Journal Name

ARTICLE TYPE

Cite this: DOI: 10.1039/xxxxxxxxxx

Supplemental Information: Investigation of Novel Crystal Structures of Bi-Sb binaries Predicted by Minima Hopping Method

Sobhit Singh,*[a] Wilfredo Ibarra-Hernández,[a] Irais Valencia-Jaime,[a,b] Guillermo Avendaño-Franco,[a] and Aldo H. Romero†[a]

This supplemental information file contains the simulated x-ray diffraction (XRD) patterns, Wyckoff positions, thermoelectric properties of all phases of Bi-Sb binaries considered in this study, and a convex-hull calculated for previously reported phases of Bi-Sb binaries. The XRD spectra was calculated for relaxed structures by using following parameters:– x-ray wavelenght = 1.54056 Å and full width at half maxima (FWHM) = 0.1. Additionally, we present the chemical potential dependence of the thermoelectric properties for all phases.

1 Bi_1Sb_7 (P_1m_1 space group no. – 06)

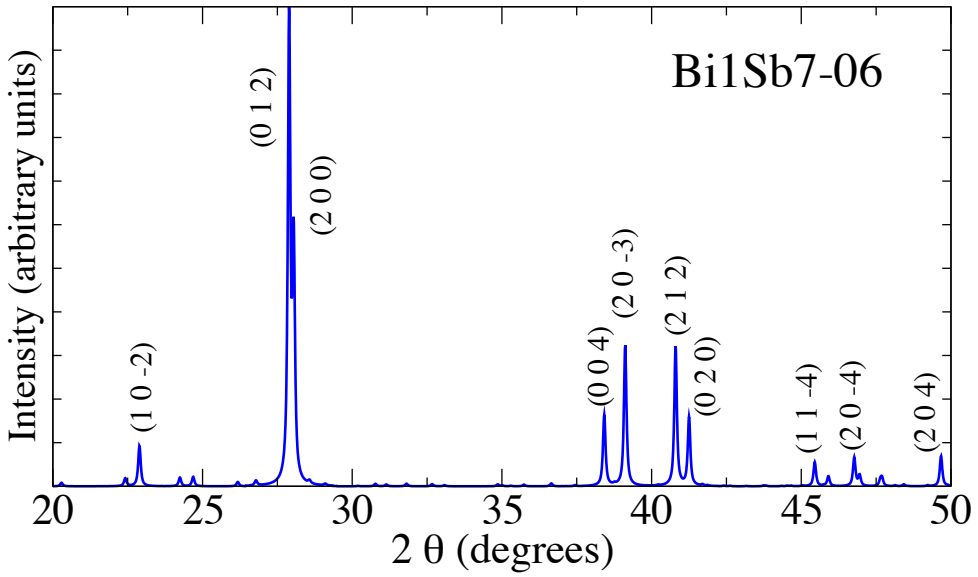

Fig. 1 (Color online) Simulated X-ray diffraction pattern of Bi_1Sb_7 in P_1m_1 space group.

[a] *Department of Physics and Astronomy, West Virginia University, Morgantown, WV-26505-6315, USA*
[b] *Centro de Investigación y Estudios Avanzados del IPN, MX-76230, Querétaro, México*
*E-mail: * smsingh@mix.wvu.edu; † alromero@mail.wvu.edu*

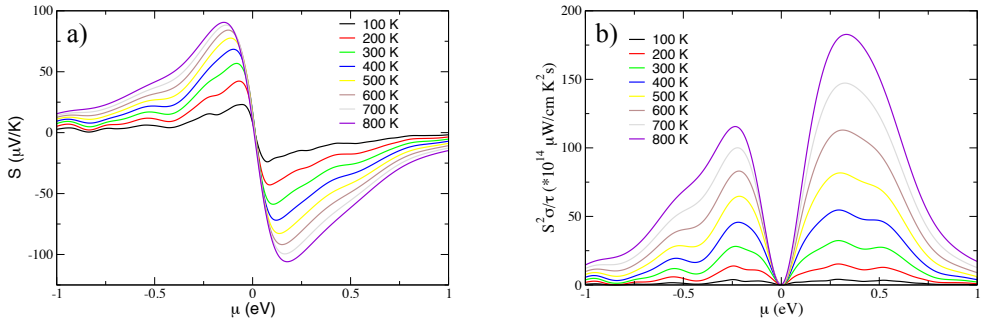

Fig. 2 (Color online) Chemical potential dependence of the a) Seebeck coefficient, and b) power factor ($S^2\sigma/\tau$) for different values of temperature for Bi_1Sb_7 composition in P_1m_1 space group.

