Electronic supplementary information : **High thermoelectric performance in Tellurium doped Paracostibite**

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Table S1. Table listing the energy of formation (eV) of intrinsic and extrinsic defects for charges -3, -2, -1, 0, 1, and 2 at the VBM ($\Delta\mu_e$=0) for the three points in Figure 3.

	Point 1						Point 2						Point 3					
Defect Charge	-3	-2	-1	0	1	2	-3	-2	-1	0	1	2	-3	-2	-1	0	1	2
Vac_Co	3.31	2.56	1.94	1.71	1.7	1.94	3.08	2.33	1.72	1.49	1.48	1.71	3.12	2.37	1.75	1.52	1.51	1.74
Vac_Sb	3.75	3.06	2.59	2.42	2.44	2.69	3.83	3.14	2.67	2.5	2.52	2.77	3.72	3.04	2.57	2.4	2.41	2.67
Vac_S	4.32	3.26	2.51	2.01	1.93	2.06	4.47	3.41	2.66	2.16	2.08	2.2	4.53	3.47	2.73	2.23	2.15	2.27
Co_Sb	4.7	3.96	3.42	3.06	3.15	3.45	5.01	4.27	3.73	3.37	3.46	3.76	4.87	4.13	3.6	3.23	3.32	3.62
Sb_Co	5.29	4.27	3.41	2.82	2.42	2.24	4.98	3.96	3.11	2.52	2.12	1.93	5.12	4.1	3.24	2.65	2.25	2.06
Co_S	4.98	3.98	3.23	3.04	3.04	3.24	5.36	4.36	3.61	3.41	3.42	3.62	5.39	4.39	3.64	3.44	3.45	3.65
S_Co	4.9	3.94	3.7	2.55	2.19	2.35	4.52	3.56	3.33	2.18	1.82	1.98	4.49	3.53	3.29	2.14	1.79	1.95
Sb_S	2.59	1.78	1.2	1.06	1.12	1.36	2.66	1.84	1.27	1.12	1.18	1.43	2.83	2.01	1.44	1.29	1.35	1.6
S_Sb	2.89	2.1	1.45	1.03	0.83	1.15	2.83	2.03	1.38	0.96	0.77	1.09	2.66	1.86	1.21	0.79	0.6	0.92
Te_Co	5.89	4.87	4.04	3.35	2.93	2.85	5.71	4.69	3.86	3.17	2.75	2.67	5.68	4.66	3.83	3.14	2.72	2.64
Te_Sb	**2.58**	**1.68**	**0.96**	**0.48**	**0.2**	**0.5**	**2.71**	**1.82**	**1.1**	**0.61**	**0.34**	**0.64**	**2.54**	**1.65**	**0.92**	**0.44**	**0.17**	**0.47**
Te_S	2.53	1.69	1.09	0.67	0.82	1.14	2.73	1.89	1.29	0.87	1.02	1.34	2.73	1.89	1.29	0.87	1.02	1.34
Se_Co	4.99	4	3.19	2.57	2.19	2.29	4.81	3.83	3.01	2.39	2.01	2.12	4.78	3.8	2.98	2.36	1.98	2.08
Se_Sb	2.54	1.7	1.07	0.62	0.41	0.7	2.67	1.84	1.2	0.75	0.54	0.83	2.5	1.67	1.03	0.58	0.37	0.66
Se_S	1.99	1.13	0.56	0.07	0.19	0.52	2.19	1.34	0.76	0.27	0.39	0.73	2.19	1.33	0.76	0.27	0.39	0.72
Sc_Co	5.1	4.17	3.97	2.93	2.97	3.19	5.09	4.16	3.97	2.93	2.97	3.19	5.23	4.3	4.1	3.06	3.1	3.32
Sc_Sb	4.73	3.97	3.57	3.34	3.32	3.41	5.03	4.27	3.87	3.64	3.62	3.71	5.03	4.27	3.87	3.64	3.62	3.71
Ru_Co	2.25	1.39	0.7	0.59	0.49	0.76	2.31	1.46	0.77	0.66	0.55	0.83	2.48	1.63	0.94	0.83	0.72	1
Ru_Sb	4.87	4.07	3.47	3.25	3.25	3.57	5.24	4.44	3.85	3.62	3.62	3.94	5.27	4.48	3.88	3.66	3.65	3.97
Pt_Co	3.05	2.13	1.41	0.86	0.54	0.82	2.99	2.07	1.35	0.79	0.47	0.75	2.82	1.9	1.18	0.62	0.3	0.58
Pt_Sb	4.52	3.82	3.35	2.99	2.88	3.17	4.76	4.06	3.59	3.24	3.12	3.41	4.45	3.75	3.28	2.93	2.81	3.11
P_Co	4.79	3.84	3.08	2.55	2.35	2.35	4.34	3.38	2.63	2.1	1.89	1.9	4.41	3.45	2.7	2.17	1.96	1.97
P_Sb	2.56	1.73	1.16	0.71	0.87	1.2	2.42	1.58	1.01	0.56	0.72	1.06	2.35	1.51	0.95	0.5	0.66	0.99
P_S	2.25	1.43	0.82	0.66	0.57	0.81	2.17	1.35	0.74	0.58	0.49	0.73	2.28	1.45	0.85	0.69	0.59	0.83
Pd_Co	**2.92**	**1.97**	**1.21**	**0.7**	**0.4**	**0.68**	**2.85**	**1.9**	**1.14**	**0.64**	**0.33**	**0.61**	**2.68**	**1.73**	**0.97**	**0.47**	**0.16**	**0.44**
Pd_Sb	4	3.29	2.83	2.55	2.49	2.78	4.24	3.53	3.07	2.79	2.73	3.02	3.93	3.23	2.77	2.48	2.42	2.71
Pb_Co	6.48	5.43	4.62	3.94	3.53	3.48	6.45	5.4	4.59	3.91	3.5	3.45	6.55	5.5	4.69	4.01	3.6	3.55
Pb_Sb	2.98	2.14	1.58	1.41	1.49	1.7	3.26	2.42	1.86	1.69	1.78	1.98	3.23	2.38	1.83	1.65	1.74	1.94
O_Co	3.62	2.85	2.75	1.91	1.77	2.14	3.45	2.68	2.57	1.74	1.59	1.96	3.41	2.64	2.54	1.71	1.56	1.93
O_Sb	4.53	3.87	3.59	3.13	3.19	3.57	4.66	4.01	3.73	3.26	3.32	3.7	4.49	3.84	3.55	3.09	3.15	3.53
N_Co	4.02	3.25	3.01	2.31	2.49	2.87	3.79	3.02	2.79	2.08	2.26	2.64	3.83	3.05	2.82	2.11	2.29	2.68
N_Sb	4.97	4.25	3.94	3.41	3.55	3.86	5.05	4.33	4.02	3.49	3.63	3.94	4.95	4.23	3.91	3.39	3.53	3.84
Ni_Co	**2.65**	**1.73**	**1.03**	**0.55**	**0.31**	**0.6**	**2.54**	**1.61**	**0.91**	**0.43**	**0.19**	**0.48**	**2.67**	**1.75**	**1.05**	**0.57**	**0.33**	**0.62**
Ni_Sb	4.34	3.63	3.15	2.91	2.9	3.21	4.53	3.82	3.34	3.1	3.09	3.39	4.52	3.82	3.34	3.1	3.09	3.39
Na_Co	5.33	4.42	3.8	3.39	3.27	3.38	5.48	4.56	3.95	3.53	3.42	3.53	5.55	4.63	4.02	3.6	3.48	3.6
Na_Sb	4.28	3.56	3.52	2.71	2.73	2.95	4.73	4.02	3.97	3.17	3.18	3.4	4.66	3.95	3.9	3.1	3.11	3.33
Mn_Co	2.66	1.87	1.42	0.88	0.95	1.2	2.58	1.79	1.34	0.8	0.87	1.12	2.68	1.89	1.44	0.91	0.97	1.22
La_Co	8	6.96	7	5.64	5.41	5.15	7.99	6.96	6.99	5.63	5.4	5.14	8.13	7.09	7.13	5.77	5.54	5.28
La_Sb	5.55	4.72	4.43	3.8	3.63	3.64	5.85	5.02	4.74	4.1	3.93	3.95	5.85	5.02	4.74	4.1	3.93	3.95
Li_Co	3.7	2.84	2.3	1.96	1.91	2.1	3.56	2.7	2.16	1.82	1.77	1.96	3.63	2.77	2.23	1.89	1.84	2.03

