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Supplementary Information – Influence of M/A substitution on material properties of intermetallic compounds MSn_2 (M = Fe, Co; A = Li, Na): A first-principles study

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Table S1. Lattice constants and their relative error, total energy and total energy difference of alloy compounds with different magnetic states such as ferromagnetic (FM), non-magnetic (NM) and anti-ferromagnetic (AFM) states. For the case of $CoSn_2$, only NM state was observed although initial magnetization were differently imposed.

	Mag. state	a (Å)	error (%)	c (Å)	error (%)	E_{tot} (Ry)	ΔE (Ry)
$FeSn_2$	FM	6.3430	−0.294	5.4759	0.324	−2304.670759	0.013
	NM	6.3879	−2.222	5.4386	2.226	−2304.602940	0.081
	AFM	6.5333	0.003	5.3271	0.130	−2304.683929	0.000
$CoSn_2$	NM	6.3442	−0.275	5.4723	0.258	−2489.977319	

Table S2. Magnetic moment of transition atom (M = Fe or Co), alkali atom (A = Li or Na) and Sn atom, and total magnetization of alloy compounds with different magnetic states in μ_B unit.

	Mag. state	μ_{M1}	μ_{M2}	μ_{A}	μ_{Sn}	μ_{tot}
$FeSn_2$	FM	1.72	1.72	-	0.00	6.00
	NM	0.00	0.00	-	0.00	0.00
	AFM	1.89	−1.89	-	0.00	0.00
$FeLiSn_2$	FM	2.30, 1.64	0.04	0.00	−0.03	3.40
$FeNaSn_2$	FM	2.38, 1.79	−1.78	0.02	−0.01	2.29
$CoSn_2$	NM	0.00	0.00	-	0.00	0.00
$CoLiSn_2$	NM	0.00	0.00	0.00	0.00	0.00
$CoNaSn_2$	NM	0.00	0.00	0.00	0.00	0.00

Table S3. Inter-atomic distance in Å unit for the inter-metallics. M = Fe or Co and A = Li or Na.

	M-Sn	M-M	Sn-Sn	M-A	Sn-A
$FeSn_2$	2.787	2.663	3.117		
$FeLiSn_2$	2.806	2.736	3.078	2.736	2.855
$FeNaSn_2$	2.843	2.837	3.108	2.837	2.994
$CoSn_2$	2.731	2.736	3.116		
$CoLiSn_2$	2.778	2.798	3.111	2.798	2.856
$CoNaSn_2$	2.802	2.869	3.124	2.869	2.984

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Table S4. Elastic compliance constants in 1/GPa unit.

	S_{11}	S_{12}	S_{13}	S_{33}	S_{44}	S_{66}
$FeSn_2$	0.00588	−0.00063	−0.00216	0.00738	0.01872	0.01444
$Fe_{3/4}Li_{1/4}Sn_2$	0.00692	−0.00123	−0.00183	0.00824	0.02211	0.01822
$Fe_{3/4}Na_{1/4}Sn_2$	0.00794	−0.00177	−0.00203	0.00941	0.02348	0.01961
$CoSn_2$	0.00557	−0.00105	−0.00138	0.00611	0.02343	0.01492
$Co_{3/4}Li_{1/4}Sn_2$	0.00757	−0.00127	−0.00214	0.00911	0.03558	0.02173
$Co_{3/4}Na_{1/4}Sn_2$	0.00855	−0.00147	−0.00275	0.01142	0.03901	0.02521

Table S5. Elastic moduli within the Reuss (B_R and G_R) and Voigt (B_V and G_V) approximation in GPa unit, and longitudinal (υ_l) and transverse (υ_t) elastic wave velocities in m/s unit.

	B_R	G_R	B_V	G_V	υ_l	υ_t
$FeSn_2$	108.271	59.530	108.278	61.047	4693.0629	2652.9847
$Fe_{3/4}Li_{1/4}Sn_2$	81.486	50.807	81.722	51.533	4367.6808	2552.4578
$Fe_{3/4}Na_{1/4}Sn_2$	73.489	46.264	73.989	46.653	4261.6229	2493.7009
$CoSn_2$	104.087	55.637	104.144	59.067	4495.3979	2533.3857
$Co_{3/4}Li_{1/4}Sn_2$	76.015	37.706	76.144	40.847	4003.8153	2213.9901
$Co_{3/4}Na_{1/4}Sn_2$	68.549	33.211	69.122	35.553	3859.7698	2113.4270