Table 1 Wyckoff positions for Bi_1Sb_7 in P_1m_1 space group

site	Multiplicity and Wyckoff letter	x	y	z
Sb1	1b	0.071	0.500	0.716
Sb2	1b	0.603	0.500	0.685
Sb3	1a	0.109	0.000	0.446
Sb4	1a	0.568	0.000	-0.032
Sb5	1a	0.101	0.000	-0.072
Sb6	1a	0.574	0.000	0.473
Sb7	1b	0.593	0.500	0.180
Bi1	1b	0.079	0.500	0.221

2 Bi_1Sb_1 ($R3m$ space group no. – 160)

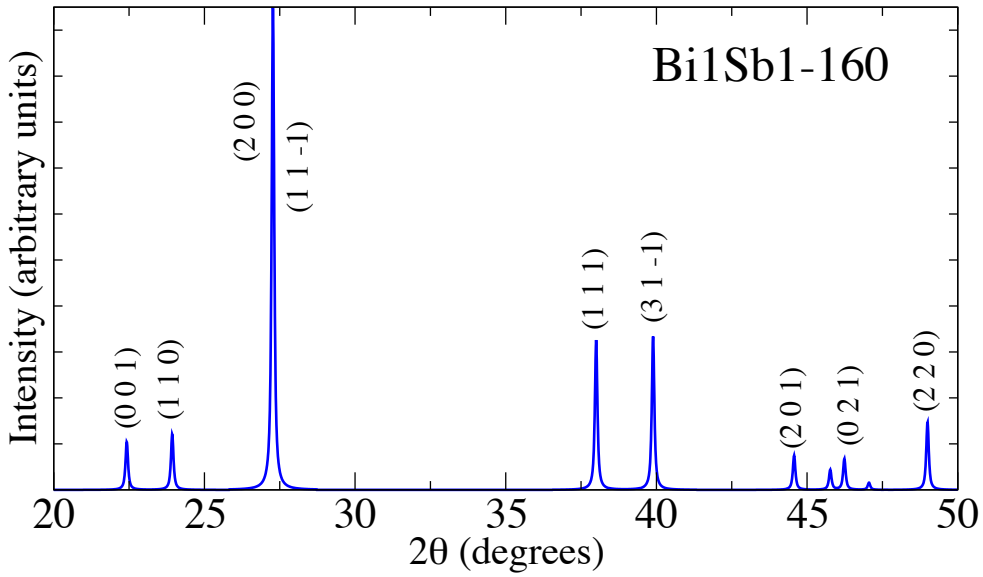

Fig. 3 (Color online) Simulated X-ray diffraction pattern of Bi_1Sb_1 in $R3m$ space group.

Table 2 Wyckoff positions for Bi_1Sb_1 in $R3m$ space group

site	Multiplicity and Wyckoff letter	x	y	z
Sb1	3a	0.000	0.000	0.353
Bi1	3a	0.000	0.000	0.818

