Electronic, Topological, and Magneto-Optical Properties of NiFeMnSn: A First-Principles Study

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Mechanical Properties

Table S1: Mechanical properties of NiFeMnSn

Mechanical properties	**Voigt**	**Reuss**	**Hill**
Bulk modulus (GPa)	155.12	155.12	155.12
Shear modulus (GPa)	76.96	62.65	69.80
Young's modulus (GPa)	198.13	165.65	181.89
Poisson's ratio (GPa)	0.28	0.32	0.30
Bulk/Shear (Pugh's) ratio	2.01	2.47	2.22

Table S2: Mirror parity of Mn atomic orbitals with respect to the mirror plane $M_{(110)}$ along the W–K–U high-symmetry path.

Orbital Type	**Orbital**	**Functional Form**	**Mirror Parity**
d	d_{xy}	xy	$+1$
	d_{z^2}	z^2	$+1$
	$d_{x^2-y^2}$	x^2-y^2	-1
	d_{xz}	xz	-
	d_{yz}	yz	-
d (combinations)	$d_{xz}+d_{yz}$	$xz+yz$	$+1$
	$d_{xz}-d_{yz}$	$xz-yz$	-1

Table S3: Mirror parity of atomic orbitals with respect to the mirror plane $M_{1\bar{1}0}$ relevant for the X–W–U plane.

Orbital Type	**Orbital**	**Mirror Parity**
d	d_{xy}	$+1$
	d_{z^2}	$+1$
	$d_{x^2-y^2}$	-1
	d_{xz}	-
	d_{yz}	-
d (combinations)	$d_{xz}+d_{yz}$	$+1$
	$d_{xz}-d_{yz}$	-1

Table S4: Mirror parity of atomic orbitals with respect to the mirror plane M_z, relevant for the $X - \Gamma - K$ path.

Orbital Type	**Orbital**	**Mirror Parity**
d	d_{xy}	$+1$
	$d_{x^2-y^2}$	$+1$
	d_{z^2}	$+1$
	d_{xz}	-1
	d_{yz}	-1

Table S5: Momentum coordinates (k_x, k_y, k_z) and chirality of the Weyl points obtained after including spin–orbit coupling (SOC). All k values are given in reciprocal lattice units.

S.No.	Weyl Point	k_x	k_y	k_z	Chirality
1	W1+	0.090520	0.164950	-0.652880	1
2	W1-	0.101470	0.163370	-0.643380	-1
3	W2+	0.003890	0.501820	-0.012800	1
4	W2-	0.005120	0.500460	0.016370	-1
5	W3+	0.500390	0.000460	-0.020290	1
6	W3-	0.501960	0.002610	0.011890	-1
7	W4-	0.161310	0.177900	-0.538490	-1
8	W4+	0.144310	0.207580	-0.534200	1
9	W5+	0.007710	-0.502880	-0.017800	1
10	W5-	0.008120	-0.501180	0.019620	-1
11	W6+	-0.500690	-0.004140	-0.022140	1
12	W6-	-0.502520	-0.007100	0.016900	-1
13	W7+	-0.148010	-0.211020	-0.526860	1
14	W7-	-0.164610	-0.176300	-0.538820	-1
15	W8-	0.214250	-0.152650	0.518590	-1
16	W8+	0.176270	-0.164920	0.537820	1
17	W9-	-0.218130	0.149040	0.519070	-1
18	W9+	-0.174340	0.163280	0.538970	1
19	W10-	-0.479010	-0.411880	-0.018200	-1
20	W10+	-0.469650	-0.403610	0.034800	1
21	W11-	0.408930	-0.475410	-0.024720	-1
22	W11+	0.405050	-0.473530	0.030090	1
23	W12-	0.159230	-0.101700	-0.644180	-1
24	W12+	0.133910	-0.061600	-0.681530	1
25	W13+	0.109320	0.162400	0.632740	1
26	W13-	0.070310	0.135490	0.678790	-1
27	W14-	-0.121120	0.070240	0.684520	-1
28	W14+	-0.159610	0.111910	0.636010	1
29	W15+	-0.267290	0.265690	-0.269040	1
30	W15-	-0.272290	0.342290	-0.252820	-1
31	W16+	-0.669450	0.213830	-0.016800	1
32	W16-	-0.701450	0.286380	-0.000020	-1
33	W17-	-0.266680	-0.267920	0.269850	-1
34	W17+	-0.346320	-0.276220	0.245810	1
35	W18-	-0.207590	-0.670780	0.019020	-1
36	W18+	-0.284340	-0.700570	-0.000150	1

Table S6: Momentum coordinates (k_x, k_y, k_z) and chirality of the Weyl points obtained after including spin–orbit coupling (SOC). All k values are given in reciprocal lattice units.

S.No.	Weyl Point	k_x	k_y	k_z	Chirality
37	W19-	0.204280	0.671020	0.022480	-1
38	W19+	0.285060	0.701640	0.000070	1
39	W20-	0.363620	0.298620	-0.213410	-1
40	W20+	0.408200	0.342340	-0.142400	1
41	W21+	-0.299200	0.361420	0.214760	1
42	W21-	-0.341740	0.407500	0.143650	-1
43	W22+	-0.409410	-0.346570	-0.137890	1
44	W22-	-0.366220	-0.300890	-0.209680	-1