# Supplementary Material

## 1 SUPPLEMENTARY TABLES

In this section we list the important results of the calculations in tabular form. Listed in Table S1 are the calculated lattice constants, cohesive energy, and formation energy of the considered Heusler compounds. Table S2 lists the calculated magnetic ground state, total spin moment, atomic spin magnetic moments, magnetization energy, spin polarization, Curie temperature, as well as the total magnetization derived by Slater-Pauling rule. Mechanical properties of the Heusler compounds are listed in Table S3, it includes elastic constants, bulk modulus $B$, shear modulus $G$, Young's modulus $E$, anisotropy factor $A$, Poisson's ratio $\nu$, and Pugh's ratio $B/G$. Table S4 lists calculated thermodynamics related results such as the density $\rho$, longitudinal $v_l$, transverse $v_t$, average $v_m$ sound velocity, Debye temperature $\Theta_D$, melting temperature $T_m$, and minimum thermal conductivity $\kappa_{min}$.

**Table S1.** Calculated equilibrium lattice constant (Å), cohesive energy (eV/f.u.), and formation energy (eV/f.u.) of $X_2YZ$ Heusler alloys. $L2_1$ and XA denote the normal and inverse structure, respectively.

| $X_2YZ$ | stru-cture | lattice constant Å | | | cohesive energy eV/f.u. | | | formation energy eV/f.u. | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | Z= Al | Ga | Si | Z= Al | Ga | Si | Z= Al | Ga | Si |
| $Fe_3Z$ | $L2_1$ | 5.736 | 5.750 | 5.601 | 19.870 | 18.691 | 21.449 | -0.924 | -0.603 | -1.479 |
| $Fe_2CrZ$ | $L2_1$ | 5.658 | 5.680 | 5.583 | 18.621 | 17.297 | 20.074 | -1.131 | -0.665 | -1.561 |
| | XA | 5.785 | 5.810 | 5.649 | 18.257 | 17.222 | 19.973 | -0.768 | -0.590 | -1.460 |
| $Cr_2FeZ$ | $L2_1$ | 5.889 | 5.845 | 5.687 | 16.513 | 15.505 | 17.882 | -0.480 | -0.330 | -0.825 |
| | XA | 5.754 | 5.777 | 5.616 | 17.102 | 15.916 | 18.795 | -1.069 | -0.740 | -1.738 |
| $Cr_3Z$ | $L2_1$ | 5.909 | 5.917 | 5.726 | 15.809 | 14.783 | 17.475 | -1.233 | -1.064 | -1.874 |
| $Fe_2MnZ$ | $L2_1$ | 5.668 | 5.692 | 5.582 | 18.553 | 17.318 | 20.231 | -0.939 | -0.561 | -1.593 |
| | XA | 5.730 | 5.724 | 5.589 | 18.318 | 17.006 | 19.986 | -0.703 | -0.248 | -1.347 |
| $Mn_2FeZ$ | $L2_1$ | 5.705 | 5.729 | 5.623 | 16.757 | 15.640 | 15.189 | -0.473 | -0.214 | 2.119 |
| | XA | 5.743 | 5.772 | 5.577 | 17.175 | 16.048 | 14.797 | -0.891 | -0.622 | 2.510 |
| $Mn_3Z$ | $L2_1$ | 5.787 | 5.814 | 5.641 | 15.778 | 14.709 | 17.664 | -0.826 | -0.614 | -1.687 |
| $Fe_2CoZ$ | $L2_1$ | 5.726 | 5.756 | 5.583 | 19.744 | 18.541 | 21.104 | -0.744 | -0.399 | -1.081 |
| | XA | 5.700 | 5.720 | 5.602 | 20.213 | 18.970 | 21.687 | -1.214 | -0.828 | -1.664 |
| $Co_2FeZ$ | $L2_1$ | 5.699 | 5.717 | 5.623 | 20.636 | 19.343 | 21.684 | -1.583 | -1.147 | -1.607 |
| | XA | 5.686 | 5.717 | 5.577 | 19.941 | 18.692 | 21.293 | -0.887 | -0.496 | -1.215 |
| $Co_3Z$ | $L2_1$ | 5.672 | 5.693 | 5.578 | 20.148 | 18.854 | 21.338 | -1.041 | -0.604 | -1.207 |

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**Table S2.** Calculated magnetic ground state, total spin magnetization ($m_t$), atomic spin magnetization ($m_{X(1)}$, $m_{X(2)}$, $m_Y$ and $m_Z$ for X(1), X(2), Y, and Z atom, respectively), total magnetization $M_t = N_v$-24 given from Slater-Pauling rule, magnetization energy $E_M = E_{FM}$-$E_{NM}$, spin polarization P and Curie temperature $T_c$. FM, Fi, AHM, and HM are ferromagnetic, ferrimagnetic, antiferromagnetic, and half-metallic metal, respectively. $L2_1$ and XA denote the normal and inverse structure, respectively.