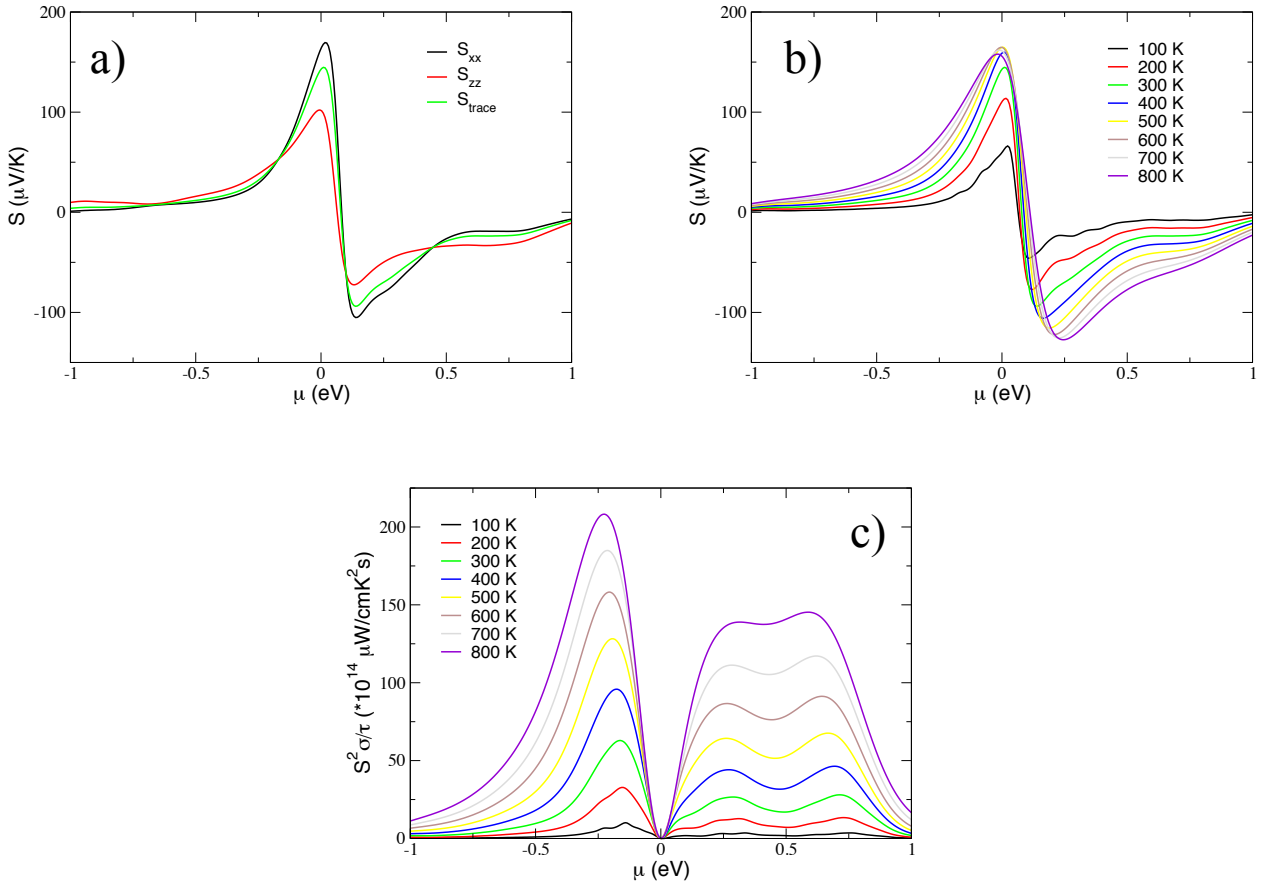

Fig. 4 (Color online) Carrier concentration dependence of a) two non-degenerate cartesian components and the average of the trace of the Seebeck coefficient at 300K, b) the average of the trace of the Seebeck coefficient, and c) the power factor ($S^2\sigma/\tau$) for different values of temperature for Bi_1Sb_1 in $R3m$ space group.

3 Bi_1Sb_1 ($Imm2$ space group no. – 44)

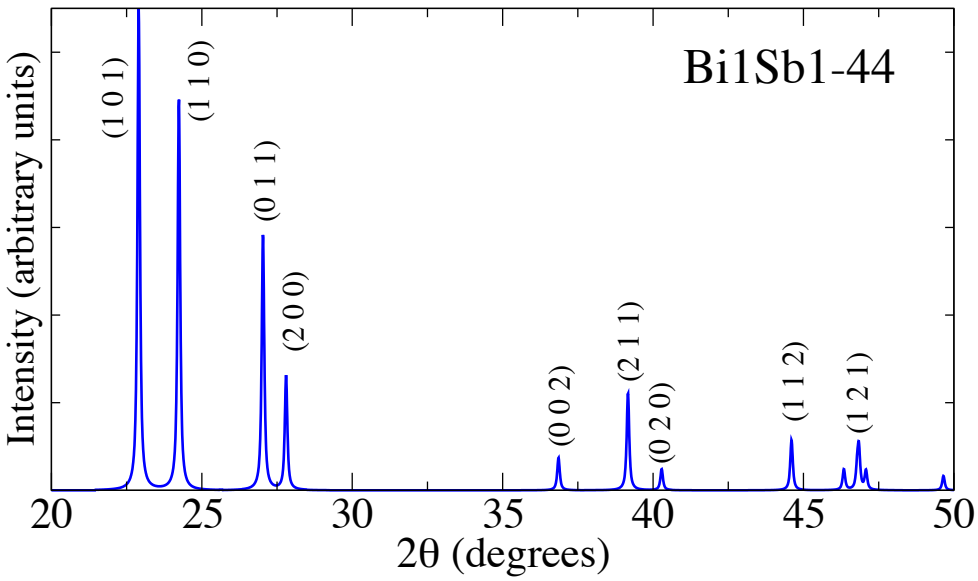

Fig. 5 (Color online) Simulated X-ray diffraction pattern of Bi_1Sb_1 in $Imm2$ space group.

