Effect of lattice misfit on stability of the misfit layer compound $(SnS)_{1+x}NbS_2$

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Supplementary Materials

Table S1. Designed approximants and related symmetry for the $(SnS)_{1+x}NbS_2$ (x = 0.200, 0.167, 0.143) misfit compounds and those containing Sn or S deficiencies. *Pseudo-orthorhombic unit cells. The experimental values are included for comparison.

Structure	Symmetry	lattice paras.(Å)* *a*, *b*, *c*	Remarks
(a) $(SnS)_{1.200}NbS_2$	C2 (no. 5)	16.605, 5.571, 11.761	10 Nb, 12 Sn and 32 S
(b) $(SnS)_{1.167}NbS_2$-a	Pa (no.7)	39.852, 5.571, 11.761	24 Nb, 28 Sn and 76 S
(c) $(SnS)_{1.167}NbS_2$-b	Pa (no.7)	39.852, 5.571, 11.761	24 Nb, 28 Sn and 76 S
(d) $(SnS)_{1.143}NbS_2$	C2 (no. 5)	23.247, 5.571, 11.761	14 Nb, 16 Sn and 44 S.
(e) $(SnS_{0.929})_{1.167}NbS_2$	C2 (no. 5)	39.852, 5.571, 11.761	24 Nb, 28 Sn and 74 S
(f) $(Sn_{0.929}S)_{1.167}NbS_2$	C2(no. 5)	39.852, 5.571, 11.761	24 Nb, 26 Sn and 76 S
Experimental [1,4] $(SnS)_{1.171}NbS_2$	Cm2a C2m2	SnS (Z = 4) 5.673, 5.751, 11.761 NbS_2 (Z=2) 3.321, 5.751, 11.761	

Table S2. Calculated results (coordinates of atoms, interatomic distances and Bader charges at the atomic sites) using the DFT + vdW approach for the $(SnS)_{1.20}NbS_2$ misfit layer compound, case a). This structure has a pseudo-orthorhombic lattice, space group C2 (no. 5) with Nb1 at 2a (0, y ,0) and (½, ½+y, 0); and the rest atoms at the 4c sites (x, y, z) + (-x, y, -z), (½+x, ½+y, z) and (½-x, ½+y, z). The calculated lattice parameters are shown in Table 2.

Specie and atomic coordinates site x/a, y/b, z/c	Bonds (Å)	Charge (e/atom)
Nb1 2a (0.0000, 0.9147, 0.0000) Nb2 4c (0.0996, 0.4152, 0.9982) Nb3 4c (0.2004, 0.9151, 0.9987)	Nb-S(Nb): 2.49 (×6) Nb-S(Nb): 2.49 (×4), 2.50 (×2) Nb-S(Nb): 2.48, 2.49 (×4), 2.50	+1.38 +1.29 +1.30 Av:+1.31
S1 4c (0.0007, 0.2482, 0.1245) S2 4c (0.1006, 0.7487, 0.1304) S3 4c (0.1001, 0.7516, 0.8677) S4 4c (0.1988, 0.2481, 0.1314) S5 4c (0.2000, 0.2500, 0.8676)	S1-Nb: 2.49(×2), 2.50 S2-Nb: 2.49(×3); S2-Sn: 3.16 S3-Nb: 2.49(×3); S3-Sn: 3.22 S4-Nb: 2.49(×2); 2.50; S4-Sn: 3.25 S5-Nb: 2.48, 2.49, 2.50.	-0.73 -0.76 -0.81 -0.78 -0.68 Av:-0.75
S6 4c (0.0839, 0.4898, 0.5930) S7 4c (0.0824, 0.9864, 0.4071) S8 4c (0.2514, 0.4892, 0.4072)	S6-Sn: 2.68, 2.76, 2.84, 2.85, 3.08 S7-Sn: 2.66, 2.82, 2.84, 2.87, 3.03 S8-Sn:2.67, 2.80, 2.82, 2.88, 3.05	-0.76 -0.77 -0.81 Av.:-0.78
Sn1 4c (0.0839, 0.0175, 0.6302) Sn2 4c (0.0829, 0.5044, 0.3674) Sn3 4c (0.2503, 0.0115, 0.3683)	Sn-S(Sn): 2.66, 2.76, 2.82, 2.84, 3.08; Sn-S(Nb): 3.22 Sn-S(Sn): 2.68, 2.82, 2.85, 2.88, 3.03; Sn-S(Nb): 3.16 Sn-S(Sn): 2.67, 2.80, 2.84, 2.87, 3.05; Sn-S(Nb): 3.25	+1.08 +0.86 +0.91 Av.:+0.95

Table S3. Calculated results (coordinates of atoms, interatomic distances and Bader charges at the atomic sites) using the DFT + vdW correction for the $(SnS)_{1.167}NbS_2$ misfit layer compound, case b). This structure had a monoclinic lattice with space group Pa (no. 7) with all atoms at the 2a sites (*x*, *y*, *z*) + (*x*+½, *y*, -*z*). The calculated unit cell can be described as a pseudo-orthorhombic unit cell with lattice parameters in Table 2.