| $X_2YZ$ | stru-cture | mag. state | $m_t$ $\mu_B$/f.u. | $m_{X(1)}$ | $m_{X(2)}$ $\mu_B$/atom | $m_Y$ | $m_Z$ | $M_t$ $\mu_B$/f.u. | $E_M$ eV/f.u. | P % | $T_c$ K |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $Fe_3Al$ | $L2_1$ | FM | 5.95 | 1.87 | 1.87 | 2.38 | -0.06 | 3 | -1.1018 | -48.875 | 710 (713[b]) |
| $Fe_2CrAl$ | $L2_1$ | Fi2 | 1.00 | -0.10 | -0.10 | 1.19 | -0.01 | 1 | -0.0724 | 98.385 | 93 |
| | XA | Fi3 | 2.38 | 1.74 | 2.38 | -1.68 | -0.01 | 1 | -0.8937 | -30.323 | 1152 |
| $Cr_2FeAl$ | $L2_1$ | Fi2 | 0.94 | 1.68 | 1.68 | -2.60 | -0.01 | 1 | -0.6649 | -46.581 | 857 |
| | XA | Fi2 | 1.01 | 1.49 | -1.17 | 0.67 | -0.00 | 1 | -0.1149 | -96.599 | 148 |
| $Cr_3Al$ | $L2_1$ | Fi2 | 2.92 | 2.22 | 2.22 | -1.64 | -0.01 | 3 | -0.4313 | -66.422 | 278 |
| $Fe_2MnAl$ | $L2_1$ | Fi2 | 2.00 | -0.18 | -0.18 | 2.34 | -0.01 | 2 | -0.5970 | 78.925 | 770 |
| | XA | Fi3 | 1.95 | 1.43 | 2.32 | -1.74 | -0.00 | 2 | -0.7960 | 43.716 | 1026 |
| $Mn_2FeAl$ | $L2_1$ | Fi2 | -0.96 | 0.74 | 0.74 | -2.45 | -0.03 | 1 | -0.6163 | -90.811 | 795 |
| | XA | Fi1 | 1.00 | -1.76 | 2.63 | 0.13 | 0.01 | 1 | -0.4782 | 99.416 | 617 |
| $Mn_3Al$ | $L2_1$ | AF-HM | 0.00 | -1.40 | -1.40 | 2.79 | 0.02 | 0 | -0.4804 | 100.000 | 309 (342[a]) |
| $Fe_2CoAl$ | $L2_1$ | FM | 5.68 | 2.03 | 2.03 | 1.77 | -0.04 | 4 | -0.8675 | -57.675 | 1119 |
| | XA | FM | 4.98 | 1.59 | 2.53 | 1.03 | -0.05 | 4 | -1.2235 | -54.334 | 1578 (830[c]) |
| $Co_2FeAl$ | $L2_1$ | FM | 4.99 | 1.19 | 1.19 | 2.76 | -0.03 | 5 | -1.4923 | 79.433 | 1924 (1261[c]) |
| | XA | FM | 4.51 | 1.00 | 1.75 | 1.92 | -0.03 | 5 | -0.7502 | -55.171 | 967 |
| $Co_3Al$ | $L2_1$ | FM | 4.00 | 1.23 | 1.23 | 1.69 | -0.03 | 6 | -0.7049 | -68.590 | 454 |
