.50	0.00	0.00	3.18
			Co2	8g	3	0.00	0.00	-2.80	0.00	-0.01	-3.18
			Co3	8g	3	0.00	0.00	3.50	0.01	-0.01	3.18
0.416	LaCrO ₃	167.103	Cr	6b	3	0.00	0.00	1.67	0.00	0.00	2.80
0.417	LaCrO ₃	62.448	Cr	4b	3	0.98	0.00	0.00	2.82	-0.02	-0.03
0.420	Sr ₂ LuRuO ₆	14.75	Ru	2c	2	3.90	0.00	0.00	2.04	0.00	0.00
0.432	KMnF ₃	62.448	Mn	4a	4	0.00	0.00	4.8	0.00	0.01	4.65
0.433	KMnF ₃	140.541	Mn	4c	4	0.00	0.00	1.00	0.00	0.00	4.65
0.45	La ₂ NiO ₄	56.369	Ni	4a	6	1.68	0.00	0.00	1.68	-0.00	-0.01
0.475	Sr ₂ TbIrO ₆	14.75	Tb	2b	6	0.00	0.00	6.60	0.01	0.11	11.95
0.499	UCr ₂ Si ₂ C	47.252	Cr1	1f	3	0.66	0.00	0.00	0.00	0.01	0.00
			Cr2	1d	3	-0.66	0.00	0.00	-0.01	-0.00	-0.00
0.50	MnTiO ₃	9.39	Mn	6a	4	3.91	0.00	0.00	4.59	0.00	0.00
0.501	LiFe ₂ F ₆	136.499	Fe	4e	4	0.00	0.00	4.43	0.00	0.00	4.11
0.513	YRuO ₃	62.448	Ru	4b	2	0.00	0.00	0.33	0.00	0.00	0.41
0.528	CrSb	194.268	Cr	2a	3	0.00	0.00	2.45	0.00	0.00	3.54
0.56	Ba ₂ CoGe ₂ O ₇	35.167	Co	2c	3	2.05	2.05	0.00	1.89	1.89	0.00
0.575	ZnFeF ₅ (H ₂ O) ₂	44.229	Fe	4c	4	0.00	3.78	0.00	0.00	4.34	0.00
0.581	FeF ₃	15.89	Fe	6d	4	4.45	0.00	0.00	4.33	-0.01	0.00
0.586	YCrO ₃	62.448	Cr	4b	3	2.96	0.00	0.00	2.83	-0.05	-0.06
0.587	TmCrO ₃	62.448	Cr	4b	3	2.58	0.00	0.00	2.84	0.00	0.00

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ID	Compound	MSG	Element	Wyckoff	U	M_x^{in}	M_y^{in}	M_z^{in}	M_x^{out}	M_y^{out}	M_z^{out}
0.591	ErCrO ₃	62.448	Cr	4b	3	2.45	0.00	0.00	2.83	0.00	0.00
0.592	DyCrO ₃	62.446	Cr	4b	3	0.00	0.00	2.60	0.00	0.00	2.80
0.607	RuO ₂	136.499	Ru	2a	2	0.00	0.00	1.50	0.00	0.00	1.11
0.608	PrMnO ₃	62.448	Mn	4b	4	0.00	1.77	0.00	0.00	3.87	0.00
0.609	NdMnO ₃	11.50	Mn1	2b	4	-1.01	1.38	0.00	-2.22	3.01	0.00
			Mn2	2c	4	-1.01	1.38	0.00	-2.17	3.05	0.00
0.62	SrMn ₂ V ₂ O ₈	45.237	Mn	8c	4	0.00	-3.99	0.00	0.00	-4.50	-0.01
0.642	LaMnO ₃	62.448	Mn	4a	4	3.71	0.00	0.00	3.82	0.01	0.04
0.65	α -Fe ₂ O ₃	15.89	Fe1	12f	4	4.12	0.00	0.00	4.12	0.00	0.00
0.66	α -Fe ₂ O ₃	2.4	Fe1	6i	4	0.78	0.00	4.15	0.76	0.00	4.05
0.708	CrNb ₄ S ₈	194.268	Cr	2a	2	0.00	0.00	1.50	0.00	0.00	3.12
