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Supplementary Information

"A Simple Chemical Guide for Finding Novel n-type Dopable Zintl Pnictide Thermoelectric Materials"

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Predicted Thermoelectric Performance of n-type Dopable Zintl Phases

Table S1: Computed parameters used in determining the descriptor of thermoelectric performance β. The following are tabulated: compound, Inorganic Crystal Structure Database (ICSD) identification number, β_p and β_n for valence (p-type) and conduction (n-type) band transport, lattice thermal conductivity (κ_L) in $\mathrm{Wm^{-1}K^{-1}}$, bulk modulus (B) in GPa, valence band density-of-states effective mass ($m^*_{DOS,VB}$) and conduction band density-of-states effective mass ($m^*_{DOS,CB}$) in the units of m_e, and valence band ($N_{b,VB}$) and conduction band ($N_{b,CB}$) degeneracy.

Compound	ICSD	β_p	β_n	κ_L	B	$m^*_{DOS,VB}$	$m^*_{DOS,CB}$	$N_{b,VB}$	$N_{b,CB}$
$ZnAs_2$	002021	6.63	29.46	5.98	86	0.531	0.044	2	2
NaSb	026473	26.80	26.60	1.06	20	1.061	0.417	6	4
$KGaSb_4$	300158	5.04	23.03	1.03	21	0.303	0.121	1	2
NaAs	182159	5.99	22.67	1.41	25	4.571	0.497	4	4
Na_2As_2	421420	5.97	22.37	1.42	25	4.556	0.504	4	4
$KAlSb_4$	300157	5.29	20.79	1.08	21	0.261	0.135	1	2
$CdAs_2$	020518	5.26	19.25	6.30	49	0.717	0.083	3	3
KSb	056529	4.45	18.37	0.87	14	3.220	0.592	3	4
Li_3As_7	409657	8.64	17.99	1.08	14	1.489	3.717	4	10
Cs_4ZnAs_{14}	423082	11.93	14.69	0.67	7	4.299	4.849	9	11
Ba_3As_{14}	001404	4.86	9.38	1.01	18	3.462	3.805	3	5
KSb_2	080945	4.69	8.95	0.95	19	1.685	0.114	2	1
Cs_3Sb_7	092473	8.71	8.93	0.53	6	4.526	4.341	7	7
CsBi	055067	6.35	8.77	0.66	14	1.121	0.655	2	2
KBi	055065	8.98	8.72	0.63	10	3.461	1.102	5	3
$RbSb_2$	419402	2.97	7.98	0.73	15	0.718	0.138	1	1
KBa_2As_5	414140	15.21	7.86	1.21	28	0.760	0.886	3	2
LiAs	026472	26.73	7.53	1.82	34	0.672	0.654	5	2
CsAs	412595	12.86	7.51	0.76	12	1.863	2.713	5	4
K_3As_{11}	036591	4.38	6.26	0.82	10	9.826	3.538	6	5
Rb_3As_7	412597	5.07	5.62	0.76	9	3.126	2.631	4	4

Compound	ICSD	β_p	β_n	κ_L	B	$m^*_{DOS,VB}$	$m^*_{DOS,CB}$	$N_{b,VB}$	$N_{b,CB}$
RbBi	055066	13.89	5.56	0.58	10	2.741	0.972	6	2
CsSb	412154	5.39	5.13	0.64	10	0.910	0.989	2	2
NaAs	610971	5.29	5.10	1.38	23	0.989	0.209	2	1
Cs_3As_7	412598	3.28	5.07	0.67	8	6.523	1.613	4	3
Rb_4As_6	409381	2.64	4.87	0.76	12	0.602	1.094	1	2
RbSb	014030	4.05	3.92	0.71	11	1.467	0.307	2	1
$MgAs_4$	001079	26.18	3.68	2.39	43	0.680	2.110	5	2
RbAs	412594	3.42	3.60	0.88	14	1.889	0.344	2	1
CsSb	014031	2.67	3.49	0.55	8	2.729	0.345	2	1
$BaAs_2$	414139	7.11	3.41	1.21	30	3.035	0.798	3	1
KAs	409653	1.44	3.27	1.10	16	1.393	0.353	1	1
Na_3As_7	409658	6.56	3.26	0.99	12	5.560	1.375	6	2
Cs_3As_{11}	412873	1.36	3.16	0.65	8	5.371	3.383	2	3
Rb_3As_{11}	412872	5.93	2.90	0.73	8	8.448	3.854	7	3
Cs_5Sb_8	412155	19.15	2.63	0.68	11	2.070	3.040	7	2
K_3As_7	412596	7.02	2.53	0.83	9	3.787	1.597	6	2
Rb_3As_7	409652	4.10	2.39	0.72	8	3.763	1.842	4	2
$NaCs_2As_7$	423080	1.26	2.23	0.77	11	1.548	0.600	1	1
Cs_4As_6	409382	2.57	2.15	0.64	11	0.660	0.891	1	1
Rb_4Sb_6Sn	300212	5.32	1.45	0.65	9	5.817	1.183	5	1
$CdCs_4As_{14}$	423081	1.94	1.38	0.49	4	4.720	3.253	3	2