| $Fe_3Ga$ | $L2_1$ | FM | 6.05 | 1.89 | 1.89 | 2.42 | -0.15 | 3 | -1.2222 | -48.428 | 788 |
| $Fe_2CrGa$ | $L2_1$ | Fi2 | 1.00 | -0.16 | -0.16 | 1.30 | -0.02 | 1 | -0.1184 | 99.082 | 153 |
| | XA | Fi3 | 2.23 | 1.76 | 2.48 | -1.99 | -0.03 | 1 | -1.0320 | -38.511 | 1331 |
| $Cr_2FeGa$ | $L2_1$ | FM | 5.00 | 1.78 | 1.78 | 1.33 | -0.02 | 1 | -0.5965 | 97.270 | 769 |
| | XA | Fi2 | 0.99 | 1.70 | -1.39 | 0.67 | 0.01 | 1 | -0.1482 | -96.130 | 191 |
| $Cr_3Ga$ | $L2_1$ | Fi2 | 2.87 | 2.27 | 2.27 | -1.75 | -0.00 | 3 | -0.4692 | -35.693 | 303 |
| $Fe_2MnGa$ | $L2_1$ | Fi2 | 2.03 | -0.26 | -0.25 | 2.48 | -0.02 | 2 | -0.7122 | 75.072 | 917 |
| | XA | Fi3 | 2.01 | 1.53 | 2.38 | -1.87 | -0.01 | 2 | -0.8738 | 59.656 | 1127 |
| $Mn_2FeGa$ | $L2_1$ | Fi2 | -0.99 | 0.79 | 0.79 | -2.53 | -0.04 | 1 | -0.7104 | -89.173 | 916 |
| | XA | Fi1 | 1.03 | -2.03 | 2.78 | 0.24 | -0.00 | 1 | -0.6920 | 96.560 | 892 |
| $Mn_3Ga$ | $L2_1$ | AF-HM | 0.01 | -1.53 | -1.53 | 2.99 | 0.05 | 0 | -0.7105 | 100.000 | 458 (482[a]) |
| $Fe_2CoGa$ | $L2_1$ | FM | 5.96 | 2.17 | 2.17 | 1.75 | -0.11 | 4 | -0.9114 | -72.853 | 1175 |
| | XA | FM | 5.13 | 1.68 | 2.57 | 1.01 | -0.13 | 4 | -1.3053 | -40.000 | 1683 |
| $Co_2FeGa$ | $L2_1$ | FM | 5.00 | 1.17 | 1.17 | 2.77 | -0.10 | 5 | -1.5135 | 74.957 | 1952 |
| | XA | FM | 4.80 | 1.09 | 1.73 | 2.11 | -0.10 | 5 | -0.7685 | -66.488 | 991 |
| $Co_3Ga$ | $L2_1$ | FM | 4.06 | 1.25 | 1.25 | 1.70 | -0.08 | 6 | -0.6843 | -70.627 | 441 |
| $Fe_3Si$ | $L2_1$ | FM | 5.04 | 1.30 | 1.30 | 2.53 | -0.05 | 4 | -1.0999 | -39.975 | 709 (840[b]) |
| $Fe_2CrSi$ | $L2_1$ | FM-HM | 2.00 | 0.25 | 0.25 | 1.51 | -0.02 | 2 | -0.2861 | 100.000 | 369 |
| | XA | Fi3 | 2.03 | 0.93 | 2.35 | -1.27 | 0.02 | 2 | -0.7130 | 41.296 | 919 |
