SUPPLEMENTARY MATERIAL

Ultrathin nanowire PdX_2 (X= P, As): stability, electronic transport and thermoelectric properties

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Table S1: Our calculated lattice constant, bond length and cohesive energy of PdP_2 and $PdAs_2$ monolayer. Previous reported results are also listed in brackets from ref [1].

Material	Lattice constant (Å)	Pd-X (Å)	X-X (Å)	E_{coh} (eV per atom)
PdP_2	5.99 (5.86)	2.38 (2.32)	2.08 (2.06)	4.01 (3.67)
$PdAs_2$	6.29 (6.19)	2.47 (2.42)	2.31 (2.31)	3.56 (3.18)

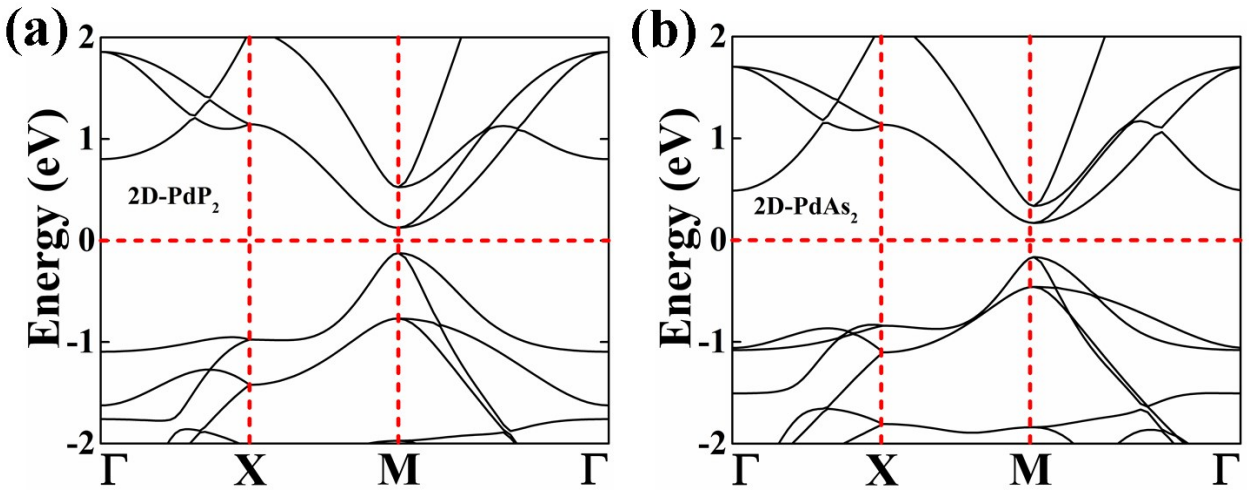

Figure S1: The electronic band structure of penta PdP_2 and $PdAs_2$ monolayer. The Fermi level is set at 0K.

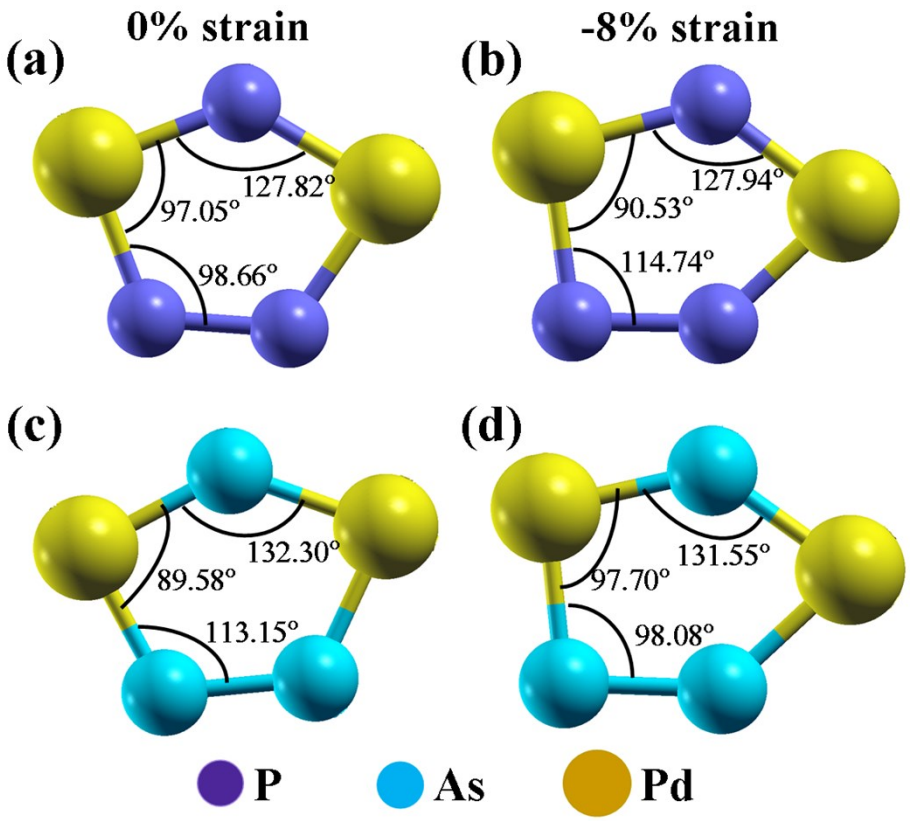

Figure S2: The electronic structure of pentagonal PdP_2 and $PdAs_2$ at 0% and 8% compressive strain.