KBa_2As_5: Native Defect Energetics and Predicted Free Electron Concentration

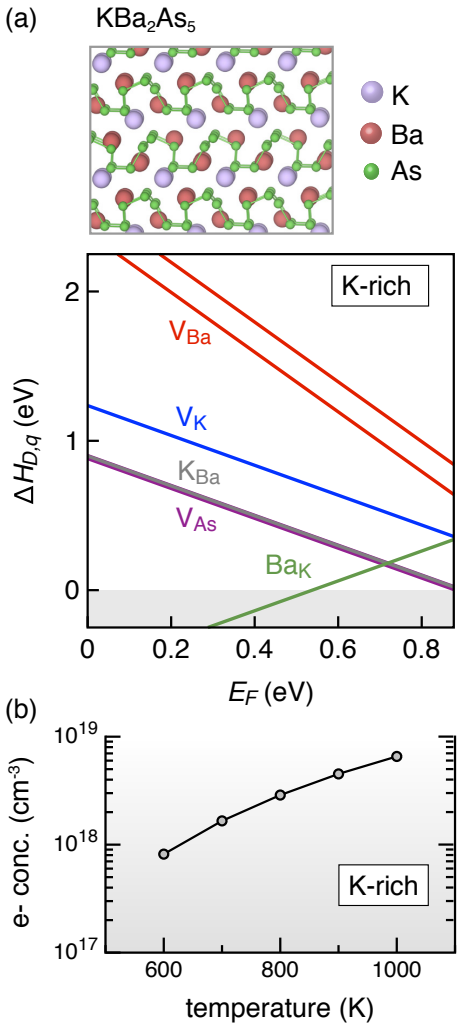

Figure S1: Crystal structure, defect energetics, and carrier concentrations: (a) Formation energetics of native defects in KBa_2As_5 reveal that under K-rich growth conditions, the antisite donor Ba_K self dopes KBa_2As_5 n-type. (b) Predicted free electron concentrations in self-doped KBa_2As_5 ranges from $\sim 10^{18}$ cm^{-3} at 600K to $\sim 10^{19}$ cm^{-3} at 1000K.

List of Zintl Pnictides in ICSD

Numbers in parenthesis are the ICSD numbers.

As_3Rh (034052), $As_{11}Cs_3$ (412873), As_3Ca_4 (252055), AsCa (026263), As_2Ru (000994), As_2Na (182161), AsIn (043973), AsIn (156105), As_7Cs_3 (412598), As_4Cu_3 (041169), As_2Fe (065168), As_3Co (009188), AsRb (412594), As_7Rb_3 (409652), As_7Rb_3 (412597), $As_{11}K_3$ (036591), AsSb (042576), As_2Mo (016820), As_2Zn (002021), As_2Ge (610601), As_3Sr (041831), As_3Sr (611440), As_2Nb (018143), As_2Nb (081218), As_3Ca (086400), As_3Ba (086402), As_7Na_3 (409658), As_4Sr_3 (100110), AsGa (043951), AsGa (043950), As_2Si (611405), As_2Si (024801), As_2Ni (076940), As_2Ni (034851), As_2Ni (042569), As_2Sr_2 (083353), As_2Cr (043898), As_2Cu (610303), AsZn (427612), As_2Cd (016037), As_2Cd (020518), As_2Ti (611500), AsCd (000432), As_3Sr_4 (402110), $As_{14}Ba_3$ (001404), As_2Pt (056021), AsSr (026264), As_2V (611574), As_2Zr (168665), As_7K_3 (412596), As_2W (611576), As_2Na_2 (421420), As_2Ta (044069), As_2Ta (107966), As_3Ca_2 (043876), As_6Cs_4 (409382), AsCs (412595), AsLi (026472), As_2Pd (043101), As_3Mo_2 (043184), As_3W_2 (043185), $As_{11}Rb_3$ (412872), AsNa (610971), AsNa (182159), As_2Hf (610636), As_2Co (610039), As_2Co (610034), As_6Rb_4 (409381), As_4Mg (001079), As_2Ba (414139), As_2Rh (611271), As_2La (280294), As_2La (610769), AsLa (098427), As_3V_5 (611571), AsK (409653), As_4Na_5 (182165), As_7Li_3 (409657), Sb_2Ti (651676), $RhSb_2$ (659978), Ag_3Sb (064716), AlSb (107877), $RuSb_2$ (042608), KSb_2 (080945), Sb_2Sr (052307), Sb_2Zr (042878), In_5Sb_3 (640434), CdSb (620395), $LaSb_2$ (641892), Cs_3Sb_7 (092473), KSb (056529), Ba_5Sb_4 (280022), Ba_5Sb_4 (052693), AsSb (042576), Sb_4Zr_5 (189947), $Sb_{10}Zn_{13}$ (159092), $NiSb_2$ (646409), Li_2Sb (100020), $CoSb_2$ (076120), $CoSb_2$ (063553), $BaSb_2$ (409517), Mo_3Sb_7 (173974), Mo_3Sb_7 (164763), Cs_5Sb_8 (412155), $HfSb_2$ (066780), $HfSb_2$ (638876), $AuSb_3$ (043504), CsSb (014031), CsSb (412154), LaSb (044806), $NbSb_2$ (645350), $Ca_{11}Sb_{10}$ (000433), $RhSb_3$ (044716), Rb_4Sb_4 (280591), $Sb_{18}Zr_{11}$ (280817), $CaSb_2$ (000862), RbSb (014030), Hf_5Sb_9 (413979), SbZn (043265), $RbSb_2$ (419402), K_5Sb_4 (056530), Sb_2Y (651733), Sb_2Ta (052311), Sb_2Ta (651600), $AuSb_2$ (612288), $PdSb_2$ (043102), Sb_3Sr_2 (032033), $Sb_{10}Sr_{11}$ (659275), $CrSb_2$ (042601), $CrSb_2$ (088093), Cs_4Sb_2 (092474), $Cd_{13}Sb_{10}$ (260098), $Ba_{11}Sb_{10}$ (413518), SbSn (154085), Sb_2V (052331), Ba_2Sb_3 (061089), Cd_6Sb_5 (420110), PbSb (648506), $Sb_{65}Zn_{84}$ (418213), $PtSb_2$ (057470), NaSb (026473), $BaSb_3$ (049000), $FeSb_2$ (151397), $FeSb_2$ (186639), GaSb (103952), GaSb (041982), InSb (659364), InSb (655298), InSb (010021), InSb (156996), Sb_7Zn_8 (238947), $Bi_{10}Sr_{11}$ (659276), $Ba_{11}Bi_{10}$ (051797), $BiHf_2$ (168286), BiCs (055067), BiNa (058816), Bi_2Hf (616683), Bi_2Tl (058864), $BaBi_3$ (058634), BiRb (055066), Bi_2K (055068), Bi_2K (058794), $Bi_{14}Rh_3$ (245517), $Bi_{14}Rh_3$ (195777), BiNi (058820), Bi_2Zr (042880), Bi_3Sr (058858), Bi_4Rh (058854), Bi_2Rh (617009), BiLi (616780), BiSn (058857), BiSn (160382), $Bi_{10}Ca_{11}$ (000434), Bi_2Ca (659277), Bi_2Rb (150969), Bi_2Rb (055069), Bi_2Cs (058771), Bi_2Cs (055070), Ba_2Bi_3 (170218), BiK (055065), Bi_3Sr_2 (106329), Bi_2Pt (077111), Bi_2Pt (058846), Au_2Bi (052284), Bi_2Cs_3 (240017), As_2GaK_2 (300142),