| $Cr_2FeSi$ | $L2_1$ | Fi2 | 0.75 | -0.82 | -0.82 | 2.33 | 0.06 | 2 | -0.5936 | 2.475 | 765 |
| | XA | NM | 0.00 | | | | | 2 | 0.0000 | 0.000 | |
| $Cr_3Si$ | $L2_1$ | Fi2 | 1.86 | 1.39 | 1.39 | -0.96 | -0.02 | 4 | -0.0557 | -36.808 | 72 |
| $Fe_2MnSi$ | $L2_1$ | FM-HM | 3.00 | 0.22 | 0.22 | 2.53 | -0.01 | 3 | -0.9088 | 100.000 | 1172 |
| | XA | Fi3 | 3.06 | 0.88 | 2.34 | -0.18 | 0.01 | 3 | -0.6109 | 83.322 | 788 |
| $Mn_2FeSi$ | $L2_1$ | FM | 5.47 | 1.34 | 1.34 | 2.79 | 0.01 | 2 | -1.2635 | -58.811 | 1629 |
| | XA | FM | 3.97 | 0.90 | 1.59 | 1.58 | -0.03 | 2 | -0.5580 | -58.333 | 720 |
| $Mn_3Si$ | $L2_1$ | Fi2-HM | 1.00 | -0.81 | -0.81 | 2.54 | 0.04 | 1 | -0.4731 | 100.000 | 305 |
| $Fe_2CoSi$ | $L2_1$ | FM | 4.37 | 1.39 | 1.39 | 1.70 | -0.04 | 5 | -0.4714 | -78.869 | 608 |
| | XA | FM | 4.96 | 1.38 | 2.65 | 1.00 | -0.03 | 5 | -1.3151 | 76.749 | 1696 (1038[d]) |
| $Co_2FeSi$ | $L2_1$ | FM | 5.47 | 1.34 | 1.34 | 2.79 | 0.01 | 6 | -1.2635 | -58.811 | 1629 (1267[a]) |
| | XA | FM | 3.97 | 0.90 | 1.59 | 1.58 | -0.03 | 6 | -0.5580 | -58.333 | 720 |
| $Co_3Si$ | $L2_1$ | FM | 3.80 | 1.21 | 1.21 | 1.47 | -0.02 | 7 | -0.4630 | -65.662 | 298 |

[a] Theoretical Curie temperature from Kübler (2006). [b] Experimental Curie temperature from Burch et al. (1979). [c] Experimental Curie temperature from Ahmad et al. (2021). [d] Theoretical Curie temperature from Du et al. (2013)

**Table S3.** Calculated elastic constants $C_{ij}$, bulk modulus $B$, Voigt shear modulus $G_V$, Reuss shear modulus $G_R$, shear modulus $G$, Young's modulus $E$ (GPa), anisotropy factor $A$, Poisson's ratio $\nu$, and Pugh's ratio $B/G$ for the Heusler compounds. $L2_1$ and XA denote the normal and inverse structure, respectively.

