Supplementary Information (SI) for Journal of Materials Chemistry C.

# Orbital-Engineered Anomalous Hall Conductivity in Stable Full Heusler Compounds: A Pathway to Optimized Spintronics

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Table S1. The Anomalous Hall Conductivity ($|\sigma_{xy}|$) alongside the stability and magnetic characteristics for $Co_2MnZ$ family. The table lists the stable phase, formation energy (ΔF in eV/atom), $|\sigma_{xy}|$ (S/Cm), total magnetic moment ($M_{tot}$ in $\mu_B$), spin polarization (P in %).

| $Co_2MnZ$ | Stable phase | ΔF eV/atom | $\|\sigma_{xy}\|$ S/Cm | $M_{tot}$ $\mu_B$ | P % |
|---|---|---|---|---|---|
| $Co_2MnAl$ | $l2_1$ | -0.385<br>-0.356[a] | 1647<br>1631[b], 1600-2000[c] | 4.14<br>4.04 [b] 4.01[f] | 63<br>68[e] |
| $Co_2MnGa$ | $l2_1$ | -0.268<br>-2.237[a] | 1046<br>845-1260[d] | 4.09<br>4.11[b], 4.05[f] | 73<br>66[e], 55[g] |
| $Co_2MnB$ | $l2_1$ | 0.017<br>0.032[a] | 447<br>598 [b], 433[e] | 4.03 | 82 |
| $Co_2MnIn$ | $l2_1$ | 0.024<br>0.064[a] | 378 | 4.43<br>4.52[b] | 27<br>31[e] |
| $Co_2MnGe$ | $l2_1$ | -0.272<br>-0.257[a] | 235<br>253 [b], 228[e] | 4.99<br>5.00 [b], 5.11[f] | 99<br>100 [e], 90 [g] |
| $Co_2MnBi$ | $l2_1$ | 0.222<br>0.227[a] | 218 | 5.92<br>5.07 [f] | 93 |
| $Co_2MnSn$ | $l2_1$ | -0.132<br>-0.139[a] | 183<br>176 [b], 174[e] | 5.00<br>5.04[b], 5.08 [f] | 77<br>75[e] |
| $Co_2MnAs$ | $l2_1$ | -0.115<br>-0.129[a] | 173<br>178 [b] | 5.62<br>5.98 [b] 4.90[g] | 33 |
| $Co_2MnSi$ | l21 | -0.467<br>-0.449[a] | 172<br>187 [b], 193[e] | 5.03<br>5.00 [b] | 1<br>100[e], 93[g] |
| $Co_2MnPb$ | $l2_1$ | 0.217<br>0.240[a] | 31 | 5.06 | 65 |
| $Co_2MnSb$ | $l2_1$ | -0.104<br>-0.094[a] | 25 | 5.95<br>5.96 [b] 4.9 [f] | 100 |

[a] Theoretical data[1]

[b] Theoretical data[2]

[c] Experiment data[3]

[d] Experiment data[4]

[e] Theoretical data[5]

[f] Experiment data[6]

[g] Experiment data[7]