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Numbers in parenthesis are the ICSD numbers.

As_4Cd_2Ge (042132), $AsPb_3Zr_5$ (604204), $As_3In_2K_2$ (300198), As_2K_2Pt (610762), As_2Cs_2Pd (069647), $AsSb_3Zr_5$ (611352), $As_6Ca_5Ga_2$ (000027), As_2LaPd_2 (192474), As_2Pd_2Sr (047170), $As_6Cs_7In_3$ (411989), As_6BaPt_4 (062519), $As_6In_4K_4$ (071244), As_2K_2Pd (032009), $As_7Rb_4Zn_7$ (237457), $As_{12}LaRu_4$ (610778), $Al_2As_3Na_2$ (300193), As_2K_2Ni (300120), As_2BaPt (405112), $As_{14}CdCs_4$ (423081), As_2BaPd (405110), As_2CuY (412550), As_2BaCu_2 (236307), As_2PtRb_2 (107529), $As_3Ga_2Na_2$ (300194), $As_{18}Ca_{21}Zn_4$ (429152), As_2BaPd_2 (061196), As_2BaPd_2 (036377), As_2BaPd_2 (190705), $AsSn_3Zr_5$ (656301), $As_3Ba_2Cd_2$ (420833), As_2Cu_2Sr (610366), $As_3Sr_2Zn_2$ (262413), $As_{14}Cs_4Zn$ (423082), As_2CaPd_2 (604341), $As_{12}Fe_4La$ (168584), As_2CaNi_2 (023004), $As_3Ga_2K_2$ (300195), As_6Pt_4Sr (062518), As_3LaSi (039160), As_3LaSi (068205), As_2CaRu_2 (609914), $As_4Ba_3Cd_2$ (424761), As_2GaRb_2 (300143), $As_{11}Ca_{14}Ga$ (071176), As_7Cs_2Na (423080), $AgAs_2La$ (420609), As_5Ba_2K (414140), $As_4Ba_3Li_4$ (280027), $As_4Ba_3Zn_2$ (424760), $Ca_5In_2Sb_6$ (036467), Cs_2PtSb_2 (658700), Sb_4Sn_3Sr (165617), $AlCa_{14}Sb_{11}$ (033266), $AuSbTl$ (391381), $CaMnSb_2$ (052705), $BaPdSb_2$ (405111), $LaPdSb_2$ (658217), $In_4K_4Sb_6$ (071245), $Mn_{12}Rb_7Sb_{12}$ (237459), $Ba_3Cd_2Sb_4$ (173685), $CrLaSb_3$ (083907), $LaRu_4Sb_{12}$ (641783), La_3Sb_5Ti (080907), Ni_2Sb_2Sr (646442), Hf_3NiSb_7 (195051), GaK_2Sb_2 (053579), $Fe_4Sb_{12}Sr$ (658733), $HfLa_3Sb_5$ (083906), $MnSb_{11}Sr_{14}$ (075939), $Cd_6Sb_{12}Sr_{11}$ (418887), $Ca_{11}InSb_9$ (042371), $In_2K_2Sb_3$ (300197), $NiSb_7Zr_3$ (260035), $BaMnSb_2$ (100024), $AlKSb_4$ (300157), $MnSb_2Sr$ (643539), $Cd_3Sb_3Tl_2$ (076500), $AgSb_2Y$ (190094), $Ba_{11}Cd_6Sb_{12}$ (418886), $Ga_2K_2Sb_3$ (300196), Hf_3PdSb_7 (195052), $FeLaSb_2$ (657985), $Al_2Na_7Sb_5$ (048168), $Ba_3Li_4Sb_4$ (428114), $Ba_3Li_4Sb_4$ (615946), $Al_2Sb_6Sr_5$ (062304), $Ca_{10}Mg_2Sb_9$ (171162), Rb_4Sb_6Sn (300212), $In_5K_{10}Sb_9$ (056323), $InSb_9Sr_{11}$ (240900), $Al_2Ca_5Sb_6$ (183853), $Al_2Ca_5Sb_6$ (060146), $SbSnTi$ (097545), Na_6Sb_4Tl (096942), $AgLaSb_2$ (095222), $CoLaSb_3$ (419540), $GaRb_2Sb_2$ (300135), Pd_2Sb_2Sr (061195), $Mn_4Sb_{18}Sr_{21}$ (280280), $BaCdSb_2$ (052683), $Ba_5In_2Sb_6$ (062305), $Ca_{21}Mn_4Sb_{18}$ (281257), $Ca_{21}Mn_4Sb_{18}$ (416972), Pb_3SbZr_5 (604080), $CoLaSb_2$ (657990), $LaNiSb_2$ (658208), $BaPd_2Sb_2$ (061197), La_3Sb_5Zr (083905), $In_2Na_2Sb_3$ (300192), $Li_4Sb_4Sr_3$ (025307), $Ca_{14}MnSb_{11}$ (059710), $PdSb_7Zr_3$ (426314), Sb_2SrZn (010001), $Ca_{21}Sb_{18}Zn_4$ (429153), $BaRu_4Sb_{12}$ (616049), $Ca_5Ga_2Sb_6$ (036466), $CuSb_2Y$ (153572), $LaNiSb_3$ (249473), Cs_2PdSb_2 (658702), $AuLaSb_2$ (082589), $Cs_2In_2Sb_3$ (056387), $BaFe_4Sb_{12}$ (658735), $GaKSb_2$ (300202), $CuLaSb_2$ (658225), $Ru_4Sb_{12}Sr$ (042962), $In_2Sb_6Sr_5$ (036468), $In_2Rb_2Sb_3$ (083663), $Ba_2Cd_2Sb_3$ (420834), $GaKSb_4$ (300158), $Al_2K_2Sb_3$ (052627), $Ba_{21}Cd_4Sb_{18}$ (173283), $Al_2Na_2Sb_3$ (052628), $Ba_2Sb_6Sn_3$ (082529), $Bi_{18}Ca_{21}Mn_4$ (416520), Bi_2Cs_2Pd (658703), $Bi_{11}MnSr_{14}$ (106328), $BaBi_2Mn$ (615787), $BaBi_2Zn$ (058638), Bi_2MnSr (100025), $Ba_{11}Bi_{14}Cd_8$ (240338), Bi_2Cs_2Ni (658704), $Bi_{11}Ca_{14}Mn$ (106319), Bi_2GaLa (165559), Bi_2CaMn (010454), Bi_2Cs_2Pt (658701), $Bi_{18}Cd_4Sr_{21}$ (173284), Bi_2LaLi (415728), Bi_5K_6Zn (238106), Bi_5La_3Mg (415727), Bi_2SrZn (041924), $BaBi_2Cd$ (058635),