| $X_2YZ$ | structure | $C_{11}$ | $C_{12}$ | $C_{44}$ | $B$ | $G_V$ | $G_R$ | $G$ | $E$ | $A$ | $\nu$ | $B/G$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | GPa | | | | arbitrary unit | | |
| $Fe_3Al$ | $L2_1$ | 213.1 | 154.9 | 138.7 | 174.3 | 94.9 | 55.3 | 75.1 | 197.0 | 4.8 | 0.31 | 2.3 |
| $Fe_2CrAl$ | $L2_1$ | 366.7 | 139.7 | 120.0 | 215.3 | 117.4 | 117.3 | 117.3 | 297.9 | 1.1 | 0.27 | 1.8 |
| | XA | 176.6 | 124.4 | 138.0 | 141.8 | 93.2 | 50.8 | 72.0 | 184.8 | 5.3 | 0.28 | 2.0 |
| $Cr_2FeAl$ | $L2_1$ | 238.8 | 136.7 | 134.5 | 170.7 | 101.1 | 81.3 | 91.2 | 232.3 | 2.6 | 0.27 | 1.9 |
| | XA | 277.6 | 121.9 | 108.7 | 173.8 | 96.4 | 93.8 | 95.1 | 241.3 | 1.4 | 0.29 | 1.8 |
| $Cr_3Al$ | $L2_1$ | 252.7 | 71.2 | 106.1 | 131.7 | 100.0 | 99.4 | 99.7 | 238.8 | 1.2 | 0.20 | 1.3 |
| $Fe_2MnAl$ | $L2_1$ | 309.6 | 136.5 | 166.7 | 194.2 | 134.6 | 121.7 | 128.2 | 315.1 | 1.9 | 0.23 | 1.5 |
| | XA | 208.5 | 112.3 | 145.5 | 144.4 | 106.5 | 80.4 | 93.4 | 230.6 | 3.0 | 0.23 | 1.5 |
| $Mn_2FeAl$ | $L2_1$ | 221.7 | 168.3 | 148.6 | 186.1 | 99.8 | 52.6 | 76.2 | 201.2 | 5.6 | 0.32 | 2.4 |
| | XA | 186.7 | 128.7 | 116.2 | 148.0 | 81.3 | 52.7 | 67.0 | 174.7 | 4.0 | 0.30 | 2.2 |
| $Mn_3Al$ | $L2_1$ | 119.1 | 151.6 | 108.0 | 140.8 | 58.3 | -52.6 | 2.8 | 8.4 | -6.6 | 0.49 | 50.0 |
| $Fe_2CoAl$ | $L2_1$ | 125.3 | 153.5 | 110.3 | 144.1 | 60.6 | -43.6 | 8.5 | 24.9 | -7.8 | 0.47 | 17.0 |
| | XA | 241.9 | 148.8 | 139.8 | 179.8 | 102.5 | 77.6 | 90.1 | 231.5 | 3.0 | 0.29 | 2.0 |
| $Co_2FeAl$ | $L2_1$ | 264.5 | 148.3 | 140.7 | 187.0 | 107.7 | 89.7 | 98.7 | 251.8 | 2.4 | 0.28 | 1.9 |
| | XA | 160.1 | 161.0 | 119.5 | 160.7 | 71.5 | -1.1 | 35.2 | 98.4 | -266.7 | 0.40 | 4.6 |
| $Co_3Al$ | $L2_1$ | 210.8 | 163.9 | 127.6 | 179.5 | 86.0 | 46.0 | 66.0 | 176.3 | 5.4 | 0.34 | 2.7 |
| $Fe_3Ga$ | $L2_1$ | 181.9 | 165.7 | 127.3 | 171.1 | 79.6 | 18.5 | 49.1 | 134.4 | 15.7 | 0.37 | 3.5 |
| $Fe_2CrGa$ | $L2_1$ | 338.1 | 158.5 | 109.6 | 218.4 | 101.6 | 100.7 | 101.2 | 262.9 | 1.2 | 0.30 | 2.2 |
| | XA | 172.6 | 129.7 | 132.3 | 144.0 | 88.0 | 43.1 | 65.5 | 170.7 | 6.2 | 0.30 | 2.2 |