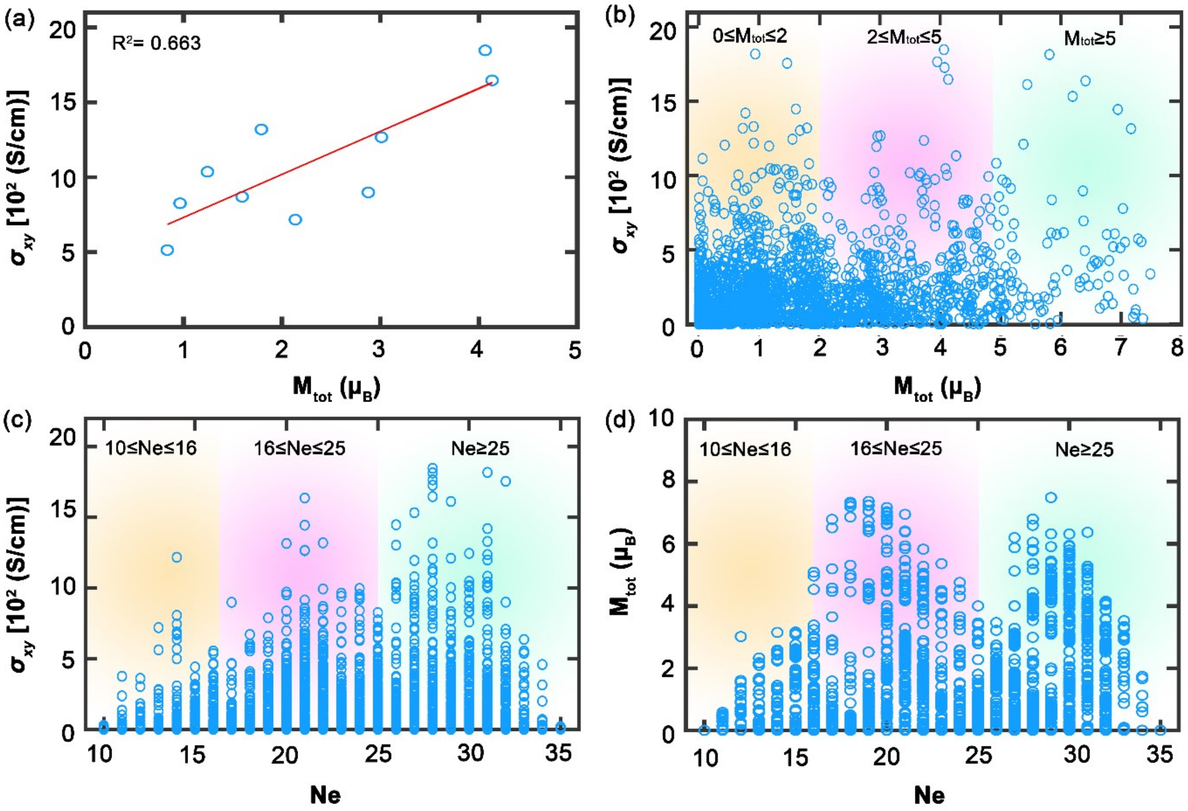

**Figure S1.** Anomalous Hall conductivity $\sigma_{xy}$ as a function of total magnetic moment $M_{tot}$ for data in (a) table 1 and (b) whole data. Yellow, purple, and cyan backgrounds distinguish three areas $0 \leq M_{tot} \leq 2$, $2 \leq M_{tot} \leq 5$, and $M_{tot} \geq 5$, respectively. (c) $\sigma_{xy}$ and (d) $M_{tot}$ as a function of total valance electrons Ne. Yellow, purple, and cyan backgrounds distinguish three areas 10≤Ne≤16, 16≤Ne≤25, and Ne≥25, respectively.