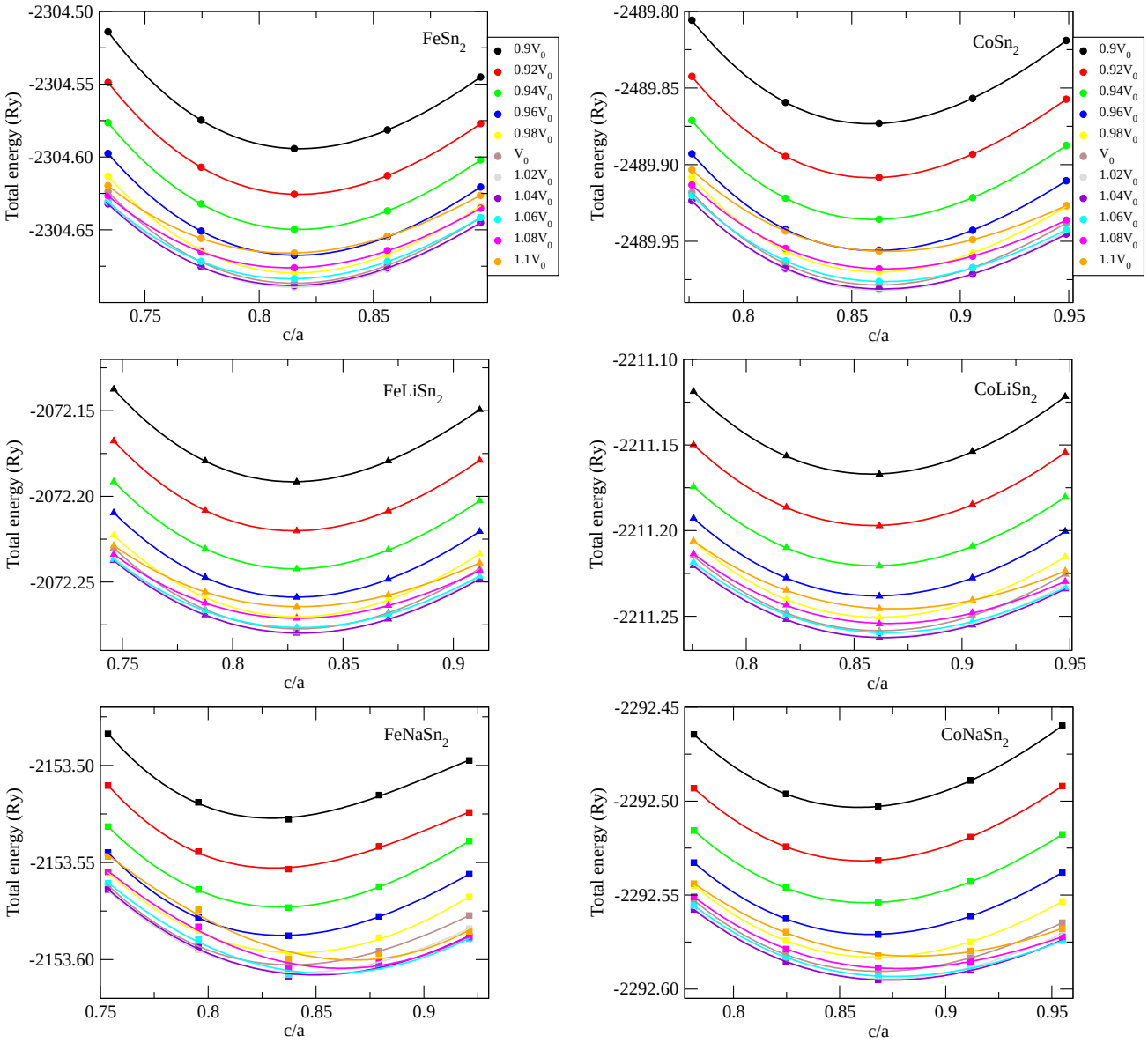

Figure S1. Total energy as a function of tetragonal lattice constants ratio c/a with gradually varying the cell volume from $0.9V_0$ to $1.1V_0$ in $FeSn_2$, $Fe_{3/4}Li_{1/4}Sn_2$, $Fe_{3/4}Na_{1/4}Sn_2$, $CoSn_2$, $Co_{3/4}Li_{1/4}Sn_2$ and $Co_{3/4}Na_{1/4}Sn_2$ in tetragonal phase.