| $Cr_2FeGa$ | $L2_1$ | 250.7 | 159.3 | 139.0 | 189.8 | 101.7 | 76.5 | 89.1 | 231.1 | 3.0 | 0.30 | 2.1 |
| | XA | 231.9 | 129.1 | 94.1 | 163.4 | 77.0 | 70.6 | 73.8 | 192.4 | 1.8 | 0.30 | 2.2 |
| $Cr_3Ga$ | $L2_1$ | 239.7 | 84.4 | 99.4 | 136.2 | 90.7 | 89.4 | 90.1 | 221.4 | 1.3 | 0.23 | 1.5 |
| $Fe_2MnGa$ | $L2_1$ | 289.3 | 148.0 | 158.0 | 195.1 | 123.1 | 105.7 | 114.4 | 287.1 | 2.2 | 0.25 | 1.7 |
| | XA | 182.9 | 122.2 | 141.3 | 142.4 | 96.9 | 57.4 | 77.2 | 196.1 | 4.7 | 0.27 | 1.8 |
| $Mn_2FeGa$ | $L2_1$ | 164.2 | 122.3 | 156.5 | 136.3 | 102.3 | 43.6 | 73.0 | 185.7 | 7.5 | 0.27 | 1.9 |
| | XA | 159.7 | 133.8 | 113.6 | 142.4 | 73.4 | 27.7 | 50.5 | 135.5 | 8.8 | 0.34 | 2.8 |
| $Mn_3Ga$ | $L2_1$ | 133.1 | 159.9 | 107.6 | 151.0 | 59.2 | -41.1 | 9.0 | 26.6 | -8.0 | 0.47 | 16.7 |
| $Fe_2CoGa$ | $L2_1$ | 133.2 | 160.7 | 92.2 | 151.5 | 49.8 | -44.3 | 2.7 | 8.2 | -6.7 | 0.49 | 55.4 |
| | XA | 197.3 | 154.8 | 132.4 | 168.9 | 87.9 | 42.8 | 65.4 | 173.7 | 6.2 | 0.33 | 2.6 |
| $Co_2FeGa$ | $L2_1$ | 253.7 | 161.1 | 129.8 | 192.0 | 96.4 | 75.4 | 85.9 | 224.3 | 2.8 | 0.31 | 2.2 |
| | XA | 152.2 | 169.5 | 106.9 | 163.8 | 60.7 | -24.6 | 18.0 | 52.2 | -12.4 | 0.45 | 9.1 |
| $Co_3Ga$ | $L2_1$ | 205.3 | 170.5 | 113.7 | 182.1 | 75.2 | 35.4 | 55.3 | 150.7 | 6.5 | 0.36 | 3.3 |
| $Fe_3Si$ | $L2_1$ | 295.6 | 184.7 | 142.4 | 221.7 | 107.6 | 87.5 | 97.6 | 255.2 | 2.6 | 0.31 | 2.3 |
| $Fe_2CrSi$ | $L2_1$ | 198.1 | 260.2 | 127.3 | 239.5 | 63.9 | -122.5 | -29.3 | -91.5 | -4.1 | 0.56 | -8.2 |
| | XA | 260.9 | 156.6 | 142.0 | 191.4 | 106.1 | 84.0 | 95.1 | 244.7 | 2.7 | 0.29 | 2.0 |
| $Cr_2FeSi$ | $L2_1$ | 202.8 | 164.8 | 140.1 | 177.5 | 91.7 | 39.5 | 65.6 | 175.1 | 7.4 | 0.34 | 2.7 |
| | XA | 360.9 | 194.6 | 80.6 | 250.0 | 81.7 | 81.6 | 81.6 | 220.9 | 1.0 | 0.35 | 3.1 |
| $Cr_3Si$ | $L2_1$ | 251.4 | 134.3 | 112.9 | 173.3 | 91.2 | 82.3 | 86.7 | 223.0 | 1.9 | 0.29 | 2.0 |
| $Fe_2MnSi$ | $L2_1$ | 242.7 | 233.2 | 168.9 | 236.4 | 103.2 | 11.5 | 57.4 | 159.2 | 35.4 | 0.39 | 4.1 |
| | XA | 320.3 | 179.3 | 157.3 | 226.3 | 122.6 | 105.4 | 114.0 | 292.8 | 2.2 | 0.28 | 2.0 |