Li_Sb	3.94	3.28	2.8	2.52	2.58	2.85	4.11	3.44	2.97	2.69	2.75	3.02	4.04	3.37	2.9	2.62	2.68	2.95
K_Co	7.87	6.96	6.7	5.92	5.76	5.68	8.02	7.11	6.85	6.07	5.9	5.83	8.08	7.18	6.92	6.13	5.97	5.89
K_Sb	5.5	4.75	4.87	3.83	3.72	3.81	5.96	5.21	5.32	4.29	4.17	4.27	5.89	5.14	5.25	4.22	4.1	4.2
I_Co	7.7	6.67	6.52	5.09	4.6	4.35	7.55	6.51	6.36	4.93	4.44	4.19	7.55	6.51	6.36	4.93	4.44	4.19
I_Sb	3.97	3.15	2.52	2.08	1.9	1.91	4.12	3.3	2.67	2.23	2.05	2.06	3.99	3.16	2.53	2.09	1.91	1.92
I_S	4.03	3.21	2.88	2.14	1.92	2.26	4.25	3.43	3.09	2.35	2.14	2.48	4.28	3.46	3.13	2.39	2.17	2.51
In_Co	5.04	4.01	3.25	2.66	2.45	2.41	5.05	4.02	3.26	2.67	2.46	2.42	5.18	4.16	3.39	2.81	2.6	2.56
In_Sb	2.64	1.87	1.62	1.34	1.34	1.51	2.96	2.19	1.94	1.65	1.66	1.83	2.96	2.18	1.93	1.65	1.66	1.83
Hf_Co	4.96	4.07	3.98	2.78	2.45	2.69	5.17	4.28	4.2	2.99	2.66	2.9	5.41	4.52	4.44	3.23	2.9	3.14
Hf_Sb	4.34	3.52	2.9	2.78	2.83	3.09	4.86	4.04	3.42	3.3	3.35	3.61	4.96	4.15	3.52	3.4	3.45	3.71
Ge_Co	4.32	3.36	2.6	2.04	1.7	1.91	4.08	3.13	2.37	1.81	1.47	1.68	4.21	3.26	2.5	1.94	1.6	1.81
Ge_Sb	2.02	1.22	0.66	0.59	0.74	1.09	2.1	1.29	0.73	0.67	0.82	1.16	2.08	1.28	0.72	0.65	0.81	1.15
Gd_Co	9.43	8.53	8.73	7.4	7.2	7.5	9.42	8.53	8.72	7.39	7.19	7.5	9.56	8.66	8.86	7.53	7.33	7.63
Gd_Sb	8.03	7.44	6.91	6.51	6.25	6.42	8.33	7.75	7.21	6.81	6.55	6.72	8.33	7.75	7.21	6.81	6.55	6.72
Ga_Co	4.1	3.12	2.39	1.87	1.79	1.91	4.09	3.12	2.38	1.86	1.78	1.9	4.23	3.25	2.52	2	1.92	2.04
Ga_Sb	2.45	1.71	1.54	1.31	1.4	1.6	2.75	2.01	1.84	1.61	1.7	1.9	2.75	2.01	1.84	1.61	1.7	1.9
F_Co	4.29	3.48	3.23	2.47	2.18	2.45	4.09	3.28	3.03	2.27	1.98	2.25	4.09	3.28	3.03	2.27	1.98	2.25
F_Sb	3.68	3.04	2.68	2.4	2.43	2.64	3.79	3.15	2.78	2.51	2.54	2.75	3.65	3.02	2.65	2.38	2.4	2.61
F_S	3.5	2.67	2.22	1.72	1.54	1.82	3.67	2.84	2.39	1.89	1.71	1.99	3.71	2.88	2.43	1.93	1.75	2.02
Fe_Co	2.22	1.39	0.76	0.65	0.63	0.91	2.22	1.39	0.77	0.65	0.63	0.92	2.39	1.56	0.94	0.82	0.8	1.09
Eu_Co	9.34	8.7	8.46	7.34	7.47	7.2	9.26	8.62	8.38	7.26	7.39	7.11	9.36	8.72	8.48	7.36	7.49	7.22
Eu_Sb	7.83	7.07	6.64	6.17	6.13	6.04	8.05	7.3	6.87	6.4	6.36	6.27	8.02	7.26	6.83	6.36	6.32	6.23
Cu_Co	3.37	2.48	1.8	1.34	1.17	1.27	3.3	2.41	1.73	1.26	1.09	1.19	3.45	2.57	1.89	1.42	1.25	1.35
Cr_Co	3.12	2.32	1.78	1.47	1.45	1.66	3.14	2.34	1.79	1.49	1.47	1.68	3.27	2.48	1.93	1.63	1.6	1.81
C_Co	5.69	4.91	4.36	4.12	4.11	4.5	5.46	4.69	4.13	3.89	3.89	4.27	5.49	4.72	4.16	3.93	3.92	4.31
C_Sb	5.31	4.6	4.58	3.9	3.88	4.23	5.39	4.68	4.66	3.98	3.96	4.31	5.29	4.58	4.56	3.88	3.86	4.21
Cl_Co	6.42	5.45	5.65	3.99	3.55	3.34	6.22	5.25	5.45	3.79	3.35	3.14	6.22	5.25	5.45	3.79	3.35	3.14
Cl_Sb	3.63	2.85	2.48	1.92	1.86	2	3.73	2.96	2.58	2.03	1.97	2.11	3.6	2.82	2.45	1.89	1.83	1.97
Cl_S	3.54	2.67	1.99	1.52	1.27	1.57	3.71	2.84	2.16	1.69	1.45	1.74	3.75	2.88	2.2	1.73	1.48	1.77
Ce_Co	6.72	5.81	5.72	4.46	4.07	4.14	6.71	5.8	5.71	4.45	4.07	4.13	6.85	5.94	5.85	4.59	4.2	4.27
Ce_Sb	4.5	3.68	3.04	2.79	2.75	2.89	4.8	3.98	3.35	3.09	3.05	3.19	4.8	3.98	3.34	3.09	3.05	3.19
Ca_Co	6.55	5.62	5.05	4.59	4.37	4.45	6.47	5.54	4.97	4.51	4.29	4.37	6.58	5.64	5.07	4.61	4.4	4.47
Ca_Sb	5.19	4.47	4.38	3.56	3.41	3.61	5.42	4.7	4.61	3.79	3.64	3.84	5.39	4.66	4.57	3.76	3.6	3.81