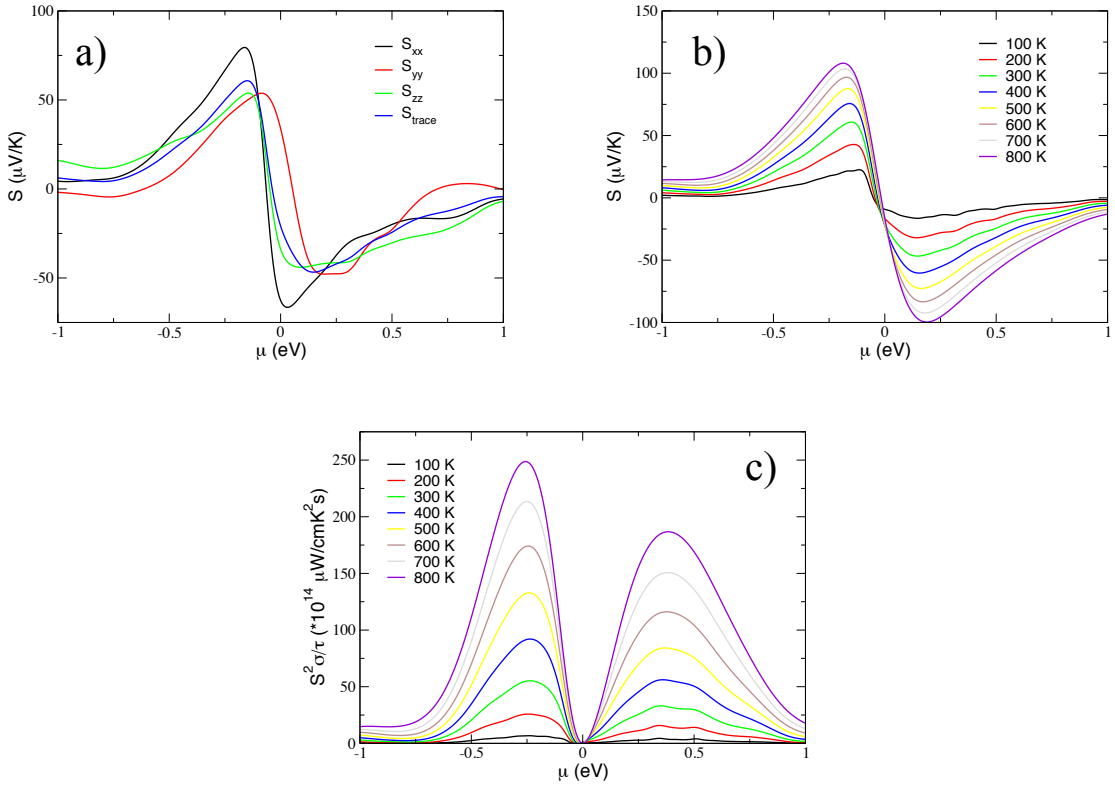

Fig. 6 (Color online) Carrier concentration dependence of a) three cartesian components of the Seebeck coefficient at 300 K, b) the average of the trace of the Seebeck coefficient, and c) the power factor ($S^2\sigma/\tau$) for different values of temperature for Bi_1Sb_1 in $Imm2$ space group.

Table 3 Wyckoff positions for Bi_1Sb_1 in $Imm2$ space group

site	Multiplicity and Wyckoff letter	x	y	z
Sb1	2a	0.000	0.000	0.719
Bi1	2b	0.000	0.500	0.133

4 Bi_1Sb_1 ($R\bar{3}m$ space group no. – 166)

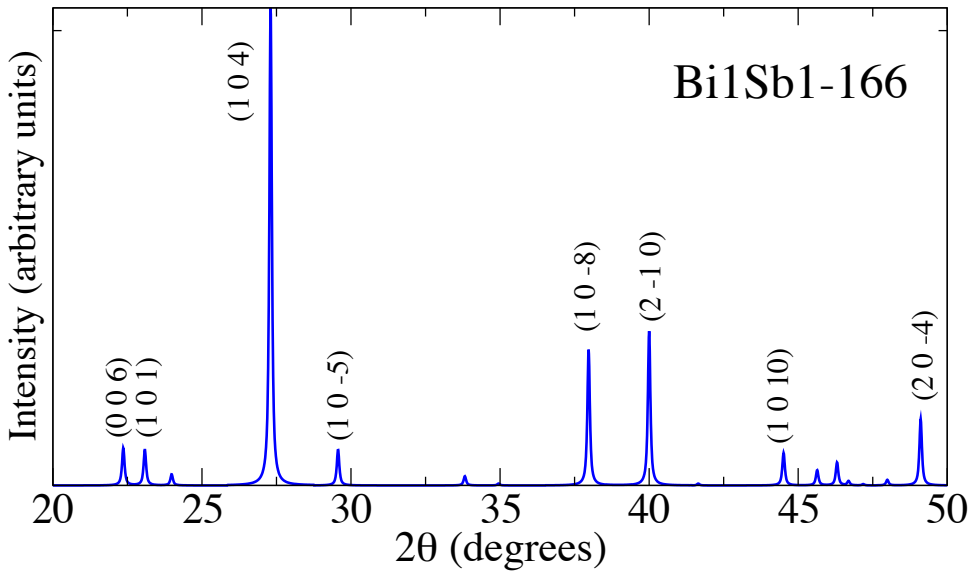

Fig. 7 (Color online) Simulated X-ray diffraction pattern of Bi_1Sb_1 in $R\bar{3}m$ space group.