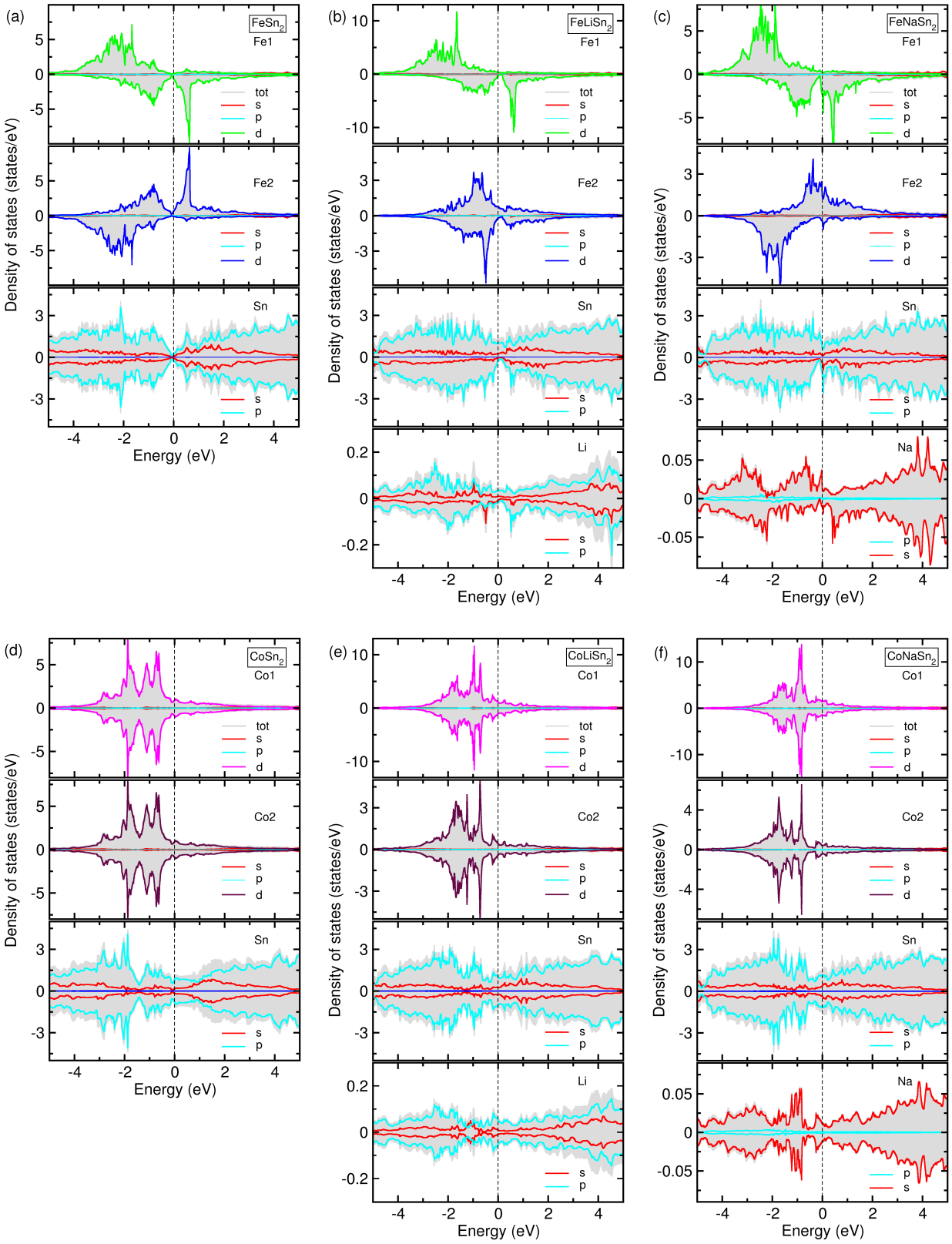

Figure S2. Partial density of states in (a) $FeSn_2$, (b) $FeLiSn_2$, (c) $FeNaSn_2$, (d) $CoSn_2$, (e) $CoLiSn_2$ and (f) $CoNaSn_2$. The Fermi energy is set to zero as denoted by vertical dotted line.