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Numbers in parenthesis are the ICSD numbers.

Bi_5La_3Sc (416609), Bi_2CdSr (058764), $Ba_3Bi_4Li_4$ (428115), $Bi_6In_2Sr_5$ (415576), Bi_5La_3Mn (173362), $Ba_{14}Bi_{11}Mn$ (106304), $AuBi_2La$ (238704), $Bi_8Ca_3Pd_4$ (412563), As_2BaRu_2 (609861), $As_6Sn_2Sr_5$ (262646), As_2CdSr_2 (422940), As_3CoHf_5 (085884), As_2Co_2La (610073), As_2GaK_2 (300142), $As_4Ga_3K_3$ (040206), As_4NbRb_7 (380111), As_2Cs_3Ga (300115), As_4Ba_4Ti (380115), $As_7Mg_6Ni_{16}$ (078834), AsFeNa (163143), AsFeNa (187137), AsFeNa (187136), AsHfNb (424124), $AsMgPt_5$ (610830), As_4MgRh_6 (089611), $As_5K_6Sn_3$ (071009), As_2LaRu_2 (602111), AsLiZn (074504), As_2HgK_4 (402573), $AlAs_3Ca_3$ (606012), As_3CsZn_4 (262030), $Al_4As_8K_{12}$ (300121), $As_3In_2K_2$ (300198), As_2CdK_4 (300190), AsBeNa (100091), AsPdSr (404723), AsFeLi (246338), AsFeLi (042331), AsFeLi (166457), AsFeLi (187131), AsFeLi (187132), AsFeLi (187133), AsFeLi (168206), As_2K_2Pt (610762), As_3GaNa_6 (300276), As_3Ca_3Ga (060126), As_2BRb_3 (402082), $Al_2As_4Sr_3$ (423787), Ag_4As_2Sr (424309), $As_4Rb_2Zn_5$ (250688), As_2BCs_3 (300122), AsCaPt (060828), As_2HfNi_4 (610651), $AsCuK_2$ (043936), As_2KRh_2 (031474), As_2Cu_4K (059207), As_3Na_5Sn (656058), As_2BaCu_4 (089628), $As_5La_4Mn_2$ (429102), As_2CsRh_2 (610296), AsMnNa (026461), $As_4Cs_5In_3$ (280723), As_3Ba_3In (402338), As_2Cd_2Sr (023249), As_2CsFe_2 (074877), AsKMn (060745), As_2SrZn_2 (023248), As_2Cs_2Pd (069647), As_2Ru_2Sr (165118), $As_6Ca_5Ga_2$ (000027), As_2BK_3 (300105), As_2CaCo_2 (609899), $Al_2As_3K_3$ (060950), $As_6K_{10}Sn_2$ (409486), As_2Ba_2Cd (422941), $As_2Cu_3K_3$ (032015), As_2BaCo_2 (609848), As_2Co_2Sr (610122), As_2LaPd_2 (192474), As_2Ga_2Sr (422527), As_2Pd_2Sr (047170), As_2BaCu_6 (079256), As_2BaCr_2 (609849), $As_{23}Cu_{44}Sr_7$ (251516), AsCaCu (049741), As_6BaCo_{10} (092463), As_2Ni_4Y (611100), $As_4Ga_2Sr_3$ (423785), $As_6Cs_7In_3$ (411989), $Al_3As_5Ba_3$ (425292), As_2Rh_2Sr (417001), As_2Rh_2Sr (417002), AsCdK (609963), $As_4Ge_2Sr_3$ (016454), As_6BaPt_4 (062519), As_2CsRu_2 (610297), $As_6Ca_5Sn_2$ (061037), $As_6In_4K_4$ (071244), As_2CuK_5 (040699), As_2Pt_2Sr (418156), As_2Pt_2Sr (181396), $As_3Ni_3Zr_2$ (611109), AsCdNa (609968), AsCdNa (009571), AsCoHf (406953), $As_4Ba_3Si_2$ (041183), As_3Cd_4Na (262035), AsAuCa (404725), $As_{12}Sn_3Sr_{14}$ (195752), As_2K_2Pd (032009), $As_3In_2K_3$ (300199), As_3Cd_4Rb (262037), $As_3Hf_2Ni_3$ (610649), $AlAs_2Cs_3$ (300113), $Al_2As_4Ba_3$ (423779), $As_7Rb_4Zn_7$ (237457), $As_6Ge_2Na_{10}$ (300187), $As_4Ca_3In_2$ (061336), $As_{12}LaRu_4$ (610778), AsKSn (040815), $Al_2As_3Na_2$ (300193), As_2InNa_3 (300139), AsCoLi (107932), As_2K_2Ni (300120), As_2BeK_4 (300111), As_2Fe_2K (031473), AsPtY (044047), As_2BaPt (405112), $AgAsK_2$ (001154), As_2BaZn_2 (012146), As_2BaZn_2 (417000), As_2LaRh_2 (610777), As_2Na_2Sn (073307), As_2Rb_2Sn (071223), As_3NaZn_4 (262036), As_4BaCu_8 (066017), As_2BaNi_2 (164196), As_2BaNi_2 (609856), As_2Fe_2Sr (163208), As_2Fe_2Sr (610527), As_3Cs_5Si (065716), As_2BaPd (405110), $As_6Na_{10}Si_2$ (300188), $As_7Co_{12}Mg_2$ (094408), As_2CuY (412550), As_2BaCu_2 (236307), AsAuBa (420341), $As_4Cd_5Rb_2$ (290262), As_3Rb_5Si (300191), As_2PtRb_2 (107529), As_2BaRh_2 (416983), $As_3Cr_3Rb_2$ (195012), As_4SiSr_4 (611409), As_2Cu_4Sr (089626),

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Numbers in parenthesis are the ICSD numbers.

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Numbers in parenthesis are the ICSD numbers.