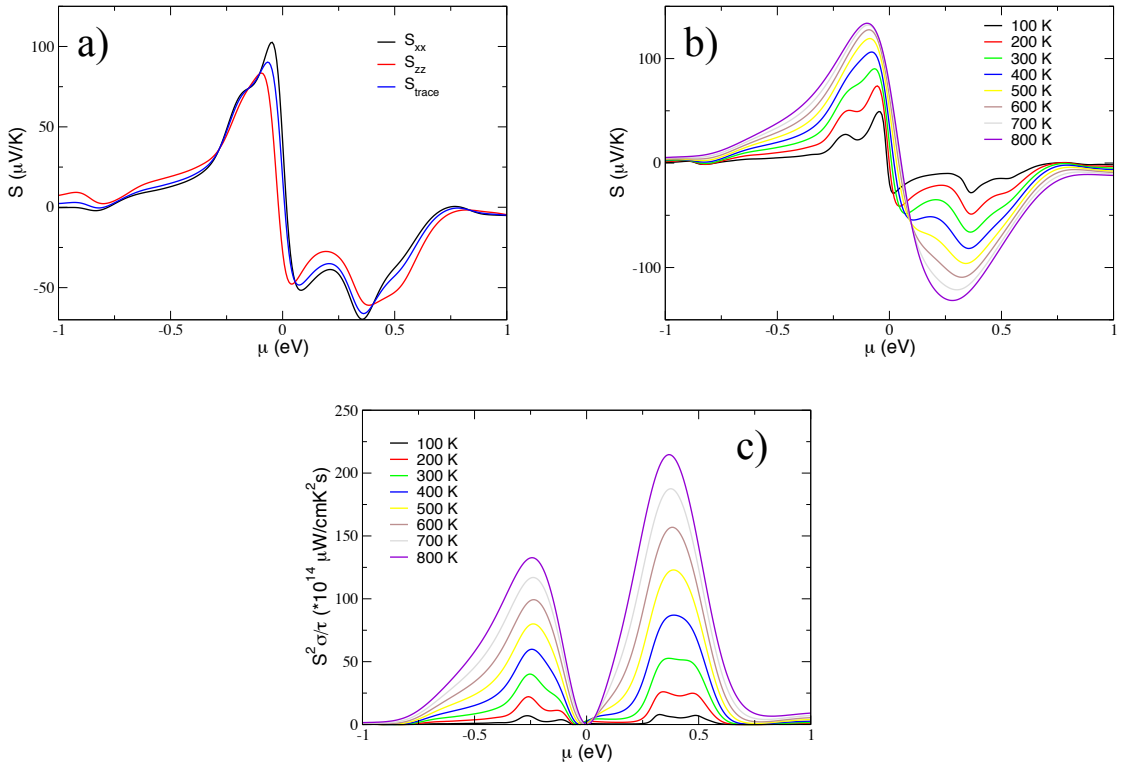

Fig. 8 (Color online) Carrier concentration dependence of a) two non-degenerate cartesian components and the average of the trace of the Seebeck coefficient at 300K, b) the average of the trace of the Seebeck coefficient, and c) the power factor ($S^2\sigma/\tau$) for different values of temperature for Bi_1Sb_1 in $R\bar{3}m$ space group.

Table 4 Wyckoff positions for Bi_1Sb_1 in $R\bar{3}m$ space group

site	Multiplicity and Wyckoff letter	x	y	z
Sb1	6c	0.000	0.000	0.121
Bi1	6c	0.000	0.000	0.612

5 Bi_3Sb_1 ($R3m$ space group no. – 160)

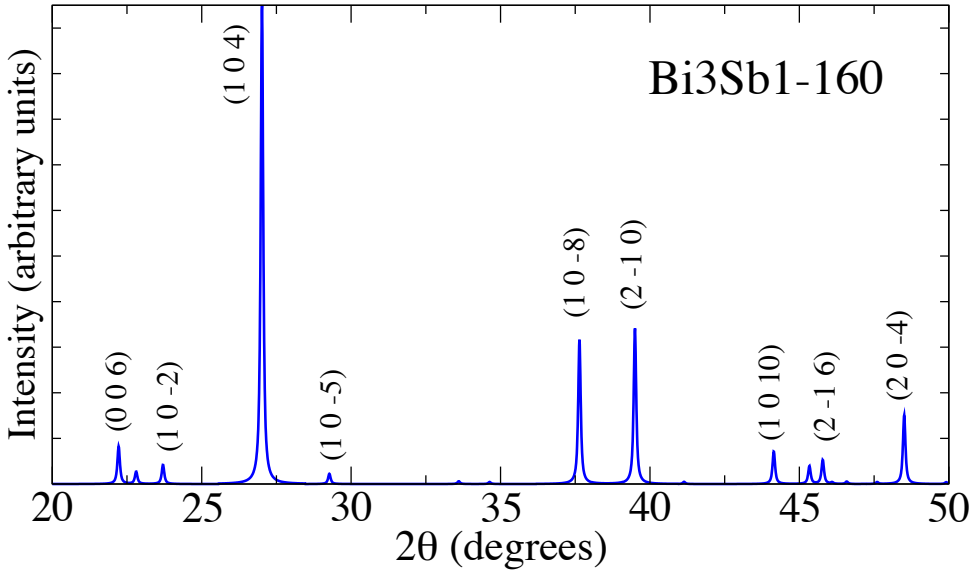

Fig. 9 (Color online) Simulated X-ray diffraction pattern of Bi_3Sb_1 in $R3m$ space group.