Br_Co	6.89	5.86	5.88	4.32	3.86	3.63	6.79	5.76	5.79	4.23	3.76	3.54	6.79	5.76	5.79	4.23	3.76	3.54
Br_Sb	3.63	2.86	2.27	1.89	1.8	1.91	3.84	3.07	2.48	2.1	2.01	2.12	3.7	2.93	2.34	1.97	1.88	1.98
Br_S	3.65	2.8	2.13	1.67	1.44	1.77	3.93	3.08	2.41	1.95	1.72	2.04	3.96	3.11	2.44	1.99	1.75	2.08
B_Co	4.54	3.7	3.06	2.64	2.64	2.54	4.39	3.55	2.92	2.5	2.5	2.4	4.53	3.69	3.05	2.64	2.64	2.53
B_Sb	4.15	3.42	2.88	2.65	2.75	3.14	4.32	3.58	3.04	2.81	2.91	3.3	4.32	3.58	3.04	2.81	2.91	3.3
Bi_Co	6.03	4.98	4.16	3.5	3.13	2.96	6.03	4.97	4.16	3.49	3.12	2.96	6.16	5.11	4.29	3.63	3.26	3.09
Bi_Sb	2.55	1.63	0.97	0.5	0.58	0.88	2.85	1.93	1.27	0.8	0.89	1.19	2.85	1.93	1.27	0.8	0.89	1.18
As_Co	4.6	3.61	2.82	2.27	2.05	2.03	4.29	3.3	2.51	1.96	1.74	1.72	4.43	3.44	2.65	2.1	1.88	1.86
As_Sb	2.11	1.26	0.63	0.21	0.35	0.69	2.11	1.26	0.63	0.21	0.35	0.69	2.11	1.26	0.63	0.21	0.35	0.69
Al_Co	4.11	3.17	2.45	1.94	1.95	2.13	4.1	3.16	2.44	1.93	1.94	2.12	4.24	3.3	2.58	2.07	2.07	2.26
Al_Sb	3.23	2.5	2.34	2.13	2.19	2.41	3.53	2.8	2.64	2.43	2.49	2.71	3.53	2.8	2.64	2.43	2.49	2.71
Ag_Co	4.06	3.09	2.31	1.74	1.47	1.46	3.83	2.86	2.08	1.52	1.24	1.23	3.87	2.9	2.12	1.55	1.28	1.27
Ag_Sb	3.31	2.65	2.41	1.93	1.97	2.19	3.39	2.73	2.49	2.01	2.05	2.27	3.29	2.63	2.38	1.91	1.95	2.17
Ag_S	4.6	3.65	2.94	2.33	2.12	2.26	4.74	3.79	3.09	2.47	2.27	2.41	4.81	3.86	3.16	2.54	2.33	2.48
Zr_Co	5.33	4.43	4.16	3.15	2.82	3.06	5.4	4.5	4.22	3.22	2.89	3.13	5.57	4.67	4.39	3.39	3.06	3.3
Zr_Sb	4.69	3.88	3.26	3.12	3.13	3.37	5.06	4.25	3.63	3.49	3.5	3.75	5.09	4.28	3.67	3.53	3.54	3.78
Y_Co	6.51	5.55	5.28	4.26	4.23	4.33	6.51	5.55	5.27	4.25	4.22	4.32	6.64	5.68	5.41	4.39	4.36	4.46
Y_Sb	5.2	4.38	4.11	3.57	3.47	3.51	5.5	4.68	4.42	3.88	3.77	3.81	5.5	4.68	4.41	3.87	3.77	3.81
Ti_Co	4.14	3.28	2.67	2.09	1.81	2.07	4.2	3.34	2.74	2.16	1.88	2.13	4.37	3.51	2.91	2.33	2.05	2.3
Zn_Co	4.07	3.19	2.48	2.11	1.94	2.09	3.99	3.1	2.4	2.03	1.86	2.01	4.1	3.21	2.5	2.13	1.96	2.12
V_Co	3.53	2.73	2.48	1.78	1.63	1.73	3.5	2.7	2.45	1.75	1.6	1.7	3.63	2.83	2.57	1.87	1.73	1.82
Tl_Co	6.14	5.1	4.34	3.7	3.36	3.19	6.18	5.14	4.37	3.73	3.39	3.22	6.24	5.2	4.44	3.8	3.46	3.29
Tl_Sb	2.95	2.16	1.91	1.59	1.58	1.72	3.29	2.51	2.25	1.93	1.92	2.06	3.22	2.44	2.19	1.86	1.85	1.99
Tb_Co	6.6	5.65	5.38	4.35	4.31	4.35	6.59	5.64	5.38	4.34	4.3	4.35	6.73	5.78	5.51	4.48	4.44	4.48
Tb_Sb	5.16	4.35	3.86	3.54	3.43	3.47	5.46	4.65	4.17	3.85	3.73	3.77	5.46	4.65	4.16	3.84	3.73	3.77
Sr_Co	7.99	7.02	6.55	5.87	5.52	5.63	8.01	7.03	6.56	5.89	5.54	5.65	8.11	7.13	6.66	5.99	5.64	5.75
Sr_Sb	5.67	4.9	4.89	3.91	3.73	3.86	5.99	5.22	5.22	4.23	4.05	4.18	5.95	5.18	5.18	4.2	4.01	4.14
Sn_Co	5.07	4.06	3.26	2.62	2.24	2.33	4.99	3.98	3.18	2.54	2.16	2.25	5.09	4.09	3.28	2.65	2.26	2.35
Sn_Sb	2.14	1.34	0.78	0.65	0.76	1.02	2.37	1.57	1	0.88	0.99	1.25	2.33	1.53	0.97	0.84	0.96	1.21
Sn_S	3.34	2.54	2.31	1.77	1.77	1.93	3.63	2.84	2.6	2.07	2.07	2.23	3.77	2.97	2.74	2.2	2.2	2.36
Si_Co	4.32	3.4	2.65	2.11	1.79	2.06	4.39	3.46	2.71	2.18	1.86	2.13	4.56	3.63	2.88	2.35	2.03	2.3
Si_Sb	2.58	1.81	1.27	1.2	1.38	1.72	2.96	2.18	1.65	1.57	1.75	2.1	2.99	2.21	1.68	1.61	1.79	2.13