| $Mn_2FeSi$ | $L2_1$ | 244.2 | 180.7 | 131.0 | 201.8 | 91.3 | 58.2 | 74.8 | 199.6 | 4.1 | 0.34 | 2.7 |
| | XA | 228.5 | 197.4 | 117.8 | 207.8 | 76.9 | 32.4 | 54.6 | 150.7 | 7.6 | 0.38 | 3.8 |
| $Mn_3Si$ | $L2_1$ | 294.8 | 168.3 | 131.7 | 210.4 | 104.3 | 91.9 | 98.1 | 254.8 | 2.1 | 0.30 | 2.1 |
| $Fe_2CoSi$ | $L2_1$ | 213.5 | 205.9 | 107.8 | 208.4 | 66.2 | 9.0 | 37.6 | 106.4 | 28.4 | 0.41 | 5.5 |
| | XA | 293.4 | 186.6 | 139.1 | 222.2 | 104.8 | 84.7 | 94.8 | 248.9 | 2.6 | 0.31 | 2.3 |
| $Co_2FeSi$ | $L2_1$ | 244.2 | 180.7 | 131.0 | 201.8 | 91.3 | 58.2 | 74.8 | 199.6 | 4.1 | 0.34 | 2.7 |
| | XA | 228.5 | 197.4 | 117.8 | 207.8 | 76.9 | 32.4 | 54.6 | 150.7 | 7.6 | 0.38 | 3.8 |
| $Co_3Si$ | $L2_1$ | 215.7 | 208.2 | 116.6 | 210.7 | 71.5 | 9.0 | 40.2 | 113.5 | 30.9 | 0.41 | 5.2 |

**Table S4.** Calculated density $\rho$ (g/cm$^3$) longitudinal v$_l$ (m/s$^2$), transverse v$_t$ (m/s$^2$), average v$_m$ (m/s$^2$) sound velocity, Debye $\Theta_D$ (K), melting T$_m$ (K) temperature, and thermal conductivity $\kappa_{min}$ (W/mK) from the elastic moduli of the Heusler compounds. Here, we exclude mechanically unstable compounds as shown in Table S3. L2$_1$ and XA denote the normal and inverse structure, respectively.

| Compounds | structure | $\rho$ g/cm$^3$ | $v_l$ m/s$^2$ | $v_t$ m/s$^2$ | $v_m$ m/s$^2$ | $\Theta_D$ K | T$_m$ $\pm$300 K | $\kappa_{min}$ W/mK |
|---|---|---|---|---|---|---|---|---|
| $Fe_3Al$ | $L2_1$ | 6.845 | 6332 | 3312 | 2464 | 347 | 1792 | 1.744 |
| $Fe_2CrAl$ | $L2_1$ | 6.997 | 7290 | 4095 | 3005 | 429 | 2700 | 2.181 |
| | XA | 6.543 | 6029 | 3318 | 2445 | 342 | 1577 | 1.699 |
| $Cr_2FeAl$ | $L2_1$ | 6.077 | 6936 | 3874 | 2846 | 391 | 1944 | 1.907 |
| | XA | 6.519 | 6791 | 3819 | 2802 | 394 | 2174 | 1.967 |
| $Cr_3Al$ | $L2_1$ | 5.893 | 6701 | 4113 | 2956 | 404 | 2026 | 1.951 |
| $Fe_2MnAl$ | $L2_1$ | 7.061 | 7190 | 4260 | 3089 | 440 | 2363 | 2.224 |
| | XA | 6.843 | 6270 | 3696 | 2683 | 378 | 1765 | 1.893 |
| $Mn_2FeAl$ | $L2_1$ | 6.814 | 6498 | 3344 | 2495 | 352 | 1843 | 1.772 |
| | XA | 6.762 | 5925 | 3149 | 2336 | 329 | 1636 | 1.649 |
| $Fe_2CoAl$ | XA | 7.085 | 6506 | 3565 | 2629 | 373 | 1963 | 1.882 |