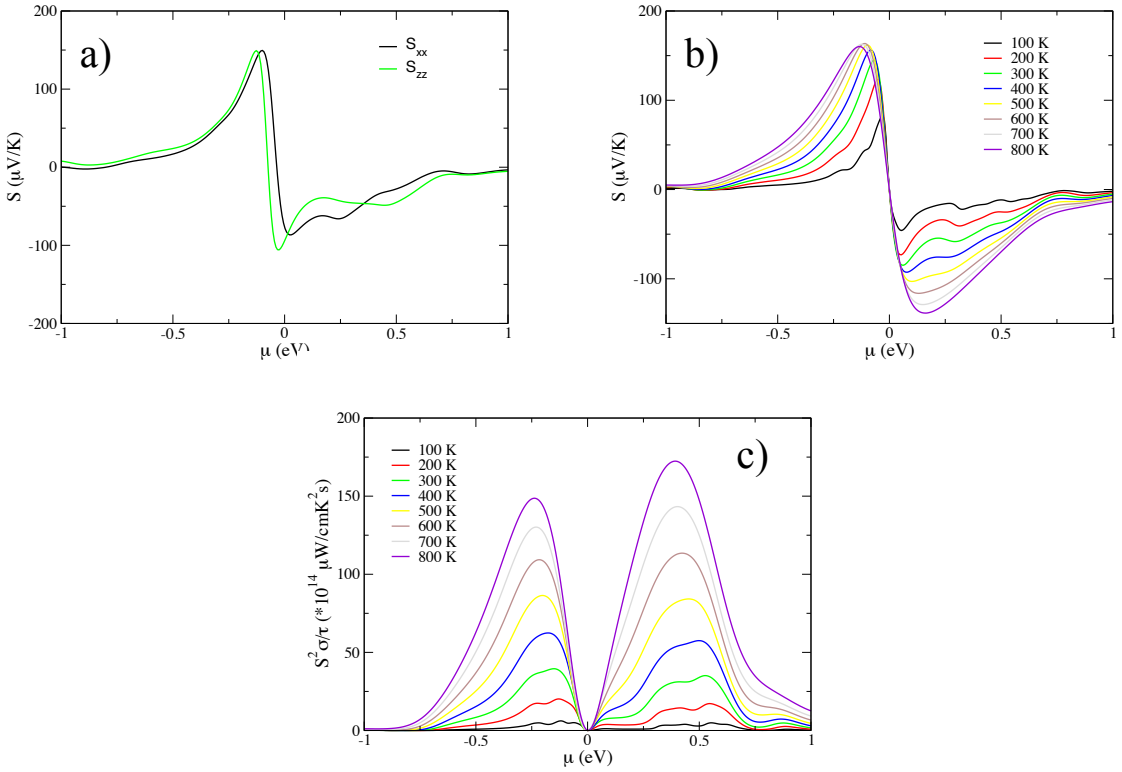

Fig. 10 (Color online) Carrier concentration dependence of a) two non-degenerate cartesian components of the Seebeck coefficient at 300K, b) the average of the trace of the Seebeck coefficient, and c) the power factor ($S^2\sigma/\tau$) for different values of temperature for Bi_3Sb_1 in $R3m$ space group.

Table 5 Wyckoff positions for Bi_3Sb_1 in $R3m$ space group

site	Multiplicity and Wyckoff letter	x	y	z
Sb1	3a	0.000	0.000	0.063
Bi1	3a	0.000	0.000	0.791
Bi2	3a	0.000	0.000	0.297
Bi3	3a	0.000	0.000	0.564