Specie and atomic coordinates x/a, y/b, z/c	Bonds (Å)	Charge (e/atom)
Nb1 (0.9930, 0.9197, 0.9993)	Nb-S(Nb): 2.48 (×3), 2.49 (×3)	+1.49
Nb2 (0.0764, 0.9198, 0.9995)	Nb-S(Nb): 2.48 (×3), 2.49 (×3)	+1.43
Nb3 (0.1599, 0.9198, 0.0017)	Nb-S(Nb): 2.48 (×3), 2.49 (×2), 2.50	+1.36
Nb4 (0.2432, 0.9196, 0.9978)	Nb-S(Nb): 2.48 (×3), 2.49 (×2), 2.50	+1.32
Nb5 (0.3263, 0.9196, 0.0022)	Nb-S(Nb): 2.48 (×3), 2.49 (×2), 2.50	+1.45
Nb6 (0.4095, 0.9197, 0.9982)	Nb-S(Nb): 2.48 (×3), 2.49 (×2), 2.50	+1.40
Nb7 (0.0347, 0.4189, 0.9978)	Nb-S(Nb): 2.48 (×3), 2.49, 2.50 (×2)	+1.02
Nb8 (0.1179, 0.4191, 0.0021)	Nb-S(Nb): 2.48 (×2), 2.49 (×3), 2.50	+1.01
Nb9 (0.2013, 0.4192, 0.9987)	Nb-S(Nb): 2.48 (×3), 2.49 (×3)	+1.03
Nb10 (0.2847,0.4191, 0.0001)	Nb-S(Nb): 2.48 (×3), 2.49 (×3)	+1.15
Nb11 (0.3681, 0.4190, 0.0011)	Nb-S(Nb): 2.48 (×3), 2.49 (×3)	+1.14
Nb12 (0.4516, 0.4190, 0.9980)	Nb-S(Nb): 2.48 (×2), 2.49 (×3), 2.50	+1.06 Av:+1.24
S1 (0.9935, 0.2516, 0.1330)	S1-Nb: 2.48, 2.49, 2.50	-0.67
S2 (0.4929, 0.2530, 0.1333)	S2-Nb: 2.48, 2.49, 2.50	-0.50
S3 (0.0760, 0.2518, 0.1331)	S3-Nb: 2.48, 2.49, 2.50	-0.59
S4 (0.5766, 0.2528, 0.1333)	S4-Nb: 2.48, 2.49, 2.50	-0.61
S5 (0.1598, 0.2544, 0.1333)	S5-Nb: 2.48(×2), 2.49; -Sn: 3.27	-0.59
S6 (0.6592, 0.2516, 0.1319)	S6-Nb: 2.48, 2.49(×2)	-0.63
S7 (0.2428, 0.2516, 0.1310)	S7-Nb: 2.48 (×3); -Sn: 3.22	-0.74
S8 (0.7431, 0.2556, 0.1334)	S8-Nb: 2.48, 2.49(×2), -Sn: 3.24	-0.62
S9 (0.3264, 0.2557, 0.1334)	S9-Nb: 2.48(×2), 2.49; -Sn: 3.24	-0.62
S10 (0.8265, 0.2515, 0.1309)	S10-Nb: 2.48(×3); -Sn: 3.22	-0.71
S11 (0.4102, 0.2515, 0.1317)	S11-Nb: 2.48, 2.49(×2)	-0.76
S12 (0.9097, 0.2545, 0.1333)	S12-Nb: 2.48(×2), 2.49; -Sn: 3.27	-0.50
S13 (0.0347, 0.7513, 0.1307)	S13-Nb: 2.48(×3); -Sn: 3.21	-0.79
S14 (0.5347, 0.7557, 0.1332)	S14-Nb: 2.48(×2), 2.49; -Sn: 3.24	-0.83
S15 (0.1180, 0.7553, 0.1332)	S15-Nb: 2.48, 2.49(×2); -Sn: 3.25	-0.79
S16 (0.6184, 0.7515, 0.1310)	S16-Nb: 2.48, 2.49(×2); -Sn: 3.24	-0.77
S17 (0.2019, 0.7514, 0.1322)	S17-Nb: 2.48, 2.49(×2).	-0.62
S18 (0.7013, 0.7537, 0.1331)	S18-Nb: 2.48, 2.49, 2.50.	-0.61
S19 (0.2844, 0.7522, 0.1332)	S19-Nb: 2.48, 2.49, 2.50	-0.69
S20 (0.7851, 0.7520, 0.1332)	S20-Nb: 2.48, 2.49, 2.50	-0.70
S21 (0.3682, 0.7533, 0.1332)	S21-Nb: 2.48, 2.49, 2.50	-0.58
S22 (0.8676, 0.7513, 0.1324)	S22-Nb: 2.48, 2.49, 2.50	-0.67
S23(0.4510, 0.7514, 0.1312)	S23-Nb: 2.48, 2.49(×2); -Sn: 3.25	-0.77
S24(0.9514, 0.7549, 0.1332)	S24-Nb: 2.48, 2.49(×2); -Sn: 3.25	-0.81 Av:-0.71
S25 (0.0357, 0.4892, 0.5977)	S25-Sn: 2.69, 2.81, 2.87, 2.88, 3.00	-0.62
S26 (0.9651, 0.9898, 0.5991)	S26-Sn: 2.65, 2.84, 2.87, 2.93, 2.95	-0.91
S27 (0.1795, 0.4913, 0.5984)	S27-Sn:2.66, 2.83, 2.86, 2.93, 2.96	-0.89
S28 (0.8216, 0.9891, 0.5977)	S28-Sn: 2.69, 2.81, 2.86, 2.89, 3.00	-0.60
S29 (0.3210, 0.4882, 0.6001)	S29-Sn: 2.64, 2.87, 2.88, 2.92, 2.95	-0.60
S30 (0.6778, 0.9915, 0.5982)	S30-Sn: 2.67, 2.83, 2.85, 2.93, 2.97	-0.80
S31 (0.4637, 0.4907, 0.5980)	S31-Sn: 2.68, 2.83, 2.84, 2.91, 2.99	-0.74
S32 (0.5358, 0.9882, 0.6004)	S32-Sn: 2.64, 2.88, 2.89, 2.90, 2.94	-0.66
S33 (0.6076, 0.4906, 0.5978)	S33-Sn: 2.68, 2.82, 2.84, 2.90, 2.99	-0.70
S34 (0.3936, 0.9911, 0.5981)	S34-Sn: 2.67, 2.83, 2.84, 2.92, 2.98	-0.92
S35 (0.7505, 0.4886, 0.5999)	S35-Sn: 2.64, 2.87, 2.88, 2.92, 2.95	-0.67
S36 (0.2497, 0.9895, 0.5977)	S36-Sn: 2.69, 2.81, 2.86, 2.89, 3.00	-0.69
S37 (0.8919, 0.4907, 0.5986)	S37-Sn: 2.66, 2.83, 2.86, 2.93, 2.96	-0.92
S38 (0.1064, 0.9895, 0.5994)	S38-Sn: 2.65, 2.85, 2.87, 2.93, 2.95	-0.72

