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Supplementary Materials

Synthesis and characterization of $NaCd_{0.92}Sn_{1.08}$, $Na(Cd_{0.28}Sn_{0.72})_2$, and Na_2CdSn_5 with three-dimensional Cd–Sn frameworks

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Supplementary Materials

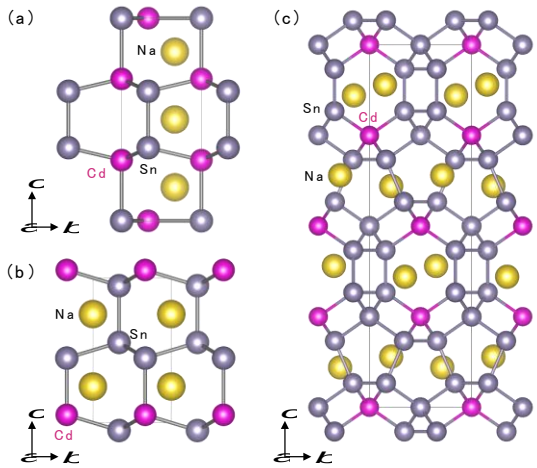

Figure S1. Ordered structure models of NaCdSn (**a**), Na $(Cd_{1/4}Sn_{3/4})_2$ (**b**), and Na_2CdSn_5 (**c**) for DOS calculation.

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Table S1. Anisotropic displacement parameters of $NaCd_{0.92}Sn_{1.08}$, Na $(Cd_{0.28}Sn_{0.72})_2$, and *tI*-Na_2CdSn_5.

Atom	U_{11}(Å)	U_{22}(Å)	U_{33}(Å)	U_{23} (Å)	U_{31}(Å)	U_{12}(Å)
$NaCd_{0.92}Sn_{1.08}$						
Na1	0.021(3)	0.021(3)	0.029(4)	0	0	0.0107(14)
Na2	0.0241(18)	0.0241(18)	0.024(2)	0	0	0.0121(9)
Cd/Sn1	0.0115(4)	0.0115(4)	0.0565(10)	0	0	0.0058(2)
Cd/Sn2	0.0151(4)	0.0151(4)	0.0406(7)	0	0	0.0076(2)
Sn1	0.0106(4)	0.0106(4)	0.0230(7)	0	0	0.0053(2)
Sn2	0.0113(3)	0.0113(3)	0.0141(4)	0	0	0.00563(17)
$Na(Cd_{0.28}Sn_{0.72})_2$						
Na1	0.0243(8)	0.0243(8)	0.0333(14)	0	0	0.0121(4)
Cd/Sn1	0.01462(11)	0.01462(11)	0.01802(14)	0	0	0.00731(6)
***tI*-Na_2CdSn_5**						
Na1	0.0317(18)	0.063(6)	0.096(8)	−0.056(5)	−0.009(2)	0.011(2)
Cd1	0.01860(12)	0.01860(12)	0.01720(16)	0	0	0
Sn1	0.01393(9)	0.01525(9)	0.01454(8)	0.00150(7)	0.00029(7)	0.00181(7)
Sn2	0.01443(10)	0.01443(10)	0.01148(13)	0	0	0

Table S2. Structure refinement results of NaCdSn based on the crystal structure of LiZnGe [1] with various arrangement of Cd and Sn atoms.

Wycoff Position	1*a*	1*e*	2*g*	2*i*	*R*1 (all data)	*wR*2 (all data)
LiZnGe [1]	Ge	Zn	Zn	Ge	1.94	3.51
NaCdSn (this study)	Sn	Cd	Cd	Sn	1.78	4.20
	Cd	Sn	Cd	Sn	2.06	4.58
	Sn	Cd	Sn	Cd	2.38	5.06
	Cd	Sn	Sn	Cd	2.96	6.67
	Cd/Sn	Cd/Sn	Cd/Sn	Cd/Sn	2.19	4.67

Table S3. Selected interatomic distances for Na_2CdSn_5 (this study) and related dimorphs *tI*-Na_2ZnSn_5 [2].

Compounds and atomic sites		Distance (Å)
***tI*-Na_2CdSn_5**		
Sn1	Sn1	2.8854(4), 2.9115(4)
Sn1	Sn2	2.8400(2)
Cd1	Sn1	2.8699(2)
Na1	Na1	0.824(14), 3.363(16), 3.819(5)
Na1	Sn1	3.176(8), 3.287(9), 3.419(5), 3.495(5), 3.598(5), 3.670(5)
Na1	Cd1	3.266(8), 3.604(8)
Na1	Sn2	3.634(6)
Sn1	Sn1	2.8854(4), 2.9115(4)
***tI*-Na_2ZnSn_5[2]**		
Sn1	Sn1	2.9181(6), 2.9222(7)
Sn1	Sn2	2.8272(3)
Zn1	Sn1	2.7509(3)
Na1	Na1	0.872(12), 3.320(15), 3.790(6)
Na1	Sn1	3.109(8), 3.194(9), 3.331(5), 3.505(6), 3.532(6), 3.697(5)
Na1	Zn1	3.195(8), 3.572(8)
Na1	Sn2	3.546(5)

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