Table S2. The summary of transport characterization carried out on non-effective dopants tested experimentally.

Dopant	Hall effect at RT		PSM at RT		
	Charge conc. n, cm^{-3}	Mobility, $cm^2/(V.s)$	Resistivity, mΩ.cm	Seebeck, $\mu V.K^{-1}$	PF, $\mu W.m^{-1}.K^{-2}$
undoped	-4.75×10^{18}	5.3	293±2.2	-459 ± 36	72 ± 0.5
+2 at. % P	$+2.59 \times 10^{19}$	0.3	1710 ± 5.7	+204 ± 44	2.4 ± 0.01
+2 at. % Zn	$+1.54 \times 10^{19}$	0.4	1344±3.7	+262 ± 56	5.1 ± 0.015
+2 mol % $CoCl_2$	-5.22×10^{18}	2.7	554±3	-212 ±3 4	8.1 ± 0.06
+2 at. % Sn	$+4.45 \times 10^{18}$	2.6	1573 ± 5	+582 ± 35	21.5 ± 0.3
+2 at. % Ag	-3.39×10^{18}	5.3	338 ± 1.5	-389 ± 30	44.8 ± 0.27
+2 at. % Ce	-2.73×10^{18}	7.9	308 ±1.4	-396 ± 28	51 ± 0.2