		Av.:-0.74
Sn1 (0.0357, 0.0056, 0.6223)	Sn-S(Sn): 2.64, 2.81, 2.84, 2.85, 3.00; Sn-S(Nb): 3.24	+1.23
Sn2 (0.5358, 0.4941, 0.6293)	Sn-S(Sn): 2.69, 2.88, 2.90, 2.91, 2.94, Sn-S(Nb): 3.21	+1.06
Sn3 (0.1790, 0.9999, 0.6271)	Sn-S(Sn): 2.67, 2.86, 2.86, 2.93, 2.96.	+0.95
Sn4 (0.6781, 0.5023, 0.6261)	Sn-S(Sn): 2.66, 2.84, 2.85, 2.92, 2.97, Sn-S(Nb): 3.27	+1.11
Sn5 (0.3213, 0.9942, 0.6292)	Sn-S(Sn): 2.69, 2.88, 2.89, 2.92, 2.95, Sn-S(Nb): 3.22	+0.93
Sn6 (0.8217, 0.5057, 0.6227)	Sn-S(Sn): 2.64, 2.81, 2.83, 2.87, 3.00, Sn-S(Nb): 3.24	+0.91
Sn7 (0.4638, 0.0047, 0.6244)	Sn-S(Sn): 2.65, 2.83, 2.83, 2.90, 2.99, Sn-S(Nb): 3.25	+0.88
Sn8 (0.9646, 0.4972, 0.6283)	Sn-S(Sn): 2.68, 2.87, 2.87, 2.93, 2.95, Sn-S(Nb): 3.25	+0.71
Sn9 (0.6075, 0.0049, 0.6238)	Sn-S(Sn): 2.65, 2.82, 2.83, 2.89, 2.99; Sn-S(Nb): 3.25	+0.78
Sn10 (0.1068, 0.4961, 0.6287)	Sn-S(Sn): 2.68, 2.87, 2.88, 2.93, 2.95, Sn-S(Nb): 3.24	+0.99
Sn11 (0.7502, 0.9945, 0.6291)	Sn-S(Sn): 2.69, 2.88, 2.89, 2.93, 2.95, Sn-S(Nb): 3.22	+0.99
Sn12 (0.2497, 0.5055, 0.6230)	Sn-S(Sn): 2.64, 2.81, 2.83, 2.87, 3.00, Sn-S(Nb): 3.24	+0.73
Sn13 (0.8925, 0.9991, 0.6285)	Sn-S(Sn): 2.67, 2.86, 2.86, 2.93, 2.96.	+0.88
Sn14 (0.3934, 0.5035, 0.6256)	Sn-S(Sn): 2.66, 2.84, 2.84, 2.92, 2.98, Sn-S(Nb): 3.21	+0.96
		Av.:+0.89

Table S4. Calculated results (coordinates of atoms, interatomic distances and Bader charges at the atomic sites) using the DFT + vdW correction for the $(SnS)_{1.143}NbS_2$ misfit layer compound, case d. This structure has a pseudo-orthorhombic lattice with space group C2 (no. 5) with Nb1 at 2a (0, *y* ,0) and (½, ½+*y*, 0); and the rest atoms at the 4c sites (*x*, *y*, *z*) + (-*x*, *y*, -*z*), (½+*x*, ½+*y*, *z*) and (½-*x*, ½+*y*, *z*). The calculated lattice parameters are shown in Table 2.