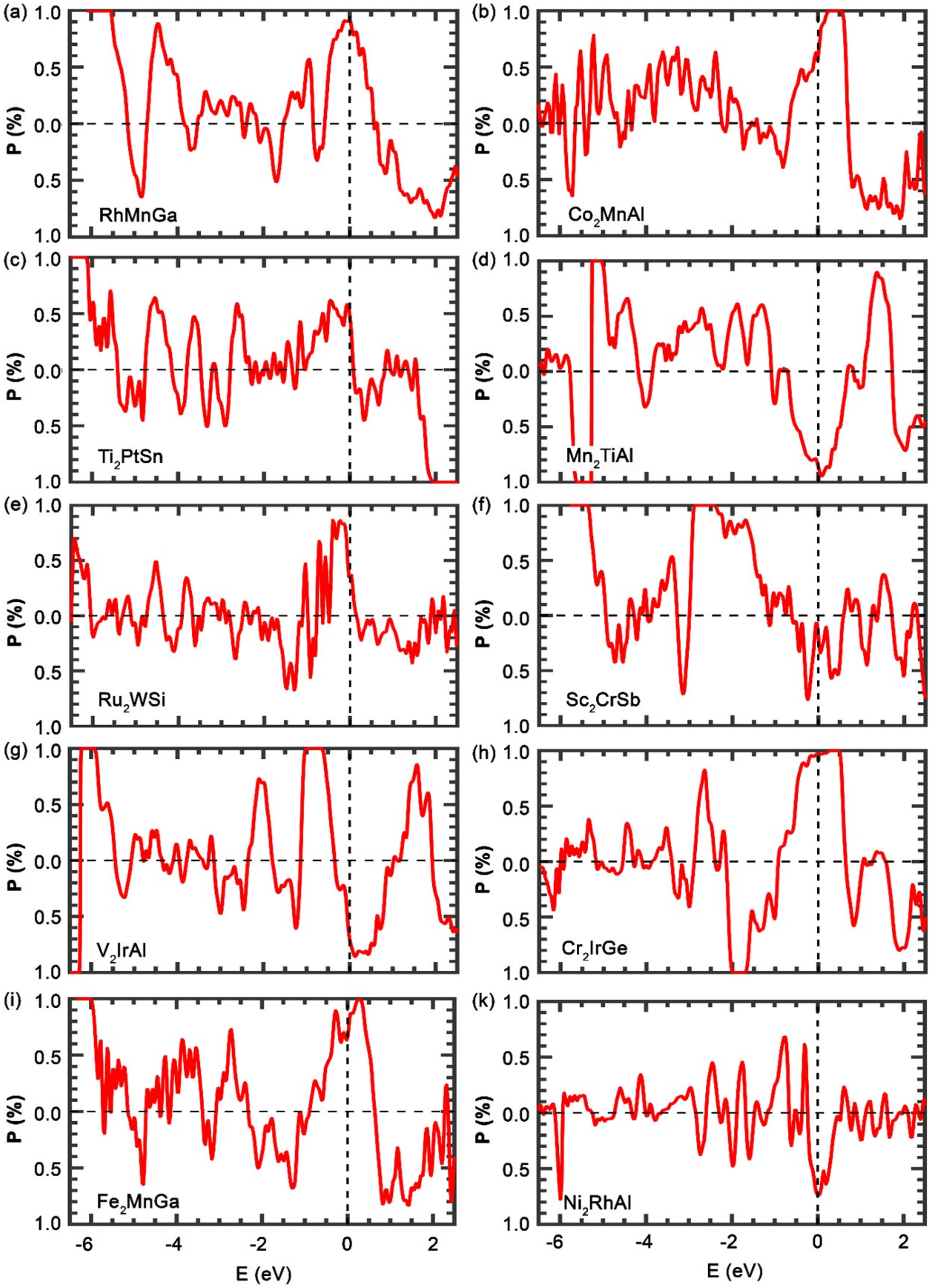

**Figure S2.** Spin polarization P (%) as the function of energy. for selected compounds (a) $Rh_2MnGa$, (b) $Co_2MnAl$, (c) $Ti_2PtSn$, (d) $Mn_2TiAl$, (e) $Ru_2WSi$, (f) $Sc_2CrSb$, (g) $V_2IrAl$, (h) $Cr_2IrGe$, (i) $Fe_2MnGa$, and (k) $Ni_2RhAl$. $E_F$ is set to zero.