0.712	VNb ₃ S ₆	20.33	V1	2b	3	1.50	0.00	0.00	1.99	0.00	0.00
0.714	Li ₂ Ni(SO ₄) ₂	14.75	Ni	2a	6	2.29	0.00	0.00	1.82	0.00	0.00
0.722	Mn ₄ Nb ₂ O ₉	9.37	Mn	4a	4	0.00	0.00	-2.68	0.00	0.00	-4.48
0.748	Ba ₃ NiRu ₂ O ₉	194.268	Ni	2a	6	0.00	0.00	1.70	0.00	0.00	1.80
			Ru	4f	2	0.00	0.00	1.50	0.00	0.00	1.91
0.755	Mn ₂ SeO ₃ F ₂	62.448	Mn	8d	4	0.00	0.00	4.34	0.00	0.00	4.65
0.757	CeFeO ₃	62.448	Fe	4b	4	3.85	0.00	0.00	4.12	0.00	0.00
0.758	CeFeO ₃	62.441	Fe	4b	4	0.00	4.05	0.00	0.00	4.12	0.00
0.760	FeOHSeO ₄	15.89	Fe	4c	4	0.00	4.09	0.00	-0.01	4.26	-0.02
0.784	NdCoO ₃	62.441	Nd	4b	4	0.00	0.00	1.39	0.00	0.00	2.90
0.786	NdVO ₃	11.54	V1	2b	3	-0.48	-0.79	0.00	-0.93	-1.53	0.00
			V2	2c	3	0.48	0.79	0.00	0.93	1.53	0.00
0.787	YVO ₃	62.446	V	4b	3	0.00	0.00	1.72	0.02	-0.02	1.80
0.79	CaIrO ₃	63.464	Ir	4a	2	0.00	0.00	1.00	0.00	0.05	0.52
0.792	Sr ₂ HoRuO ₆	14.75	Ho	2b	6	0.00	0.00	6.66	0.00	0.00	3.98
			Ru	2c	2	0.00	0.00	2.74	0.00	0.00	2.00
0.794	Sr ₂ HoRuO ₆	14.75	Ho	2b	6	0.97	0.00	-7.87	2.49	0.00	-3.10
			Ru	2c	2	0.22	1.94	-1.79	0.945	0.00	-1.181
0.795	Sr ₂ YRuO ₆	14.75	Ru	2a	2	2.16	0.00	-0.41	2.02	0.00	-0.37
0.800	MnTe	63.457	Mn	2a	4	4.62	4.62	0.00	3.17	3.17	0.00
0.802	CuFeS ₂	122.333	Fe	4b	4	0.00	0.00	3.85	0.00	0.00	3.70
0.811	Fe ₂ WO ₆	60.423	Fe1	4c	4	0.00	0.00	2.55	0.01	0.00	4.22
			Fe2	4c	4	0.00	0.00	2.15	0.01	0.00	4.16
0.813	Fe ₂ WO ₆	60.423	Fe1	4c	4	0.00	0.00	3.60	0.01	0.00	4.21
			Fe2	4c	4	0.00	0.00	4.50	0.00	0.00	4.15
0.823	Sr ₂ MnGaO ₅	46.243	Mn	4a	4	3.16	0.00	0.00	3.76	-0.01	0.00
0.825	Ca ₂ MnGaO ₅	62.447	Mn	4a	4	0.00	3.60	0.00	0.00	3.79	0.02
0.83	LiFeP ₂ O ₇	4.7	Fe	2a	4	4.84	0.00	0.90	4.24	0.00	0.79
0.836	DyFeO ₃	62.448	Fe	4b	4	3.60	0.00	0.00	4.13	0.00	0.00
0.837	DyFeO ₃	62.448	Fe	4b	4	3.70	0.00	0.00	4.13	0.00	0.00
0.838	DyFeO ₃	62.448	Fe	4b	4	3.90	0.00	0.00	4.13	0.00	0.00
0.839	DyFeO ₃	62.448	Fe	4b	4	4.00	0.00	0.00	4.13	0.00	0.00
0.840	DyFeO ₃	62.441	Fe	4b	4	0.00	4.00	0.00	0.00	4.13	0.00
0.841	DyFeO ₃	62.441	Fe	4b	4	0.00	4.00	0.00	0.00	4.13	0.00
0.896	NiCrO ₄	63.457	Ni	4a	6	0.64	0.00	0.00	1.74	0.00	0.00