Experimentally we also tested a number of dopants that resulted in poor performances. In the cases of P, Zn, Cl, Sn, Ag and Ce dopants the obtained power factors and electrical conductivities are lower than the one observed for the undoped reference (Table S1). Thus, P, Zn, Cl, Sn, Ag and Ce are not effective dopants for this system. We have also found that P, Sn and Zn cause a change of the Seebeck coefficient sign signifying a p-type characteristic. This is also evident from the defect formation energies of the corresponding defects (P_S, Sn_{Sb} and Zn_{Sb}) shown in the supplementary information, Table S1. The other dopants, i.e. Cl, Ag and Ce result in n-type characteristics. Note that the corresponding defects are very high in energy (Table S1), which results in low carrier concentrations. From the PSM measurements, we have found that all the p-type dopants result in very high resistivity values, in excess of 1300 mΩ.cm. Such large resistivities were also reported by D. Parker et al, when CoSbS was p-doped with Fe. We have observed that the mobility of charge carriers is strongly suppressed when p-doped. Finally, we

investigated Ag as a dopant motivated by our previous work in tin sulfide[5]. Unfortunately, we observed very high defect formation energies and thus large measured resistivities and furthermore a decrease in evaluated Seebeck coefficient. Similarly unfavorable results were observed for Ce doped CoSbS from both the defect calculations and PSM measurements.

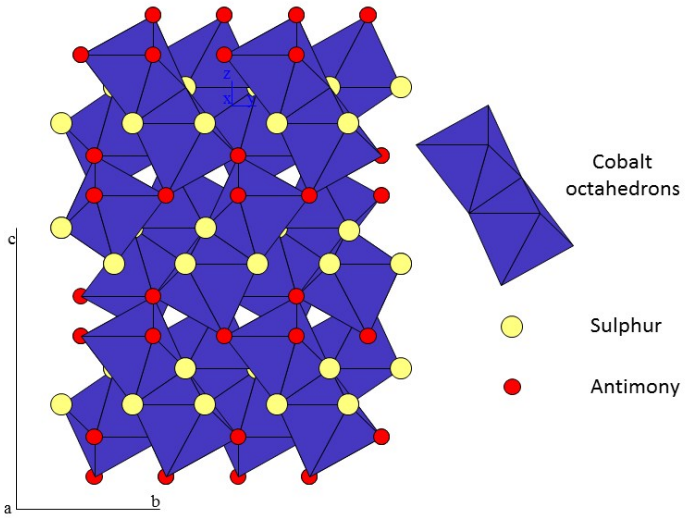

Figure S1. CoSbS structure seen along a-axis.

The unit-cell of CoSbS comprises of eight atoms each of Co, Sb and S. Every Co atom is surrounded by six nearest-neighboring anions in a distorted octahedral environment. Each anion is coordinated by one other anion and three cations in a distorted tetrahedral arrangement. The difference between the orthorhombic marcasite structure from a very similar cubic pyrite structure is that in the former, edge-sharing of the cation octahedra occurs in linear chains parallel to the orthorhombic and longest *c* direction (illustrated in Figure SI.1). As a result there is a less regular octahedral environment around the cation.

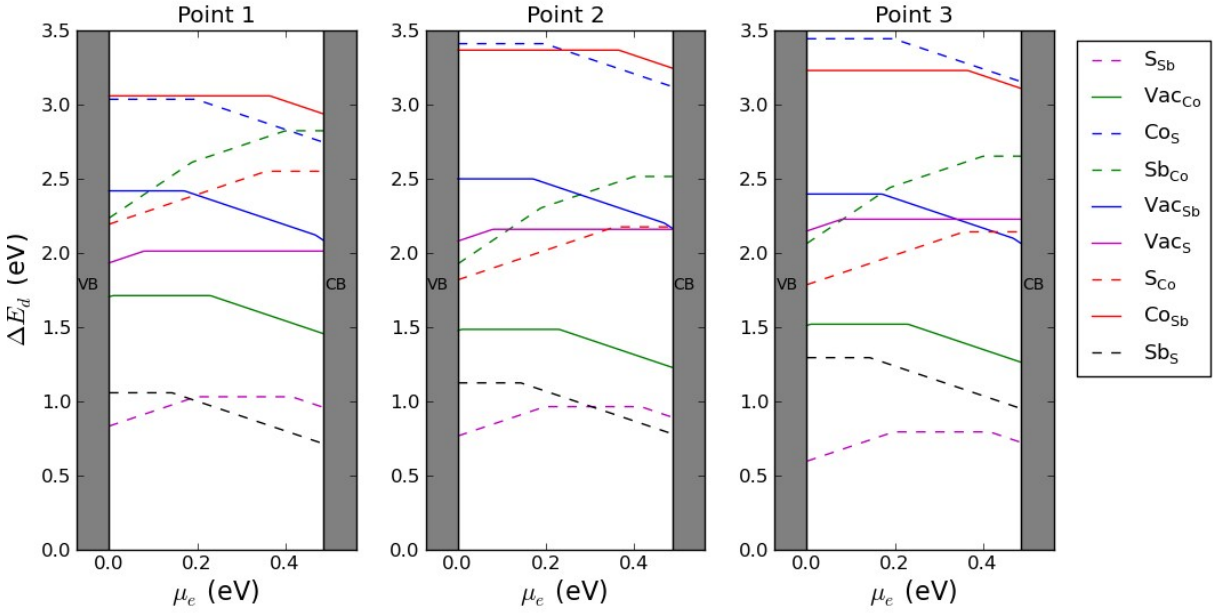

Figure S2. The defect formation energies of all the intrinsic defects are shown here. The three points correspond to the $\Delta\mu_\alpha$ (α = Co, Sb and S) values illustrated in Figure 3 and the methods section.