6 Bi_7Sb_1 (C_1m_1 space group no. – 08)

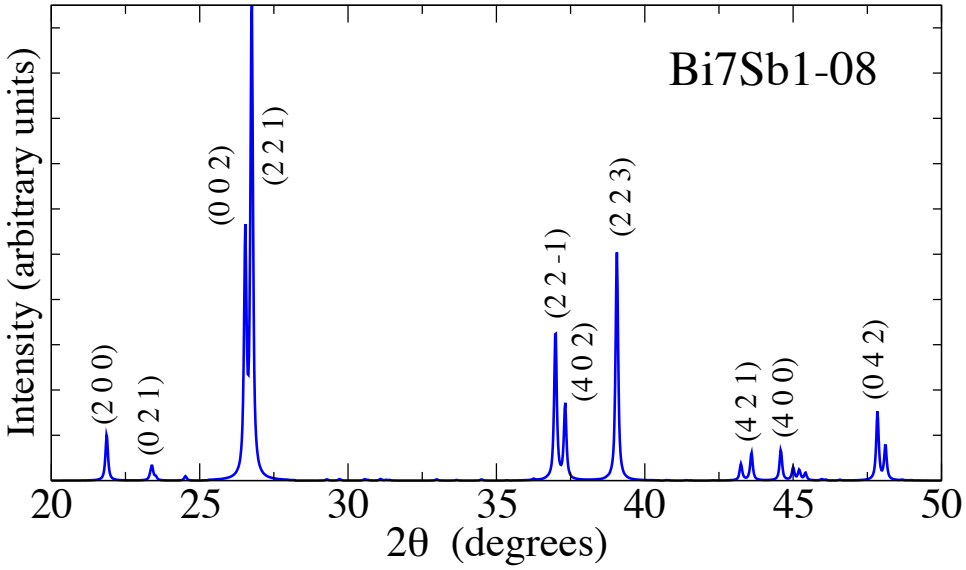

Fig. 11 (Color online) Simulated X-ray diffraction pattern of Bi_7Sb_1 in C_1m_1 space group.

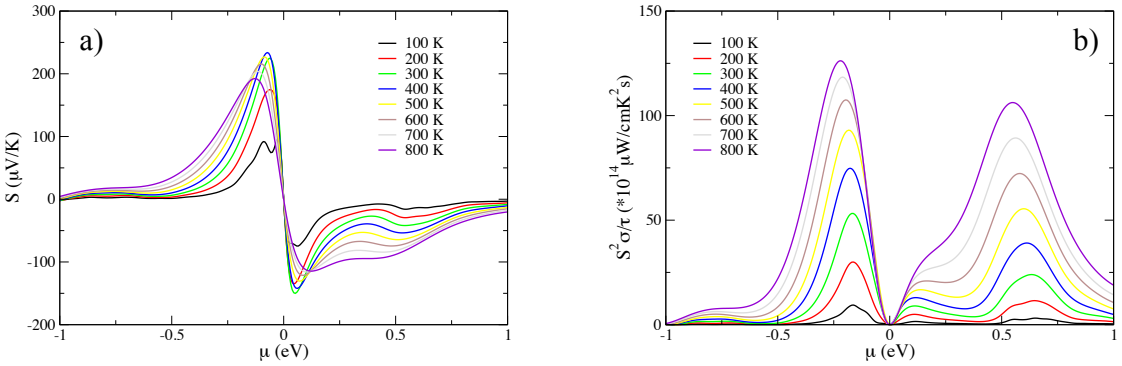

Fig. 12 (Color online) Chemical potential dependence of the a) Seebeck coefficient, and b) power factor ($S^2\sigma/\tau$) for different values of temperature for Bi_7Sb_1 in C_1m_1 space group.

Table 6 Wyckoff positions for Bi_7Sb_1 in C_1m_1 space group

site	Multiplicity and Wyckoff letter	x	y	z
Sb1	2a	0.729	0.000	0.737
Bi1	4b	0.232	0.252	0.240
Bi2	4b	0.534	0.245	0.705
Bi3	2a	0.231	0.000	0.745
Bi4	2a	0.0301	0.000	0.209
Bi5	2a	0.537	0.000	0.187

7 Bi_9Sb_1 (C_1m_1 space group no. – 08)

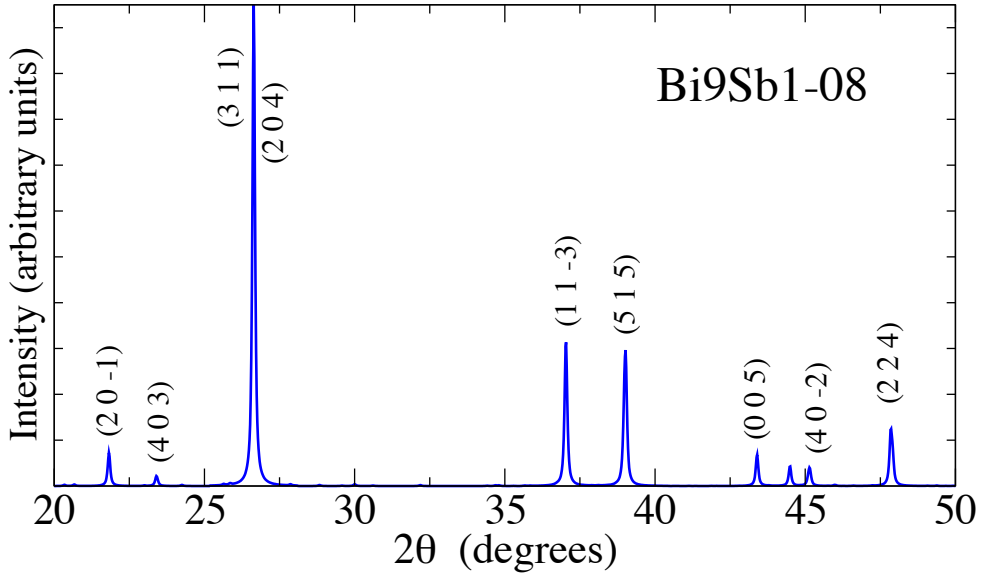

Fig. 13 (Color online) Simulated X-ray diffraction pattern of Bi_9Sb_1 in C_1m_1 space group.