Specie and atomic coordinates site x/a, y/b, z/c	Bonds (Å)	Charge (e/atom)
Nb1 2a (0.0000, 0.9277, 0.0000)	Nb1-S(Nb): 2.48 (×4), 2.49(×2)	+1.36
Nb2 4c (0.1429, 0.9275, 0.0011)	Nb2-S(Nb): 2.48(×3), 2.49(×3)	+0.91
Nb3 4c (0.2861, 0.9271, 0.9978)	Nb3-S(Nb): 2.47, 2.48, 2.49 (×4)	+0.96
Nb4 4c (0.4288, 0.9269, 0.0025)	Nb4-S(Nb): 2.47, 2.48, 2.49 (×4)	+1.20
		Av:+1.07
S1 4c (0.9994, 0.2596, 0.1335)	S1-Nb: 2.48, 2.49(×2)	-0.77
S2 4c (0.1431, 0.2607, 0.1334)	S2-Nb: 2.47, 2.49 (×2); S2-Sn: 3.26	-0.56
S3 4c (0.2849, 0.2586, 0.1314)	S3-Nb: 2.48, 2.49(×2)	-0.53
S4 4c (0.4286, 0.2630, 0.1336)	S4-Nb: 2.48(×2); 2.49; S4-Sn: 3.19	-0.65
S5 4c (0.5717, 0.2584, 0.1307)	S5-Nb: 2.48(×2), 2.49.	-0.70
S6 4c (0.7142, 0.2620, 0.1334)	S6-Nb: 2.47, 2.49(×2); S5-Sn: 3.21	-0.46
S7 4c (0.8581, 0.2587, 0.1328)	S7-Nb: 2.48, 2.48(×2)	-0.52
		Av:-0.60
S8 4c (0.0614, 0.9913, 0.6028)	S6-Sn: 2.63, 2.82, 2.90, 2.97, 3.01	-0.61
S9 4c (0.3105, 0.9963, 0.5985)	S7-Sn: 2.68, 2.81, 2.84, 2.98, 3.01	-0.59
S10 4c (0.5632, 0.9936, 0.5976)	S8-Sn: 2.70, 2.81, 2.88, 2.93, 3.00	-0.55
S11 4c (0.8151, 0.9951, 0.6004)	S9-Sn: 2.65, 2.81, 2.83, 3.01, 3.01	-0.52
		Av.:-0.57
Sn1 4c (0.0621, 0.4752, 0.6296)	Sn-S(Sn): 2.70, 2.82, 2.93, 2.98, 3.01	+0.75
Sn2 4c (0.3111, 0.4788, 0.6227)	Sn-S(Sn): 2.65, 2.81, 2.84, 2.97, 3.01; Sn-S(Nb): 3.21	+0.45
Sn3 4c (0.5632, 0.4768, 0.6190)	Sn-S(Sn): 2.63, 2.81, 2.83, 2.90, 3.00; Sn-S(Nb): 3.19	+0.71
Sn4 4c (0.8139, 0.4777, 0.6272)	Sn-S(Sn): 2.68, 2.81, 2.88, 3.01, 3.01; Sn-S(Nb): 3.26	+0.54
		Av.:+0.61

Table S5. Calculated results (coordinates of atoms, interatomic distances and Bader charges at the atomic sites) using the DFT + vdW correction for the $(Sn_{1-x}S)_{1.167}NbS_2$ (x = 0.0714) misfit layer compound, Case e). This structure had a monoclinic lattice with a pseudo-space group Pa with all atoms at the 2a sites (x,y,z) + (x+1/2, y, -z). The calculated unit cell can be described as a pseudo-orthorhombic unit cell, a = 39.889Å, b = 5.773 Å, c =11.813 Å; α = 90 °, β = 90 ° and γ = 90 °.