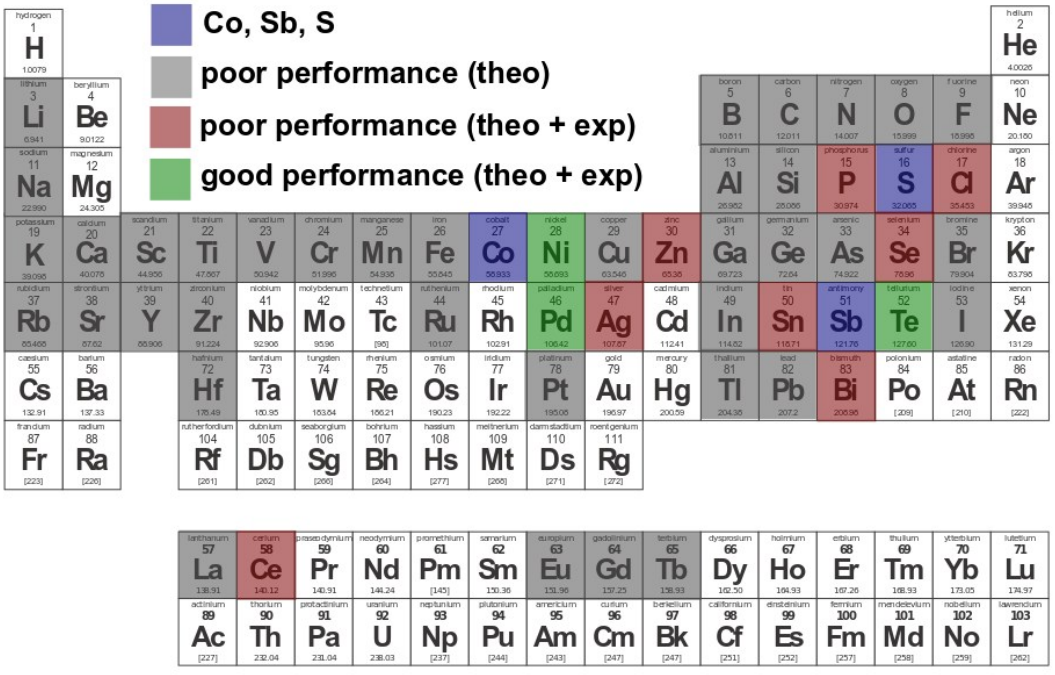

Figure S3: Extrinsic defect candidates investigated for CoSbS and their performances.

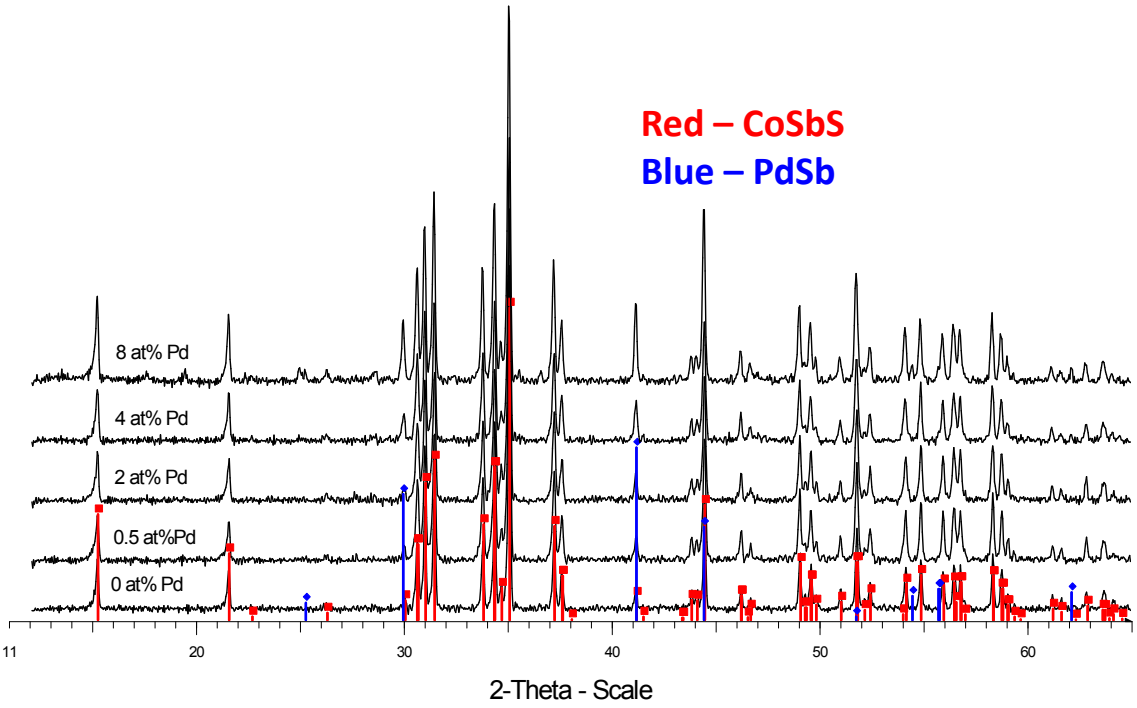

Figure S4. XRD patterns collected on CoSbS doped with various Pd contents. A PdSb pattern in blue significantly increases with Pd content increase.