BaPtSb (059186), Na_5Sb_3Sn (076495), CaPtSb (060830), $CrLaSb_3$ (083907), $LaRu_4Sb_{12}$ (641783), KMnSb (089591), La_3Sb_5Ti (080907), $Au_3K_3Sb_2$ (078977), BeNaSb (100092), CsMnSb (627028), $BaPt_2Sb_2$ (195017), Ni_2Sb_2Sr (646442), Hf_3NiSb_7 (195051), Cu_4NaSb_2 (059206), GaK_2Sb_2 (053579), $Fe_4Sb_{12}Sr$ (658733), $CaMn_2Sb_2$ (163778), CuMgSb (077364), CuMgSb (412294), $MnSb_{11}Sr_{14}$ (075939), $Cd_6Sb_{12}Sr_{11}$ (418887), AuLaSb (251686), LiSbZn (042064), $InNa_3Sb_2$ (300140), $Ca_{11}InSb_9$ (042371), $Ca_2Pd_3Sb_4$ (416139), CdNaSb (012159), $Au_3Sb_4Y_3$ (000957), $CuHf_2Sb_3$ (093243), LiSbSn (603169), Li_2PtSb (044895), MgNiSb (044925), $In_2K_2Sb_3$ (300197), $GaHf_2Sb_3$ (189076), $LaPd_2Sb_2$ (189724), $Ba_7Ga_4Sb_9$ (060583), HgKSb (056201), $NiSb_7Zr_3$ (260035), $BaMnSb_2$ (100024), Fe_4NaSb_{12} (246577), Na_8Sb_4Sn (655768), $CuSb_3Zr_2$ (195058), LaSbSc (427126), $CuSb_7Zr_4$ (427673), KSbSn (040816), $AlKSb_4$ (300157), $AlCs_6Sb_3$ (300128), $MnSb_2Sr$ (643539), $AgSb_2Y$ (190094), $AlCa_3Sb_3$ (036363), MgPdSb (044825), $Ba_{11}Cd_6Sb_{12}$ (418886), $Ga_2K_2Sb_3$ (300196), LiMnSb (642150), MnNaSb (060735), Hf_3PdSb_7 (195052), $FeLaSb_2$ (657985), Fe_4LaSb_{12} (053490), $Al_2Na_7Sb_5$ (048168), Cu_2Sb_2Sr (041923), CaCuSb (042137), RuSbZr (107126), $Al_2Sb_6Sr_5$ (062304), CoSbZr (108317), Rb_4Sb_6Sn (300212), $BaSb_2Zn_2$ (032020), $In_5K_{10}Sb_9$ (056323), $InSb_9Sr_{11}$ (240900), NiSbY (105331), $Al_2Ca_5Sb_6$ (183853), $Al_2Ca_5Sb_6$ (060146), NiSbZr (408195), Hf_2PdSb_3 (195060), Ni_2SbZr (162585), Ni_2SbZr (076703), K_5Sb_3Sn (656024), $Ga_3Na_2Sb_3$ (063617), $CaCd_2Sb_2$ (012151), $Au_3Rb_3Sb_2$ (078978), Na_6Sb_4Tl (096942), $CuLi_2Sb$ (053300), $Au_3La_3Sb_4$ (612105), $CoLaSb_3$ (419540), $AuLi_2Sb$ (058529), $Ni_3Sb_4Zr_3$ (087995), CuK_2Sb (053298), Li_2SbZn (001243), $BaCd_2Sb_2$ (032021), $NiSb_9Zr_5$ (195053), $GaRb_2Sb_2$ (300135), Cs_6GaSb_3 (300216), Pd_2Sb_2Sr (061194), Pd_2Sb_2Sr (061195), $Cd_2K_{11}Sb_5$ (425646), $Mn_4Sb_{18}Sr_{21}$ (280280), $BaCdSb_2$ (052683), $Ba_5In_2Sb_6$ (062305), $AgLi_2Sb$ (052589), $Ca_{21}Mn_4Sb_{18}$ (281257), $Ca_{21}Mn_4Sb_{18}$ (416972), LaPdSb (641676), $Ba_5In_4Sb_6$ (195087), $CoLaSb_2$ (657990), $LaNiSb_2$ (658208), KSbZn (044680), KSbZn (012161), $BaPd_2Sb_2$ (061197), $BaPd_2Sb_2$ (604350), La_2NiSb (427930), $Cu_3La_3Sb_4$ (658637), HfRuSb (107125), $CaSb_2Zn_2$ (012150), $In_2Na_2Sb_3$ (300192), AuLiSb (107996), $Ca_{14}MnSb_{11}$ (059710), $PdSb_7Zr_3$ (426314), Sb_2SrZn (010001), $Ca_{21}Sb_{18}Zn_4$ (429153), AgBaSb (056981), CoHfSb (108294), NaSbZn (160957), NaSbZn (012154), PdSbZr (092441), $BaRu_4Sb_{12}$ (616049), Ru_2Sb_2Sr (188979), AgCaSb (056982), PtSbSr (059185), $Ca_5Ga_2Sb_6$ (036466), CuK_5Sb_2 (032032), $CuSb_2Y$ (153572), $AlRb_6Sb_3$ (300217), $PdSb_3Zr_2$ (426315), $K_{10}Sb_6Sn_2$ (057401), $Rb_2Sb_4Zn_5$ (290263), $LaNiSb_3$ (249473), MgPtSb (044826), Cs_2PdSb_2 (658702), $AlBa_3Sb_3$ (032728), $AuLaSb_2$ (082589), $Cs_2In_2Sb_3$ (056387), $BaFe_4Sb_{12}$ (658735), Mn_2Sb_2Sr (416094), $GaKSb_2$ (300202), $K_6Sb_3Tl_2$ (093048), $CuLaSb_2$ (658225), CuSbSr (053339), $HfNi_2Sb$ (638718), $BaMn_2Sb_2$ (032019), Li_2PdSb (044816), $BaCu_2Sb_2$ (236308), Ba_3GaSb_3 (060124), MnRbSb (643395), $BaGa_2Sb_2$ (280662), BaCuSb (057020), $Ca_9Sb_9Zn_4$ (052787),

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Numbers in parenthesis are the ICSD numbers.