Specie and atomic coordinates x/a, y/b, z/c	Bonds (Å)	Charge (e/atom)
Nb1 (0.9929, 0.8990, 0.9995)	Nb-S(Nb): 2.47, 2.48(×2), 2.49, 2.50(×2).	+1.02
Nb2 (0.0760, 0.8995, 0.9991)	Nb-S(Nb): 2.47, 2.48(×2), 2.49, 2.50(×2).	+1.53

Nb3 (0.1597, 0.8985, 0.9974)	Nb-S(Nb): 2.47, 2.48(×2), 2.49 (×3)	+1.48
Nb4 (0.2431, 0.8976, 0.9975)	Nb-S(Nb): 2.48 (×2), 2.49(×3), 2.50	+1.75
Nb5 (0.3260, 0.8987, 0.0013)	Nb-S(Nb): 2.48 (×2), 2.49 (×4)	+1.82
Nb6 (0.4092, 0.8995, 0.0006)	Nb-S(Nb): 2.48(×2), 2.49 (×4)	+1.54
Nb7 (0.0345, 0.4022, 0.9988)	Nb-S(Nb): 2.48 (×2), 2.49 (×4)	+1.14
Nb8 (0.1178, 0.4041, 0.9968)	Nb-S(Nb): 2.48 (×3), 2.49(×2), 2.50	+0.93
Nb9 (0.2011, 0.4037, 0.9969)	Nb-S(Nb): 2.48 (×2), 2.49 (×4)	+1.02
Nb10 (0.2845, 0.4056, 0.9996)	Nb-S(Nb): 2.48 (×2), 2.49 (×4)	+1.14
Nb11 (0.3679, 0.4055, 0.0011)	Nb-S(Nb): 2.48 (×2), 2.49 (×4)	+1.13
Nb12 (0.4513, 0.4044, 0.0007)	Nb-S(Nb): 2.48 (×2), 2.49 (×3), 2.50	+1.07
		Av:+1.30
S1 (0.9922, 0.2340, 0.1303)	S1-Nb: 2.48, 2.48, 2.49	-0.62
S2 (0.4926, 0.2344, 0.1343)	S2-Nb: 2.48, 2.50, 2.50; -Sn 3.12	-0.52
S3 (0.0766, 0.2340, 0.1300)	S3-Nb: 2.48, 2.49, 2.49;	-0.65
S4 (0.5754, 0.2338, 0.1358)	S4-Nb: 2.49, 2.49, 2.50; -Sn: 3.06	-0.71
S5 (0.1592, 0.2341, 0.1291)	S5-Nb: 2.48, 2.49, 2.50	-0.69
S6 (0.6952, 0.2354, 0.1358)	S6-Nb: 2.48, 2.48, 2.49	-0.79
S7 (0.2425, 0.2323, 0.1299)	S7-Nb: 2.49, 2.49, 2.49	-0.82
S8 (0.7428, 0.2372, 0.1351)	S8-Nb: 2.48, 2.49, 2.49	-0.73
S9 (0.3259, 0.2357, 0.1322)	S9-Nb: 2.48, 2.49, 2.50	-0.86
S10 (0.8263, 0.2325, 0.1315)	S10-Nb: 2.49, 2.49, 2.50	-0.77
S11 (0.4094, 0.2332, 0.1328)	S11-Nb: 2.49, 2.49, 2.50	-0.79
S12 (0.9095, 0.2345, 0.1297)	S12-Nb: 2.48, 2.49, 2.49	-0.76
S13 (0.0344, 0.7302, 0.1337)	S13-Nb: 2.49, 2.49, 2.49: -Sn: 3.17	-0.79
S14 (0.5339, 0.7367, 0.1347)	S14-Nb: 2.48, 2.49, 2.49	-0.69
S15 (0.1182, 0.7362, 0.1306)	S15-Nb: 2.48, 2.50, 2.50	-0.84
S16 (0.6175, 0.7375, 0.1379)	S16-Nb: 2.47, 2.48, 2.49	-0.76
S17 (0.2011, 0.7333, 0.1310)	S17-Nb: 2.48, 2.49, 2.49, -Sn: 3.16	-0.70
S18 (0.7012, 0.7382, 0.1380)	S18-Nb: 2.48, 2.49, 2.49	-0.82
S19 (0.2841, 0.7354, 0.1342)	S19-Nb: 2.48, 2.49, 2.49	-0.78
S20 (0.7847, 0.7355, 0.1364)	S20-Nb: 2.48, 2.48, 2.49: -Sn 3.23	-0.71
S21 (0.3674, 0.7354, 0.1353)	S21-Nb: 2.47, 2.47, 2.48	-0.81
S22 (0.8677, 0.7339, 0.1327)	S22-Nb: 2.48, 2.48, 2.49	-0.73
S23 (0.4508, 0.7338, 0.1344)	S23-Nb: 2.48, 2.48, 2.49	-0.79
S24 (0.9506, 0.7364, 0.1314)	S24-Nb: 2.48, 2.48, 2.48	-0.67
		Av:-0.74
S25 (0.0356, 0.4673, 0.6010)	S25-Sn: 2.45, 2.72, 2.86, 2.98	-0.71
S26 (0.1786, 0.4902, 0.5974)	S26-Sn: 2.69, 2.77, 2.86, 3.00, 3.04	-0.70
S27 (0.3207, 0.4837, 0.6010)	S27-Sn: 2.69, 2.79, 2.84, 2.99, 3.03	-0.67
S28 (0.4637, 0.4863, 0.5964)	S28-Sn: 2.68, 2.79, 2.85, 3.02, 3.03	-0.55
S29 (0.6073, 0.4861, 0.5963)	S29-Sn: 2.65, 2.74, 2.77, 3.14	-0.78
S30 (0.7512, 0.4843, 0.6006)	S30-Sn: 2.68, 2.79, 2.90, 3.01, 3.03	-0.62
S31 (0.8928, 0.4905, 0.5984)	S31-Sn: 2.69, 2.76, 2.85, 3.00, 3.04	-0.68
S32 (0.1072, 0.9948, 0.6038)	S32-Sn: 2.66, 2.76, 2.90, 2.91, 3.16	-0.58
S33 (0.2506, 0.9821, 0.5964)	S33-Sn: 2.70, 2.78, 2.79, 3.02, 3.04	-0.64
S34 (0.3954, 0.9821, 0.5988)	S34-Sn: 2.66, 2.77, 2.82, 3.04, 3.04	-0.73
S35 (0.5357, 0.9292, 0.6064)	S35-Sn: 2.60, 2.71, 2.71, 3.15	-0.86
S36 (0.6759, 0.9848, 0.5988)	S36-Sn: 2.62, 2.69, 2.73, 3.11	-0.68
S37 (0.8210 0.9817, 0.5966)	S37-Sn: 2.69, 2.76, 2.79, 3.03, 3.12	-0.75
S38 (0.9642, 0.9954, 0.6039)	S38-Sn: 2.66, 2.77, 2.89, 2.92, 3.17	-0.97
		Av.:-0.72
Vac		-
Sn1 (0.1757, 0.0329, 0.6166)	Sn-S(Sn): 2.66, 2.79, 2.84, 2.94, 3.04	+0.99
Sn2 (0.3210, 0.0183, 0.6238)	Sn-S(Sn): 2.68, 2.79, 2.87, 2.94, 3.02; -S(Nb): 3.12	+1.05
Sn3 (0.4652, 0.0247, 0.6282)	Sn-S(Sn): 2.68, 2.76, 2.85, 2.99;	+0.96
Sn4 (0.6073, 0.0436, 0.6121)	Sn-S(Sn): 2.52, 2.65, 2.79, 2.79, 3.14; -S(nB): 3.06	+0.85
Sn5 (0.7501, 0.0180, 0.6277)	Sn-S(Sn): 2.75, 2.85, 3.01, 3.03, 3.07;	+0.92
Sn6 (0.8957, 0.0328, 0.6183)	Sn-S(Sn): 2.83, 2.90, 2.91, 2.95, 3.03	+0.54
Sn7 (0.1034, 0.5333, 0.6268)	Sn-S(Sn): 2.77, 2.82, 2.95, 3.04, 3.17	+1.00
Sn8 (0.2483, 0.5298, 0.6291)	Sn-S(Sn): 2.68, 2.73, 2.75, 3.01, 3.06, -S(Nb) 3.16	+0.87