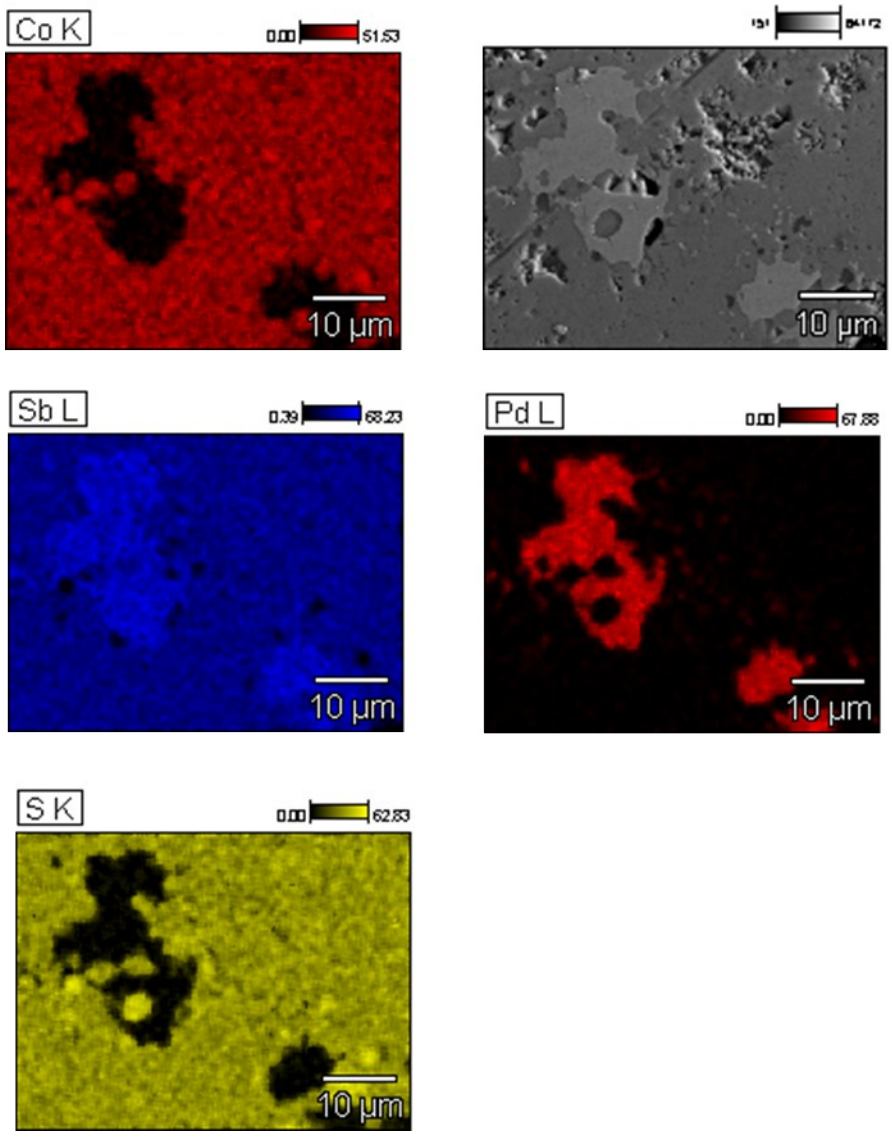

Figure S5. SEM/EDX micrographs of CoSbS doped with 4 at. % of Pd. PdSb rich areas are clearly identified.

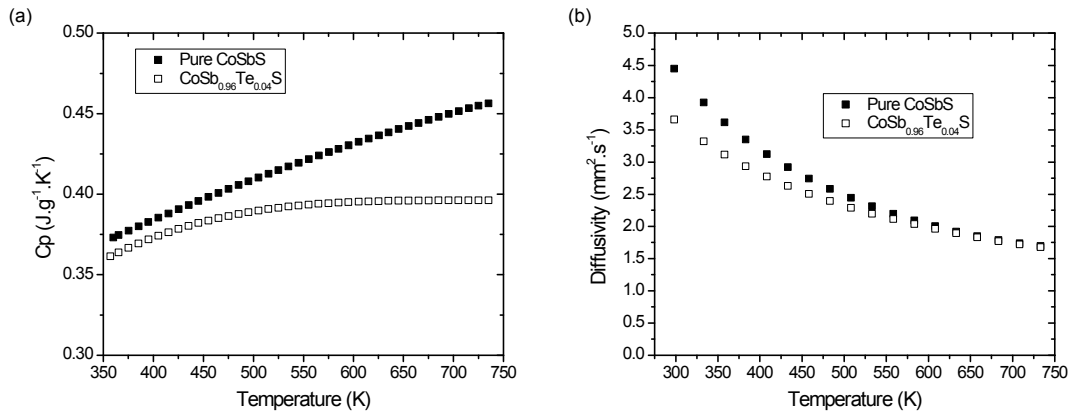

Figure SI.6. (a) Thermal capacity and (b) thermal diffusivity of pure and 4 at. % doped CoSbS.