| $Co_2FeAl$ | $L2_1$ | 7.208 | 6648 | 3700 | 2720 | 386 | 2096 | 1.948 |
| $Co_3Al$ | $L2_1$ | 7.417 | 6005 | 2982 | 2237 | 319 | 1779 | 1.621 |
| $Fe_3Ga$ | $L2_1$ | 8.277 | 5346 | 2434 | 1849 | 260 | 1608 | 1.302 |
| $Fe_2CrGa$ | $L2_1$ | 8.460 | 6462 | 3459 | 2562 | 365 | 2531 | 1.848 |
| | XA | 7.908 | 5409 | 2879 | 2135 | 297 | 1553 | 1.473 |
| $Cr_2FeGa$ | $L2_1$ | 7.642 | 6354 | 3414 | 2527 | 350 | 2015 | 1.723 |
| | XA | 7.902 | 5756 | 3057 | 2268 | 317 | 1904 | 1.581 |
| $Cr_3Ga$ | $L2_1$ | 7.244 | 5947 | 3526 | 2556 | 349 | 1950 | 1.690 |
| $Fe_2MnGa$ | $L2_1$ | 8.515 | 6389 | 3665 | 2677 | 380 | 2243 | 1.917 |
| | XA | 8.370 | 5414 | 3036 | 2228 | 315 | 1614 | 1.580 |
| $Mn_2FeGa$ | $L2_1$ | 8.322 | 5297 | 2961 | 2175 | 307 | 1503 | 1.540 |
| | XA | 8.135 | 5078 | 2491 | 1873 | 262 | 1477 | 1.310 |
| $Fe_2CoGa$ | XA | 8.504 | 5488 | 2773 | 2075 | 293 | 1699 | 1.475 |
| $Co_2FeGa$ | $L2_1$ | 8.657 | 5950 | 3150 | 2338 | 331 | 2032 | 1.666 |
| $Co_3Ga$ | $L2_1$ | 8.875 | 5369 | 2496 | 1890 | 268 | 1746 | 1.360 |
| $Fe_3Si$ | $L2_1$ | 7.393 | 6898 | 3633 | 2699 | 389 | 2280 | 2.003 |
| $Fe_2CrSi$ | XA | 7.073 | 6706 | 3666 | 2705 | 387 | 2075 | 1.973 |
| $Cr_2FeSi$ | $L2_1$ | 6.685 | 6295 | 3132 | 2349 | 332 | 1732 | 1.676 |
| | XA | 7.054 | 7133 | 3401 | 2567 | 370 | 2666 | 1.899 |
| $Cr_3Si$ | $L2_1$ | 6.531 | 6652 | 3644 | 2688 | 380 | 2019 | 1.910 |
| $Fe_2MnSi$ | $L2_1$ | 7.440 | 6484 | 2776 | 2123 | 307 | 1967 | 1.588 |
| | XA | 7.412 | 7144 | 3921 | 2891 | 418 | 2426 | 2.153 |
| $Mn_2FeSi$ | $L2_1$ | 7.553 | 6318 | 3146 | 2359 | 344 | 1976 | 1.789 |
| | XA | 7.726 | 6027 | 2660 | 2028 | 298 | 1883 | 1.561 |
| $Mn_3Si$ | $L2_1$ | 7.151 | 6908 | 3704 | 2743 | 393 | 2275 | 2.009 |
| $Fe_2CoSi$ | $L2_1$ | 7.582 | 5840 | 2227 | 1721 | 249 | 1795 | 1.285 |
| | XA | 7.514 | 6811 | 3551 | 2643 | 381 | 2267 | 1.963 |
| $Co_2FeSi$ | $L2_1$ | 7.553 | 6318 | 3146 | 2359 | 340 | 1976 | 1.741 |
| | XA | 7.726 | 6027 | 2660 | 2028 | 294 | 1883 | 1.519 |
| $Co_3Si$ | $L2_1$ | 7.836 | 5808 | 2265 | 1747 | 253 | 1808 | 1.307 |