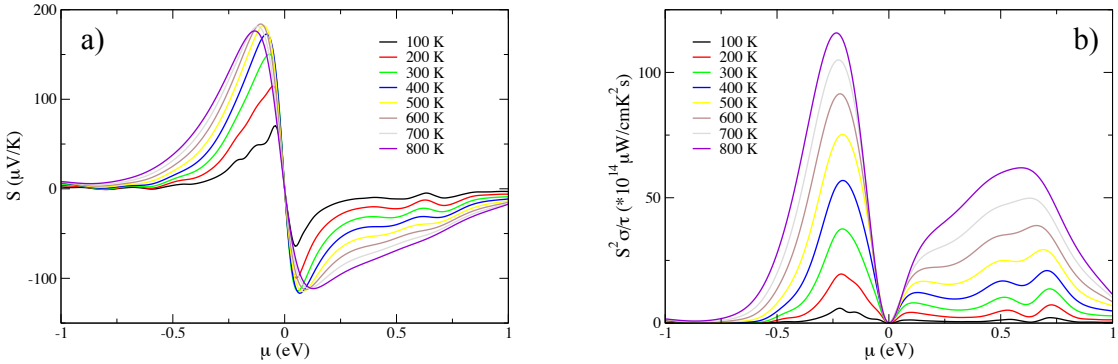

Fig. 14 (Color online) Chemical potential dependence of the a) Seebeck coefficient, and b) power factor ($S^2\sigma/\tau$) for different values of temperature for Bi_9Sb_1 in C_1m_1 space group.

Table 7 Wyckoff positions for Bi_9Sb_1 in C_1m_1 space group

site	Multiplicity and Wyckoff letter	x	y	z
Sb1	2a	0.152	0.000	0.413
Bi1	2a	0.684	0.000	0.879
Bi2	2a	0.282	0.000	0.084
Bi3	2a	0.880	0.000	0.284
Bi4	2a	0.089	0.000	0.672
Bi5	2a	-0.052	0.000	0.017
Bi6	2a	0.547	0.000	0.216
Bi7	2a	0.349	0.000	0.816
Bi8	2a	0.752	0.000	0.611
Bi9	2a	0.494	0.000	0.477

Theoretical convex-hull:

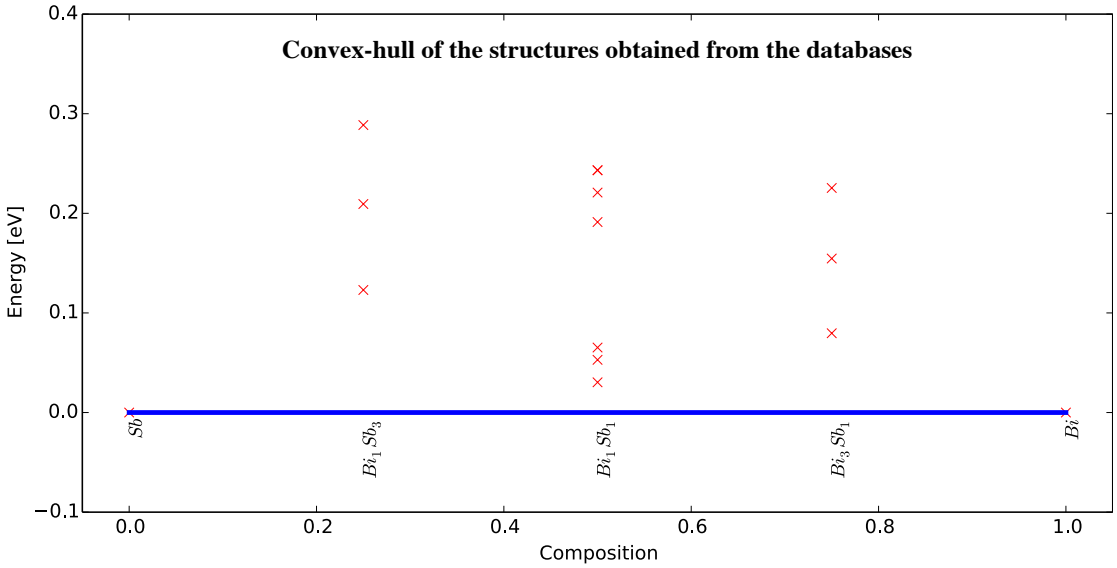

Fig. 15 (Color online) The theoretical convex-hull calculated for existing phases of Bi-Sb binaries. These structures were obtained from the Materials Project, OpenQMD and AFLOW open crystal structure databases.