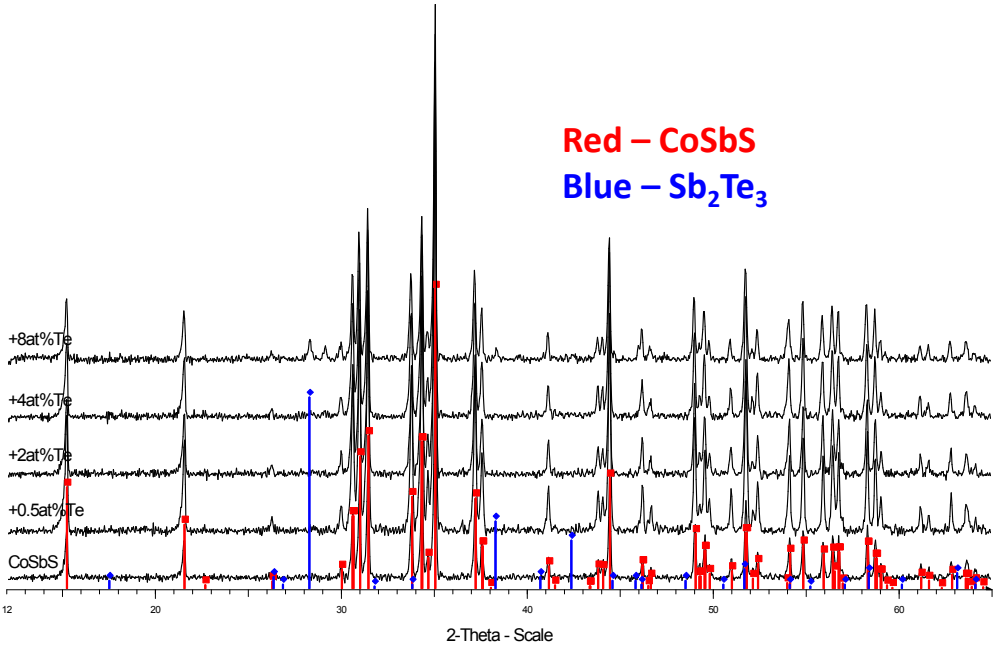

Figure S7. XRD patterns collected on CoSbS doped with various Te contents. For 8 at. % doped CoSbS a Sb_2Te_3 phase has been observed.

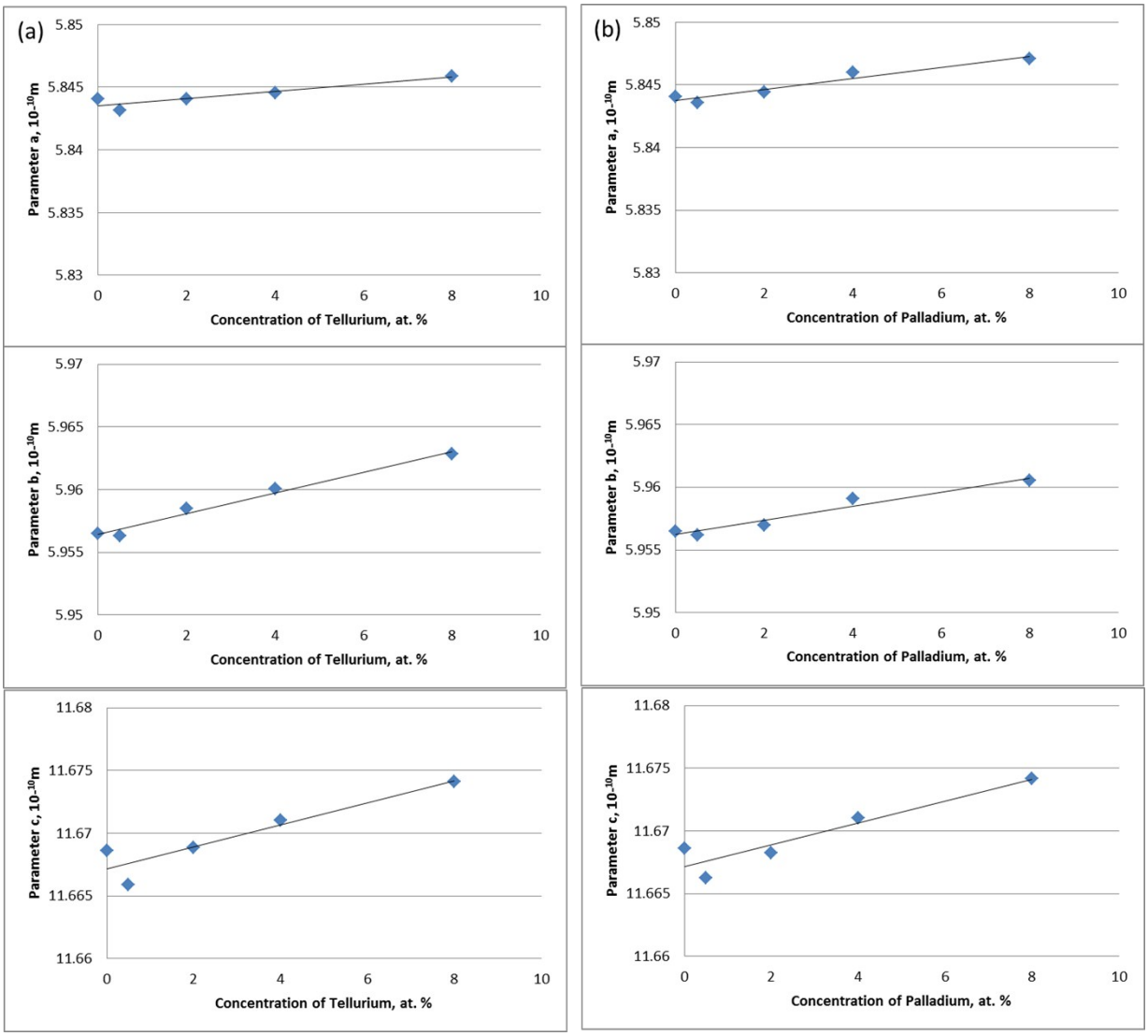

Figure S8. The evolution of the unit cell parameters for (a) Tellurium and (b) Palladium doped CoSbS.