$AgNa_2Sb$ (010010), $Ru_4Sb_{12}Sr$ (042962), AuCaSb (052662), $In_2Sb_6Sr_5$ (036468), AgK_2Sb (001155), CdKSb (620064), $GaSb_3Sr_3$ (065055), Cd_2Sb_2Sr (012153), $Sb_9V_6Zr_2$ (408565), PtSbY (649578), $AuNa_2Sb$ (023255), $In_2Rb_2Sb_3$ (083663), $Ba_2Cd_2Sb_3$ (420834), $MgSb_2Si$ (237071), AgMgSb (187150), AgMgSb (187151), AgMgSb (187149), $CaFe_4Sb_{12}$ (248622), $GaKSb_4$ (300158), $Al_2K_2Sb_3$ (052627), $AlSb_3Sr_3$ (052652), Cu_4KSb_2 (602179), Ba_2Sb_2Zn (421425), AuK_2Sb (380340), $CsFe_2Sb_2$ (658698), BeLiSb (616318), $Ba_{21}Cd_4Sb_{18}$ (173283), Ag_4Sb_2Sr (424311), $Al_2Na_2Sb_3$ (052628), $Ba_2Sb_6Sn_3$ (082529), $Bi_{18}Ca_{21}Mn_4$ (416520), Bi_2Cs_2Pd (658703), $Bi_{11}MnSr_{14}$ (106328), Bi_2CaMn_2 (041791), $BaBi_2Mn$ (615787), BiPdY (616964), Bi_2K_4Zn (192439), $Ba_2Bi_4Cd_3$ (416446), $BaBi_2Zn$ (058638), BiMnNa (060736), BiCuMg (058774), $Bi_4La_3Pt_3$ (616774), BiMgNi (076253), AgBiCa (416283), AgBiCa (659377), $BiPd_2Y$ (058842), BiK_2Sn (107616), Bi_2MnSr (100025), $Bi_9Ca_9Mn_4$ (008157), $Al_2Bi_6Ca_5$ (036364), $Bi_{12}Cs_{14}In_8$ (410420), $Bi_6K_{10}Sn_2$ (300261), $AgBiLi_2$ (057350), $AuBiNa_2$ (261790), AuBiCa (248679), AuBiCa (248676), $Ba_{11}Bi_{14}Cd_8$ (240338), Bi_2Cs_2Ni (658704), $Bi_{11}Ca_{14}Mn$ (106319), $Bi_9Ca_9Zn_4$ (008158), BaBiCu (106303), $Bi_9Ca_9Cd_4$ (058760), BiNiY (058826), BiCsMn (616575), BiCaCu (057018), Bi_2GaLa (165559), Bi_2CaMn (010454), $AuBiLi_2$ (261785), $AuBiLi_2$ (058400), Ba_2Bi_2Zn (421424), Bi_2Cs_2Pt (658701), $Bi_{18}Cd_4Sr_{21}$ (173284), BiMnRb (616824), $Bi_6In_3Na_9$ (413312), AgBaBi (056978), $AuBiK_2$ (380341), BiKMn (601586), Bi_5K_6Zn (238106), $Bi_9Cd_4Sr_9$ (058763), Bi_2SrZn (041924), BiCuSr (058777), $BaBi_2Cd$ (058635), Bi_2Pd_2Sr (416300), Bi_2Pd_2Sr (604338), $Bi_9In_6K_{11}$ (413314), $Ba_5Bi_5In_4$ (054853), Bi_5La_3Sc (416609), Bi_2CdSr (058764), Bi_2LaNi_2 (616770), $Bi_6In_2Sr_5$ (415576), Bi_5La_3Mn (173362), AgBiSr (057019), $Bi_4Cu_3La_3$ (167250), $AgBiK_2$ (001156), $BiMg_{63}Si_{32}$ (291431), $Ba_{14}Bi_{11}Mn$ (106304), BiLaPt (248481), $BaBi_2Pd_2$ (416299), $AuBi_2La$ (238704), $Bi_8Ca_3Pd_4$ (412563),