0.917	Sr ₂ ScOsO ₆	14.75	Os	2c	2	1.60	0.00	0.00	2.13	0.00	-0.20

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ID	Compound	MSG	Element	Wyckoff	U	M_x^{in}	M_y^{in}	M_z^{in}	M_x^{out}	M_y^{out}	M_z^{out}
0.934	$\text{Sr}_2\text{NiTeO}_6$	14.75	Ni	2d	6	1.18	0.00	1.34	1.19	0.00	1.34
0.936	$\text{Sr}_2\text{MnTeO}_3$	14.75	Mn	2a	4	4.55	0.00	0.00	4.57	0.00	0.00
0.937	$\text{Sr}_2\text{CoTeO}_6$	14.75	Co	2a	3	1.18	0.00	1.91	1.45	-0.05	2.26
0.947	YCrO_3	62.448	Cr	4b	3	0.00	0.00	-2.45	0.05	0.06	-2.83
0.955	$\text{Na}_2\text{Mn}(\text{H}_2\text{C}_3\text{O}_4)_2(\text{H}_2\text{O})_2$	61.433	Mn	4b	4	0.00	0.00	4.42	0.00	0.00	4.63
0.967	$\text{BaMn}_2\text{V}_2\text{O}_8$	45.237	Mn	8c	4	2.40	0.00	0.00	4.55	0.00	0.00
0.979	TmVO_3	62.446	V	4a	3	0.00	1.25	0.00	0.00	1.78	0.00
0.980	TmVO_3	62.446	V	4a	4	0.00	1.30	0.00	0.00	1.80	0.00
0.982	TmVO_3	14.75	V1	2c	6	0.93	0.36	0.00	1.67	0.62	0.00
			V2	2d	2	0.93	0.36	0.00	1.66	0.66	0.00
0.983	TmVO_3	14.75	V1	2c	6	0.99	0.00	0.00	1.80	0.00	0.00
			V2	2d	2	-0.99	0.00	0.00	-1.79	0.00	0.00
0.984	TmVO_3	62.446	V	4a	4	0.00	0.00	1.20	0.00	0.00	1.79
0.991	HoFeO_3	62.448	Fe	4a	4	4.60	0.00	0.00	4.10	0.00	0.00
0.999	Fe_4O_5	36.174	Fe1	4a	4	0.00	0.00	-3.00	0.00	0.00	-3.62
			Fe2	4a	4	0.00	0.00	3.00	0.00	-0.02	4.04
			Fe3	4a	4	0.00	0.00	3.00	-0.00	-0.06	4.11
			Fe4	4a	4	0.00	0.00	3.00	0.00	0.02	4.01
1.026	RbCoBr_3	193.259	Co1	2b	3	0.00	0.00	3.40	0.00	0.00	2.55
			Co2	4d	3	0.00	0.00	-3.40	0.00	0.00	-2.55
1.0.39	BaMnO_3	193.259	Mn1	2b	4	0.00	0.00	3.00	0.00	0.00	2.88
			Mn2	4d	4	0.00	0.00	-3.00	0.00	0.00	-2.88
1.0.47	MnSe_2	61.433	Mn1	4a	4	1.00	0.00	0.00	4.50	0.00	0.00
			Mn2	8c	4	1.00	0.00	0.00	4.50	0.00	0.00
1.0.48	MnSe_2	29.102	Mn1	4a	4	2.80	0.00	0.00	4.51	0.01	-0.01
			Mn2	4a	4	-2.80	0.00	0.00	-4.51	0.00	0.00
			Mn3	4a	4	-2.80	0.00	0.00	-4.51	0.03	-0.06
1.0.9	CsCoCl_3	193.259	Co1	2b	3	0.00	0.00	-2.80	-0.00	-0.00	-2.63
			Co2	4d	3	0.00	0.00	2.66	0.00	0.00	2.63
1.522	CrVO_4	2.4	Cr1	2a	3	1.87	0.92	0.33	2.58	1.26	0.45
			Cr2	2b	3	-1.87	-0.92	-0.33	-2.58	-1.26	-0.45