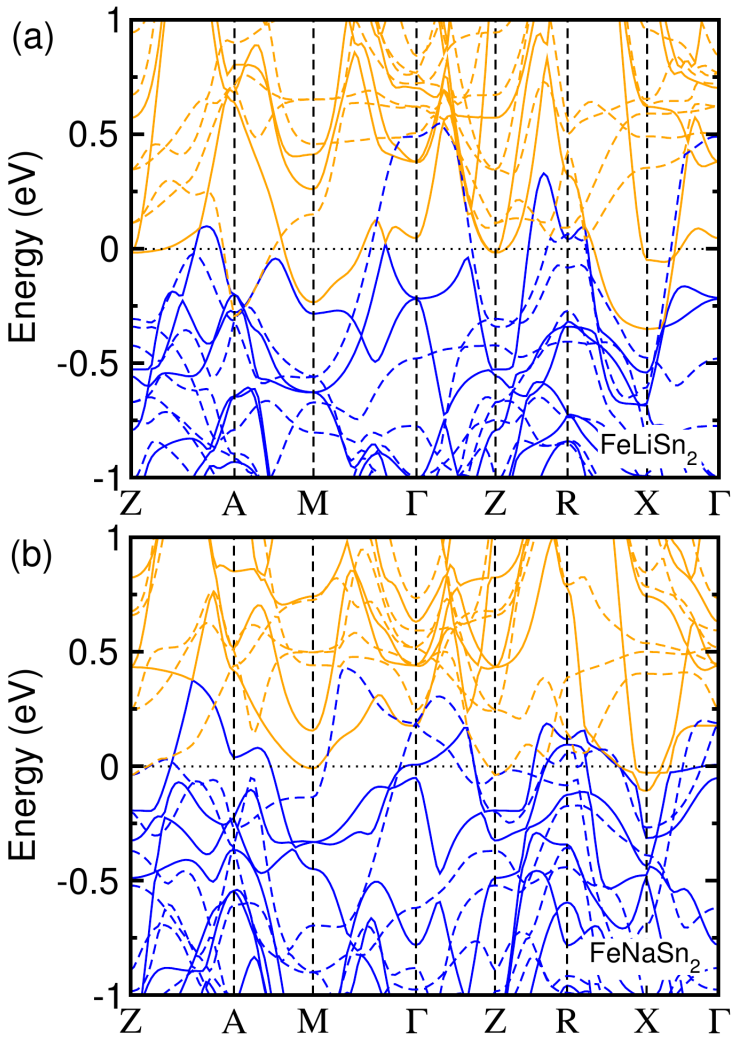

Figure S3. Both spin-up and spin-down energy band structures of (a) $Fe_{3/4}Li_{1/4}Sn_2$ and (b) $Fe_{3/4}Na_{1/4}Sn_2$. Blue and orange colors denote the occupied and empty spin-up bands, and dashed lines indicate the corresponding spin-down bands.

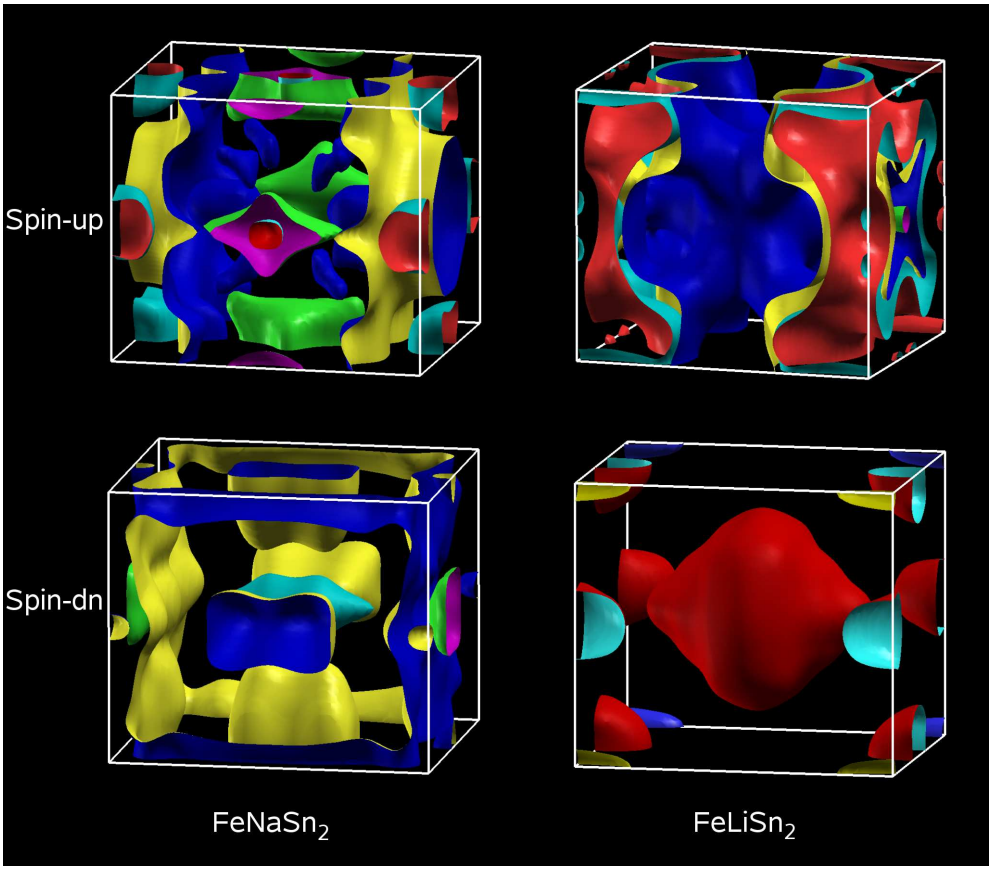

Figure S4. Fermi surface for spin-up and spin-down electronic energy bands of $Fe_{3/4}Na_{1/4}Sn_2$ and $Fe_{3/4}Li_{1/4}Sn_2$.