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Modulation of Electronic Bandgaps and Subsequent Implications on SQ Efficiencies via Strain Engineering in Ultrathin SnX (X = S, Se) Nanowires

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Table S1. Effect of strain on the structural parameters of SnS (SnSe) NW

Applied Strain ε **(%)**		**Lattice parameter** c **(Å)**	d_1 **(Å)**	d_2 **(Å)**	**X-Sn-X** θ_1 **(°)**	**Sn-X-Sn** θ_2 **(°)**	**Phonon frequencies (cm^{-1})**
Compressive	**-10**	6.79 (7.03)	2.60 (2.72)	2.67 (2.82)	82.91 (81.51)	88.79 (86.91)	+ve (-200)
	-8	6.94 (7.18)	2.60 (2.73)	2.68 (2.82)	84.80 (83.37)	89.11 (87.13)	-20 (-80)
	-6	7.09 (7.34)	2.61 (2.74)	2.68 (2.82)	88.67 (85.19)	89.43 (87.23)	+ve (+ve)
	-4	7.24 (7.49)	2.62 (2.75)	2.68 (2.82)	88.53 (86.97)	89.58 (87.51)	+ve (+ve)
	-2	7.39 (7.65)	2.63 (2.76)	2.68 (2.82)	90.36 (88.78)	89.78 (87.64)	+ve (+ve)
Unstrained	**0**	**7.54 (7.81)**	**2.65 (2.78)**	**2.67 (2.81)**	**92.18 (90.53)**	**90.08 (87.86)**	**+ve (+ve)**
Tensile	**2**	7.69 (7.96)	2.66 (2.79)	2.67 (2.81)	94.01 (92.31)	90.34 (88.03)	+ve (+ve)
	4	7.84 (8.12)	2.67 (2.80)	2.66 (2.80)	25.84 (94.06)	90.60 (88.18)	-20 (-20)
	6	7.99 (8.28)	2.68 (2.81)	2.65 (2.79)	97.73 (95.86)	90.71 (88.44)	-20 (-20)
	8	8.15 (8.43)	2.69 (2.82)	2.64 (2.78)	99.64 (97.73)	91.05 (88.50)	-40 (-30)
	10	8.30 (8.59)	2.70 (2.83)	2.64 (2.78)	101.63 (99.62)	91.32 (88.64)	-50 (-40)

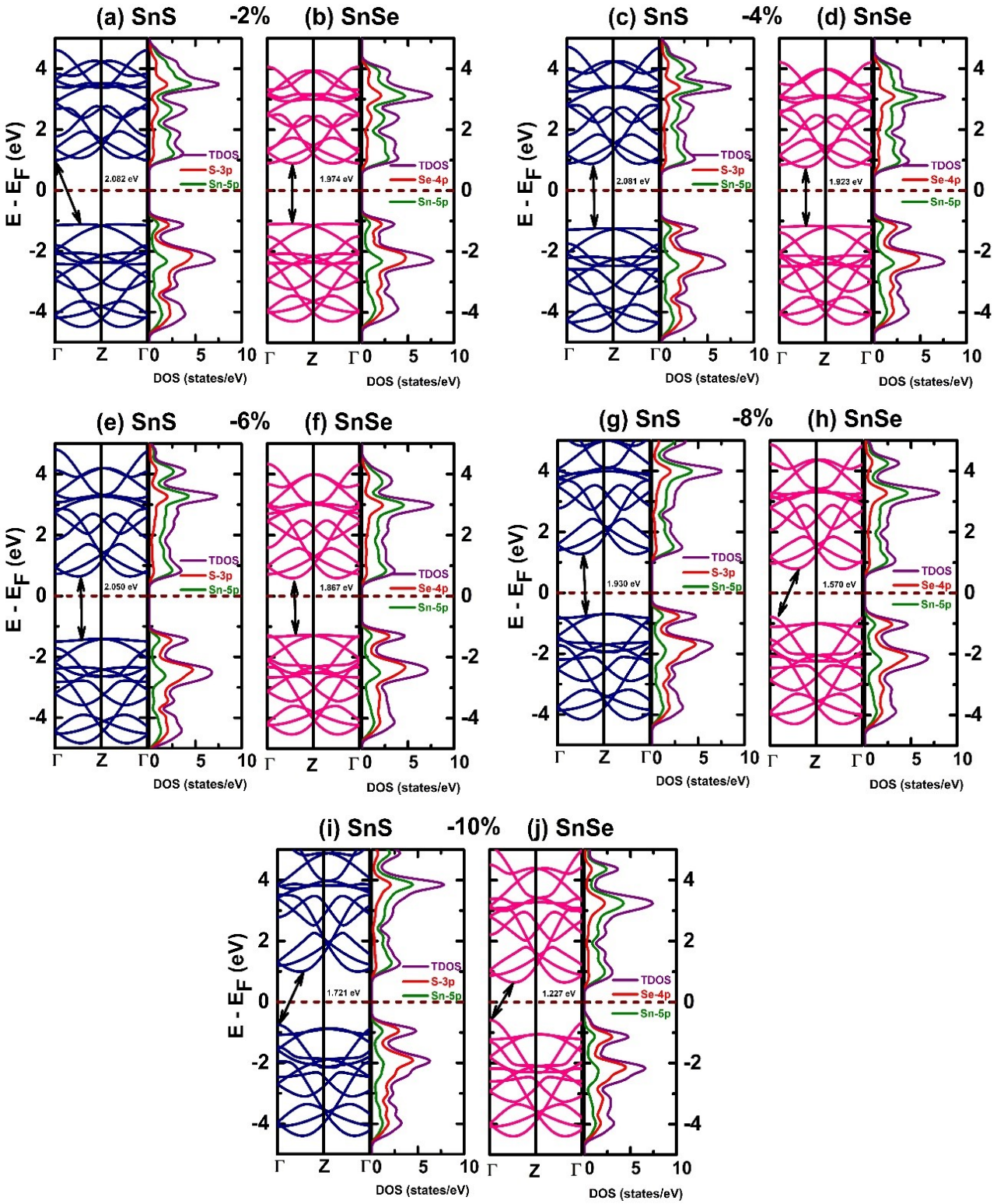

Figure S1. Electronic band structures, partial density of states (PDOS) and total density of states (TDOS) of ultrathin SnX (X = S, Se) NWs under varying compressive strains.