Sn9 (0.3927, 0.5218, 0.6173)	Sn-S(Sn): 2.65, 2.82, 2.89, 2.92, 3.03	+0.83
Sn10 (0.5390, 0.5313, 0.6155)	Sn-S(Sn): 2.45, 2.54, 2.66, 2.66; -S(Nb): 3.17	+0.93
Sn11 (0.6764, 0.5285, 0.6211)	Sn-S(Sn): 2.78, 2.78, 2.79, 3.02, 3.16	+1.06
Sn12 (0.8230, 0.5294, 0.6296)	Sn-S(Sn): 2.68, 2.71, 2.84, 2.98, 3.04, -S(Nb) 3.23	+0.91
Sn13 (0.9679, 0.5364, 0.6275)	Sn-S(Sn): 2.68, 2.76, 2.78, 3.03, 3.12	+0.94
		Av.:+0.90

Table S6. Calculated results (coordinates of atoms, interatomic distances and Bader charges at the atomic sites) using the DFT + vdW correction for the $(SnS_{1-x})_{1.167}NbS_2$ (x=0.071) misfit layer compound, case f). This structure had a monoclinic lattice with space group Pa (no. 7) with all atoms at the 2a sites (x, y, z) + (x+½, y, -z). The calculated unit cell can be described as a pseudo-orthorhombic unit cell with lattice parameters in Table 2.