Crystal Structures of Candidate Zintl Phases

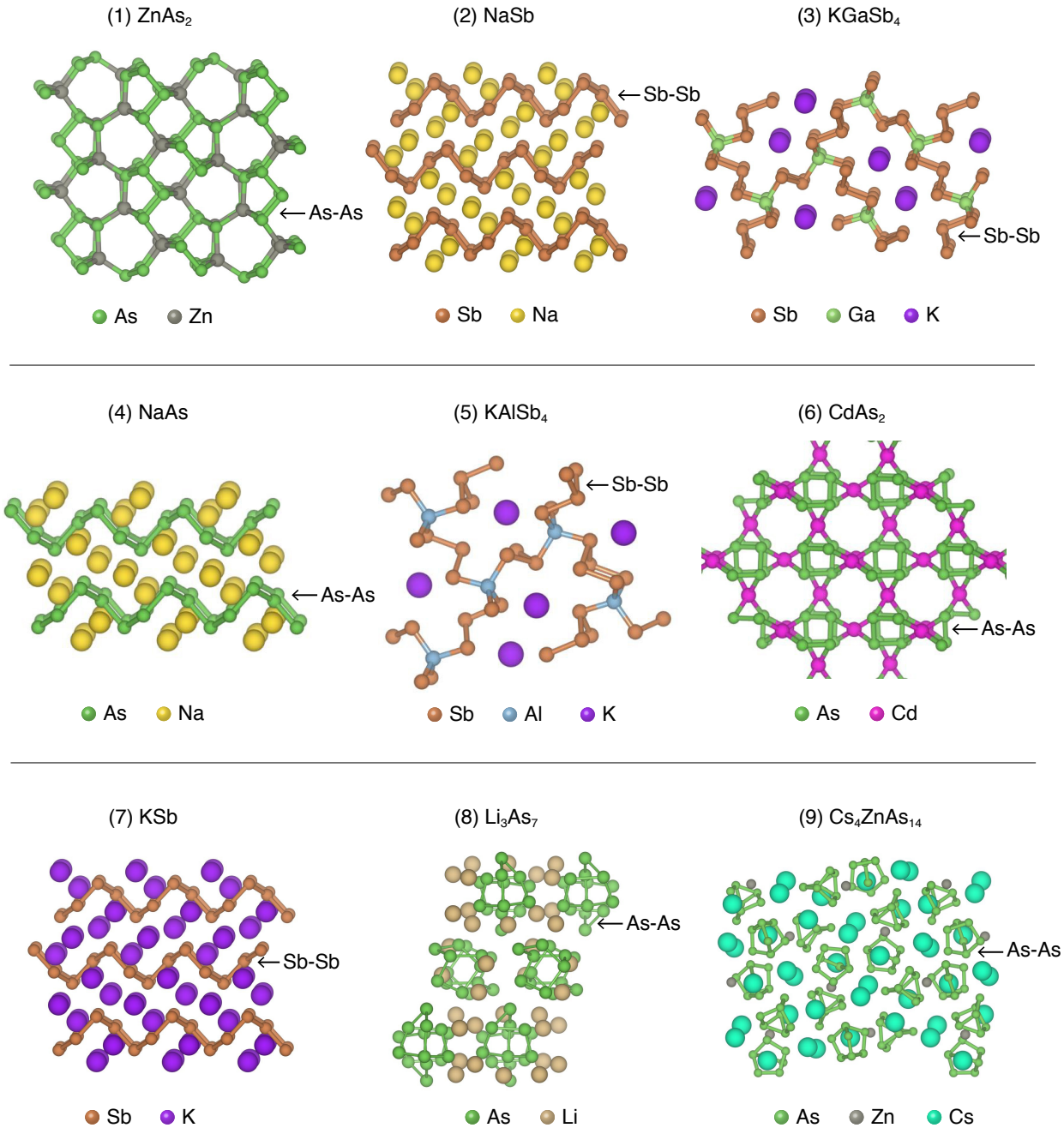

Figure S2: Crystal structures of candidate n-type dopable Zintl phases predicted to exhibit high thermoelectric performance (Table 1 in main text). The covalent pnictogen-pnictogen (Pn-Pn) bonds, which are part of the anionic framework, are indicated by arrows. Additionally, in most of these structures, the cations are highly electropositive alkali or alkaline elements (Li, Na, K, Rb, Cs, Ba).