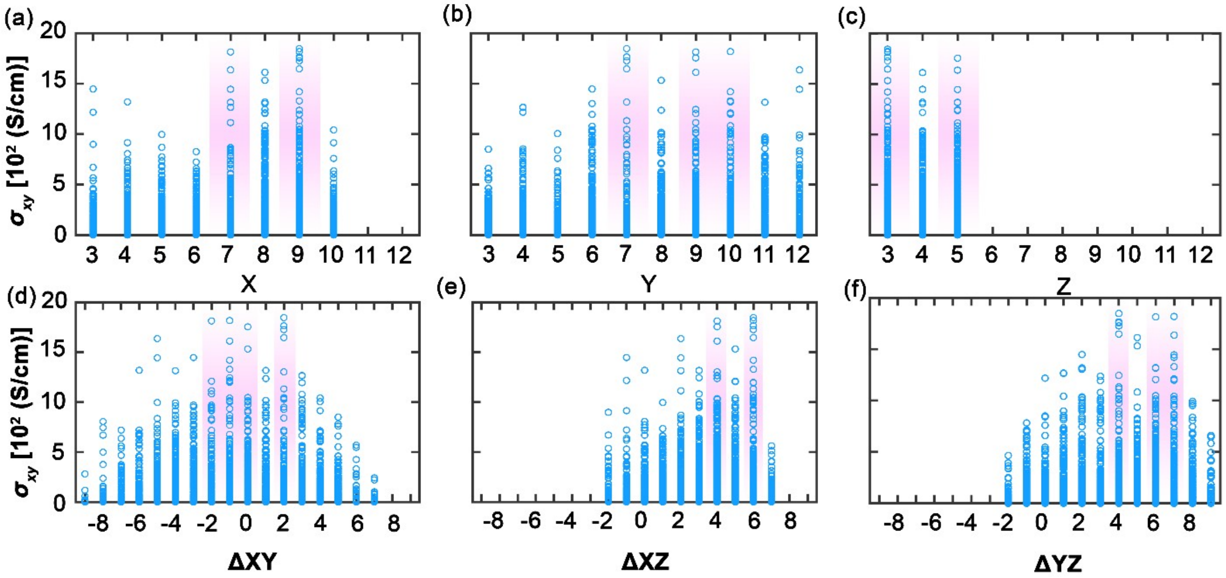

**Figure S3.** Anomalous Hall conductivity ($\sigma_{xy}$) as a function of valence electrons for (a) X, (b) Y, and (c) Z elements. $\sigma_{xy}$ as a function of valence electron differences between (d) X and Y (ΔXY), (e) X and Z (ΔXZ), and (f) Y and Z (ΔYZ). Purple backgrounds distinguish areas exhibiting large $\sigma_{xy.}$

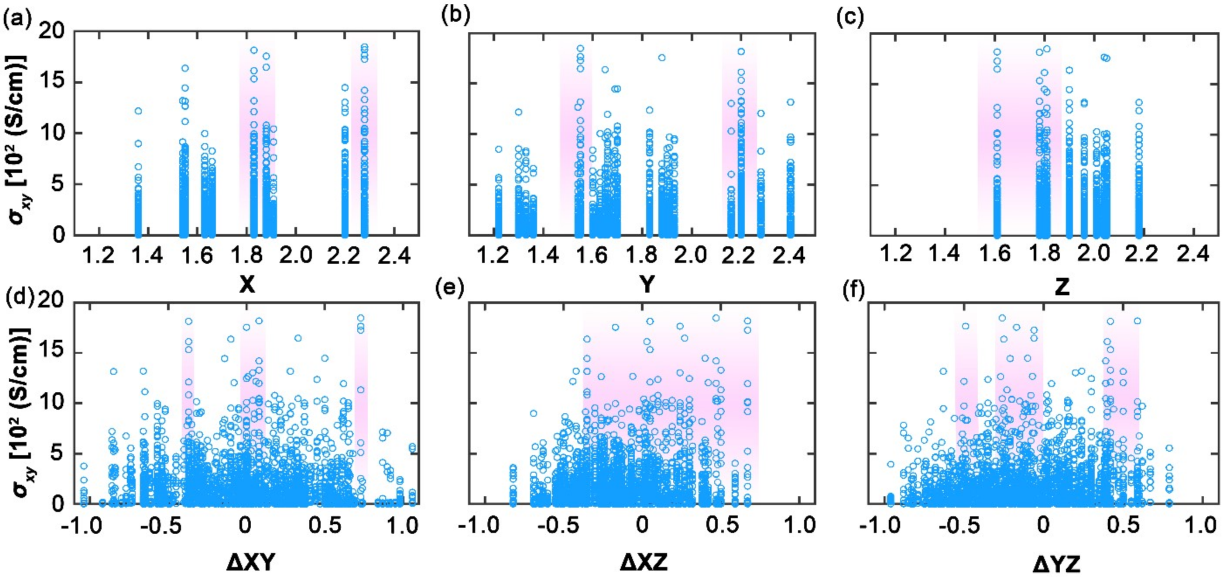

**Figure S4.** Anomalous Hall conductivity ($\sigma_{xy}$) as a function of electronegativity for (a) X, (b) Y, and (c) Z elements. $\sigma_{xy}$ as a function of electronegativity differences between (d) X and Y (ΔXY), (e) X and Z (ΔXZ), and (f) Y and Z (ΔYZ). Purple backgrounds distinguish areas exhibiting large $\sigma_{xy}$.