Specie and atomic coordinates x/a, y/b, z/c	Bonds (Å)	Charge (e/atom)
Nb1 (0.9932, 0.9202, 0.9999)	Nb-S(Nb): 2.47, 2.48 (×4), 2.49	+1.57
Nb2 (0.0763, 0.9216, 0.9999)	Nb-S(Nb): 2.48 (×3), 2.49 (×3)	+1.35
Nb3 (0.1601, 0.9203, 0.9937)	Nb-S(Nb): 2.47 (×2), 2.48, 2.49 (×3)	+1.72
Nb4 (0.2431, 0.9187, 0.9944)	Nb-S(Nb): 2.48 (×4), 2.49, 2.50	+1.58
Nb5 (0.3263, 0.9184, 0.9933)	Nb-S(Nb): 2.47, 2.48 (×3), 2.49 (×2)	+1.61
Nb6 (0.4093, 0.9193, 0.9965)	Nb-S(Nb): 2.47, 2.48 (×4), 2.49	+1.52
Nb7 (0.0348, 0.4283, 0.9986)	Nb-S(Nb): 2.48 (×4), 2.49 (×2)	+1.14
Nb8 (0.1180, 0.4268, 0.9941)	Nb-S(Nb): 2.47, 2.48 (×4), 2.49	+0.93
Nb9 (0.2013, 0.4246, 0.9991)	Nb-S(Nb): 2.47 (×2), 2.48, 2.49 (×2), 2.50	+1.11
Nb10 (0.2847,0.4237, 0.9987)	Nb-S(Nb): 2.48 (×6)	+1.12
Nb11 (0.3681, 0.4237, 0.9984)	Nb-S(Nb): 2.48 (×5), 2.49	+1.11
Nb12 (0.4515, 0.4258, 0.9986)	Nb-S(Nb): 2.48 (×4), 2.49 (×2)	+1.21
		Av:+1.33
S1 (0.9934, 0.2530, 0.1318)	S1-Nb: 2.48, 2.49, 2.49	-0.72
S2 (0.4930, 0.2595, 0.1311)	S2-Nb: 2.48, 2.48, 2.49	-0.62
S3 (0.0762, 0.2541, 0.1321)	S3-Nb: 2.48, 2.49, 2.49	-0.65
S4 (0.5767, 0.2594, 0.1310)	S4-Nb: 2.48, 2.48, 2.49	-0.71
S5 (0.1600, 0.2574, 0.1326)	S5-Nb: 2.48, 2.49, 2.50; -Sn: 2.95	-0.56
S6 (0.6592, 0.2547, 0.1298)	S6-Nb: 2.47, 2.49, 2.49	-0.59
S7 (0.2427, 0.2524, 0.1293)	S7-Nb: 2.48, 2.48, 2.48	-0.69
S8 (0.7431, 0.2572, 0.1324)	S8-Nb: 2.47, 2.48, 2.48	-0.72
S9 (0.3263, 0.2572, 0.1223)	S9-Nb: 2.48, 2.48, 2.48	-0.74
S10 (0.8266, 0.2519, 0.1292)	S10-Nb: 2.48, 2.48, 2.48	-0.71
S11 (0.4102, 0.2538, 0.1294)	S11-Nb: 2.48, 2.48, 2.48	-0.73
S12 (0.9095, 0.2566, 0.1326)	S12-Nb: 2.48, 2.48, 2.49	-0.71
S13 (0.0347, 0.7554, 0.1311)	S13-Nb: 2.48, 2.48, 2.48	-0.79
S14 (0.5348, 0.7632, 0.1355)	S14-Nb: 2.47, 2.48, 2.48	-0.91
S15 (0.1180, 0.7611, 0.1355)	S15-Nb: 2.47, 2.48, 2.49	-0.84
S16 (0.6186, 0.7577, 0.1307)	S16-Nb: 2.47, 2.47, 2.48	-0.76
S17 (0.2020, 0.7540, 0.1329)	S17-Nb: 2.48, 2.49, 2.50, -Sn: 2.94	-0.89
S18 (0.7011, 0.7568, 0.1335)	S18-Nb: 2.48, 2.49, 2.49	-0.86
S19 (0.2842, 0.7551, 0.1331)	S19-Nb: 2.47, 2.48, 2.49	-0.81
S20 (0.7852, 0.7549, 0.1331)	S20-Nb: 2.48, 2.48, 2.49	-0.85
S21 (0.3683, 0.7559, 0.1333)	S21-Nb: 2.48, 2.48, 2.49	-0.75
S22 (0.8674, 0.7531, 0.1331)	S22-Nb: 2.48, 2.48, 2.49	-0.86
S23 (0.4509, 0.7573, 0.1308)	S23-Nb: 2.48, 2.48, 2.48	-0.81
S24 (0.9515, 0.7598, 0.1353)	S24-Nb: 2.47, 2.48, 2.48	-0.92
		Av:-0.75
S25 (0.0378, 0.4909, 0.5950)	S25-Sn: 2.67, 2.70, 2.86, 2.98, 3.04	-0.70
S26 (0.9645, 0.9871, 0.5987)	S26-Sn: 2.63, 2.82, 2.85, 2.91, 3.03	-0.75
Vac	-	-
S27 (0.8213, 0.9927, 0.5929)	S27-Sn: 2.65, 2.86, 2.86, 2.87, 2.99	-0.66