Crystal Structures of Candidate Zintl Phases

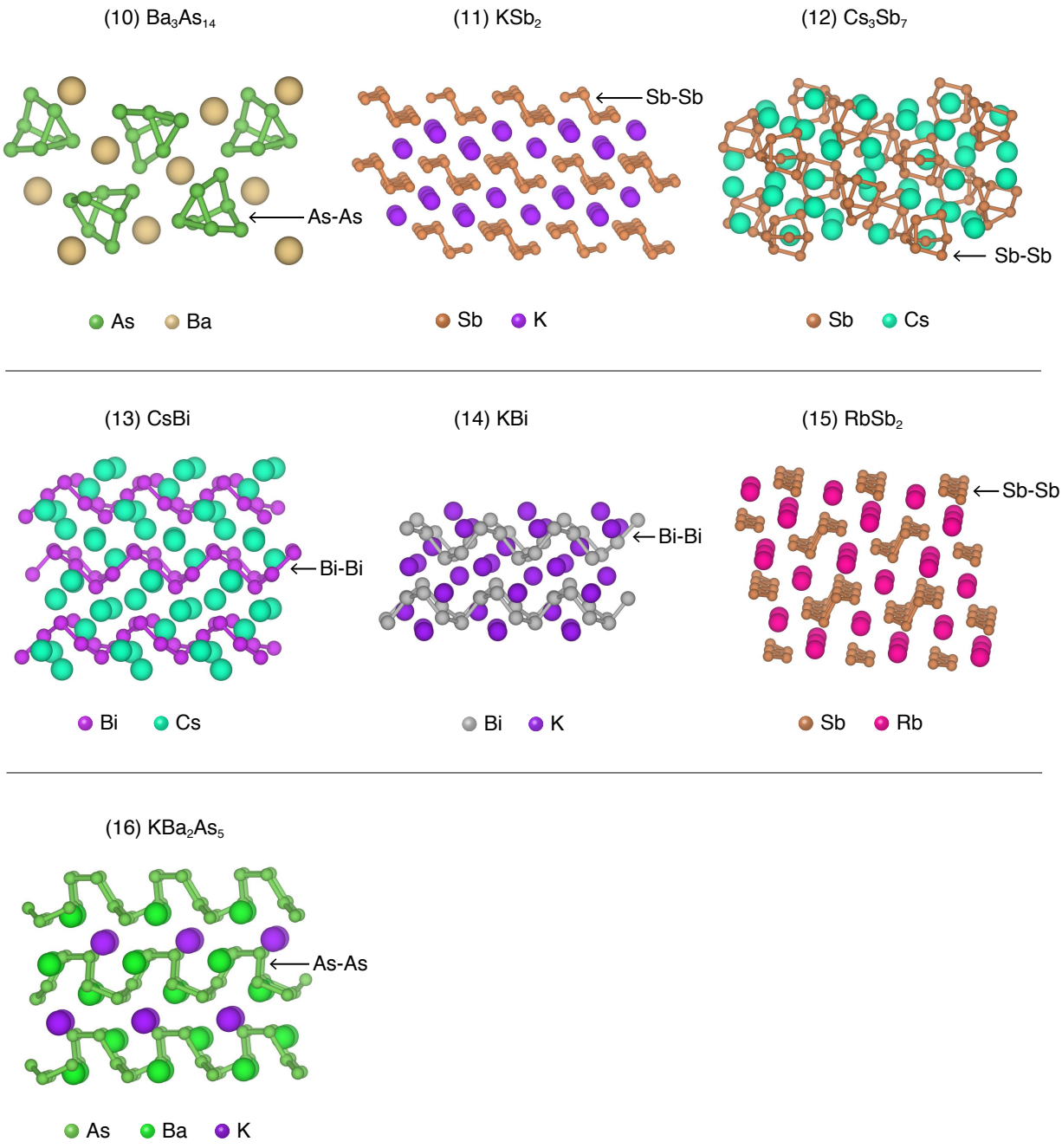

Figure S3: Crystal structures of candidate n-type dopable Zintl phases predicted to exhibit high thermoelectric performance (Table 1 in main text). The covalent pnictogen-pnictogen (Pn-Pn) bonds, which are part of the anionic framework, are indicated by arrows. Additionally, in most of these structures, the cations are highly electropositive alkali or alkaline elements (Li, Na, K, Rb, Cs, Ba).