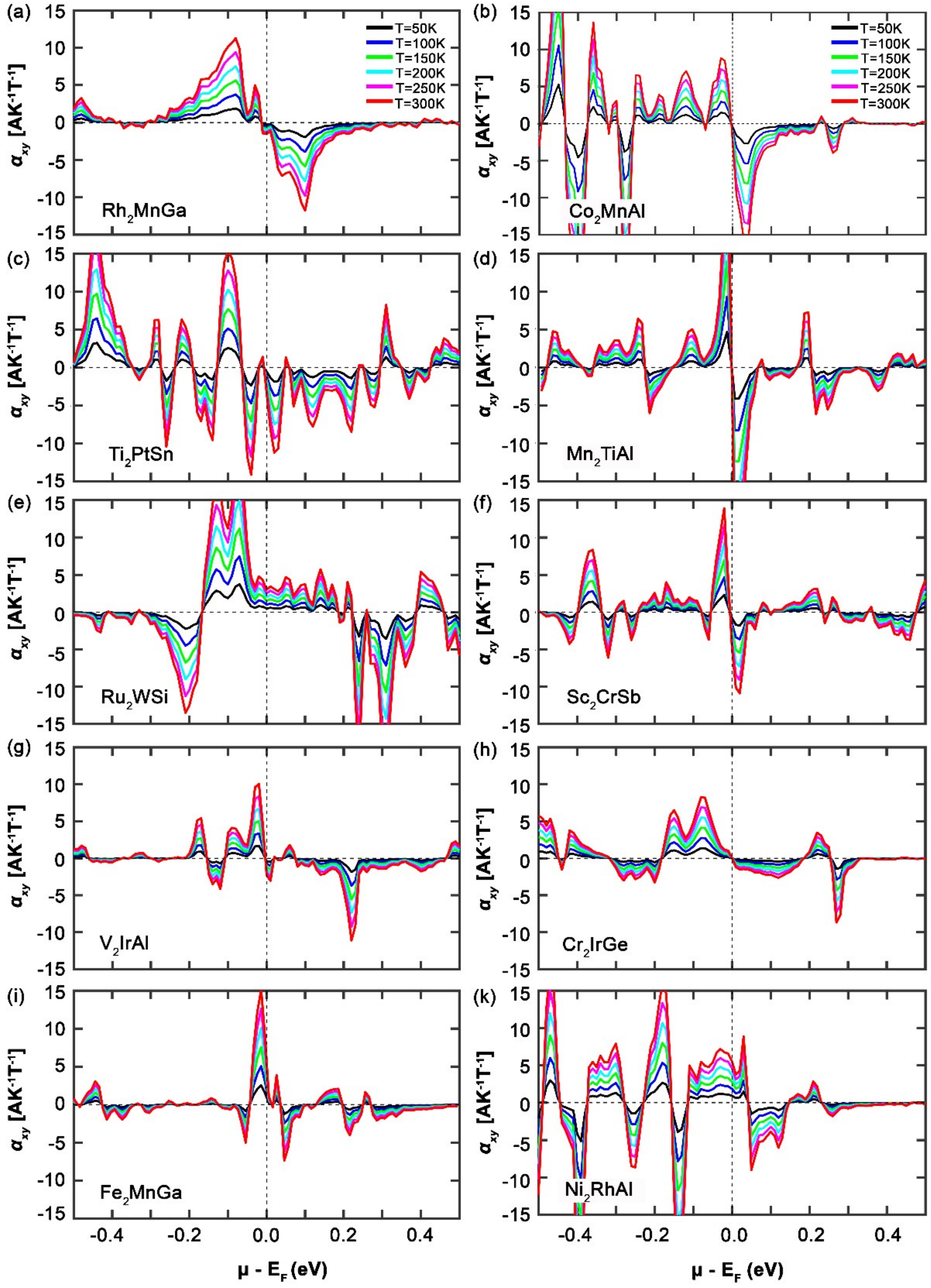

**Figure S5.** Anomalous Nernst conductivity ($\alpha_{xy}$) as a function of chemical potential μ for selected compounds (a) $Rh_2MnGa$, (b) $Co_2MnAl$, (c) $Ti_2PtSn$, (d) $Mn_2TiAl$, (e) $Ru_2WSi$, (f) $Sc_2CrSb$, (g) $V_2IrAl$, (h) $Cr_2IrGe$, (i) $Fe_2MnGa$, and (k) $Ni_2RhAl$. $E_F$ is set to zero.

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