S28 (0.3177, 0.4873, 0.5980) S29 (0.6780, 0.9819, 0.5837) S30 (0.4647, 0.4908, 0.5937) S31 (0.5355, 0.9892, 0.5971) S32 (0.6112, 0.4795, 0.5929) S33 (0.3937, 0.9889, 0.5972) S34 (0.7465, 0.4786, 0.5969) S35 (0.2498, 0.9769, 0.5955) S36 (0.8912, 0.4889, 0.5944) S37 (0.1063, 0.9749, 0.5991)	S28-Sn: 2.64, 2.69, 2.88, 3.00, 3.10 S29-Sn: 2.59, 2.86, 2.91, 2.93, 3.26 S30-Sn: 2.68, 2.82, 2.84, 2.88, 3.00 S31-Sn: 2.63, 2.87, 2.87, 2.89, 2.99 S32-Sn: 2.65, 2.76, 2.85, 3.04, 3.08 S33-Sn: 2.65, 2.82, 2.83, 2.90, 3.03 S34-Sn: 2.63, 2.80, 2.88, 2.99, 3.05 S35-Sn: 2.65, 2.73, 2.82, 2.91, 3.11 S36-Sn: 2.66, 2.84, 2.84, 2.88, 3.00 S37-Sn: 2.62, 2.76, 2.85, 3.00, 3.08	-0.74 -0.61 -0.76 -0.80 -0.69 -0.79 -0.69 -0.70 -0.71 -1.13 Av.:-0.76
Sn1 (0.0354, 0.0018, 0.6204) Sn2 (0.5360, 0.5003, 0.6286) Sn3 (0.1804, 0.0192, 0.6298) Sn4 (0.6783, 0.5135, 0.6706) Sn5 (0.3218 0.0000, 0.6265) Sn6 (0.8208, 0.5038, 0.6233) Sn7 (0.4642, 0.0044, 0.6187) Sn8 (0.9624, 0.5048, 0.6275) Sn9 (0.6074, 0.0068, 0.6176) Sn10 (0.1038, 0.5021, 0.6250) Sn11 (0.7502, 0.0010, 0.6235) Sn12 (0.2521, 0.5094, 0.6198) Sn13 (0.8921, 0.0032, 0.6218) Sn14 (0.3949, 0.5070, 0.6249)	Sn-S(Sn): 2.63, 2.85, 2.85, 2.86, 2.98 Sn-S(Sn): 2.70, 2.86, 2.88, 2.99, 3.04 Sn-S(Sn): 2.82, 3.00 Sn-S(Sn): 2.85, 2.88, 2.91, 3.26; Sn-S(Nb): 2.94, 2.95 Sn-S(Sn): 2.65, 2.85, 2.90, 2.91, 3.00 Sn-S(Sn): 2.68, 2.84, 2.86, 2.99, 2.99 Sn-S(Sn): 2.63, 2.83, 2.84, 2.87, 3.00 Sn-S(Sn): 2.68, 2.82, 2.88, 3.03, 3.04 Sn-S(Sn): 2.62, 2.76, 2.86, 2.89, 3.08 Sn-S(Sn): 2.65, 2.67, 2.76, 3.08 Sn-S(Sn): 2.65, 2.80, 2.87, 2.93, 3.05 Sn-S(Sn): 2.63, 2.64, 2.73, 3.11 Sn-S(Sn): 2.65, 2.84, 2.86, 2.91, 3.00 Sn-S(Sn): 2.66, 2.82, 2.82, 3.03, 3.10	+1.10 +1.11 +0.67 +1.20 +0.93 +0.56 +1.07 +0.71 +0.88 +0.82 +1.01 +0.82 +0.67 +0.65 Av.:+0.87

Table S7. Calculated electronic configurations in the atomic spheres (R_{Wigner} = 1.164 Å for S, R_{Wigner} = 1.270 Å for Nb and R_{Wigner} = 1.566 Å for Sn) in the parent binary compounds and the misfit layer compounds, $(Sn_{1-x}S)_{1.167}NbS_2$, case b) and $(Sn_{1-x}S)_{1.167}NbS_2$ (x=0.0714), case e).

Compound	atom	W-S(Å)	s(e)	p(e)	d(e)	total (e/atom)
α-SnS	Sn S	1.566 1.164	1.60 1.36	1.06 2.34	0.14 -	2.80 3.70
β-SnS	Sn S	1.566 1.164	1.61 1.36	1.01 2.34	0.14 -	2.76 3.70
2H-NbS_2	Nb S	1.270 1.164	2.16 1.37	6.04 2.36	2.35 -	10.55 3.73
$(SnS)_{1.167}NbS_2$	Sn S(Sn) S(Nb) Nb	1.566 1.164 1.164 1.270	1.57-1.63 1.36 1.36 2.16	0.94-1.02 2.33 2.39 6.04	0.14-0.15 - - 2.39	2.71-2.74 3.69-3.70 3.74 10.59
$(Sn_{0.9286}S)_{1.167}NbS_2$	Sn S(Sn) S(Nb) Nb	1.566 1.164 1.164 1.270	1.60 to 1.64 1.37 1.36 2.16	0.98-1.05 2.33 2.37 6.04	0.13–0.14 - - 2.37	2.75-2.79 3.70 3.73 10.56