Table S2: Variation of bond length and bond angle at different applied strain

	Strain	Bond Length (Å)			Bond Angle (°) (X-Pd-X)
		Pd-Pd	Pd-X	X-X	
PdP_2	0%	4.23	2.40	2.02	180
	-2%	4.22	2.39	2.02	180
	-4%	4.20	2.39	2.02	180
	-6%	4.19	2.39	2.02	180
	-8%	4.16	2.39	2.02	180
	-10%	4.15	2.38	2.02	180
	-12%	2.83	2.50	2.03	144.9
	-14%	3.09	2.45	2.00	101.2
$PdAs_2$	0%	4.29	2.49	2.25	180
	-2%	4.28	2.48	2.25	180

	-4%	4.27	2.48	2.24	180
	-6%	4.28	2.48	2.24	180
	-8%	4.41	2.49	2.24	180
	-10%	4.40	2.49	2.25	180
	-12%	4.40	2.50	2.25	180
	-14%	4.41	2.50	2.26	180

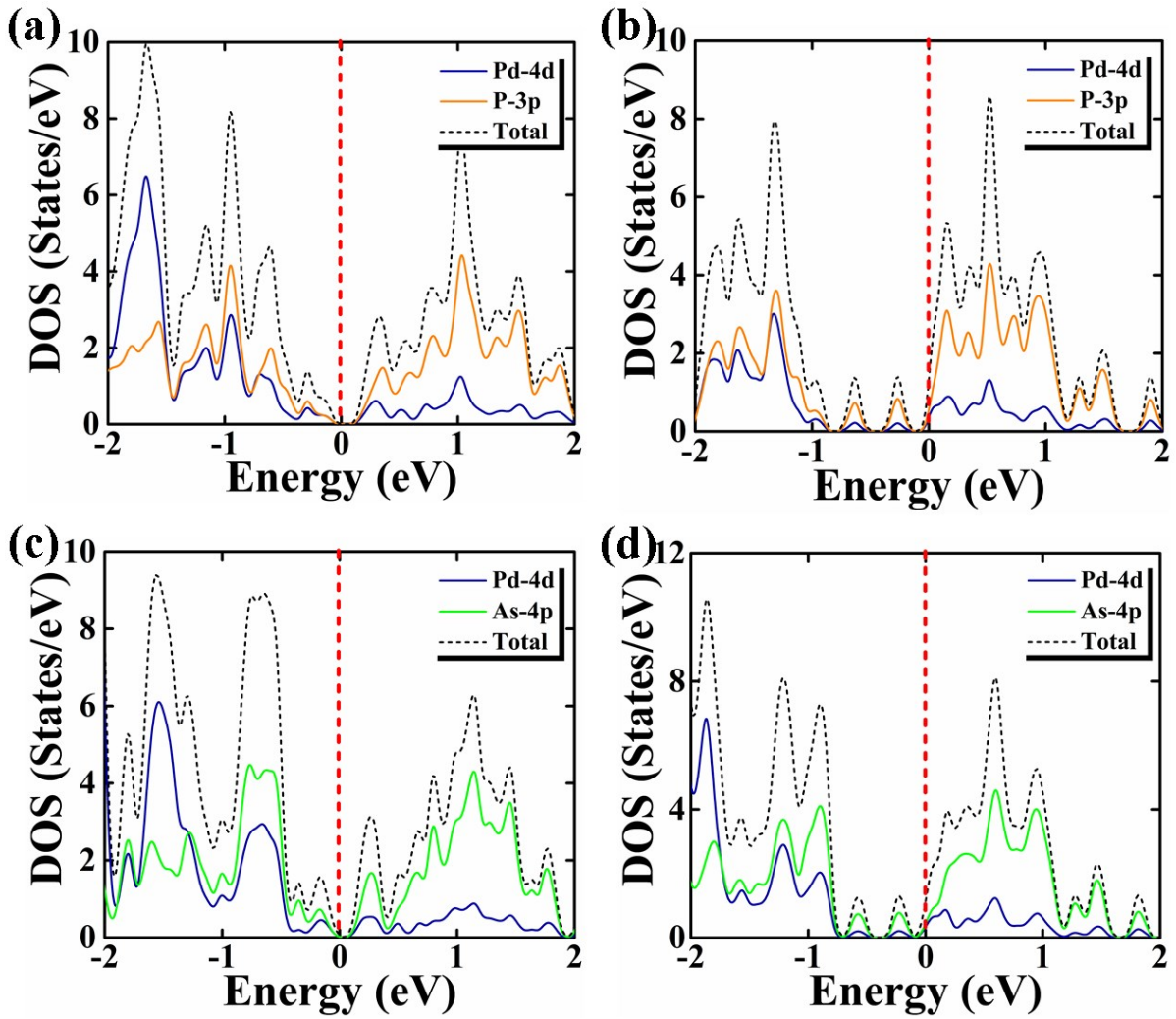

Figure S3: The calculated total density of states (TDOS) and partial density of states (PDOS) graph of unstrained (Ɛ=0%) (a) PdP_2-NW and (c) $PdAs_2$-NW is shown. Correspondingly, strained (Ɛ=-8%) PDOS of (b) PdP_2 and (d) $PdAs_2$ is also shown.

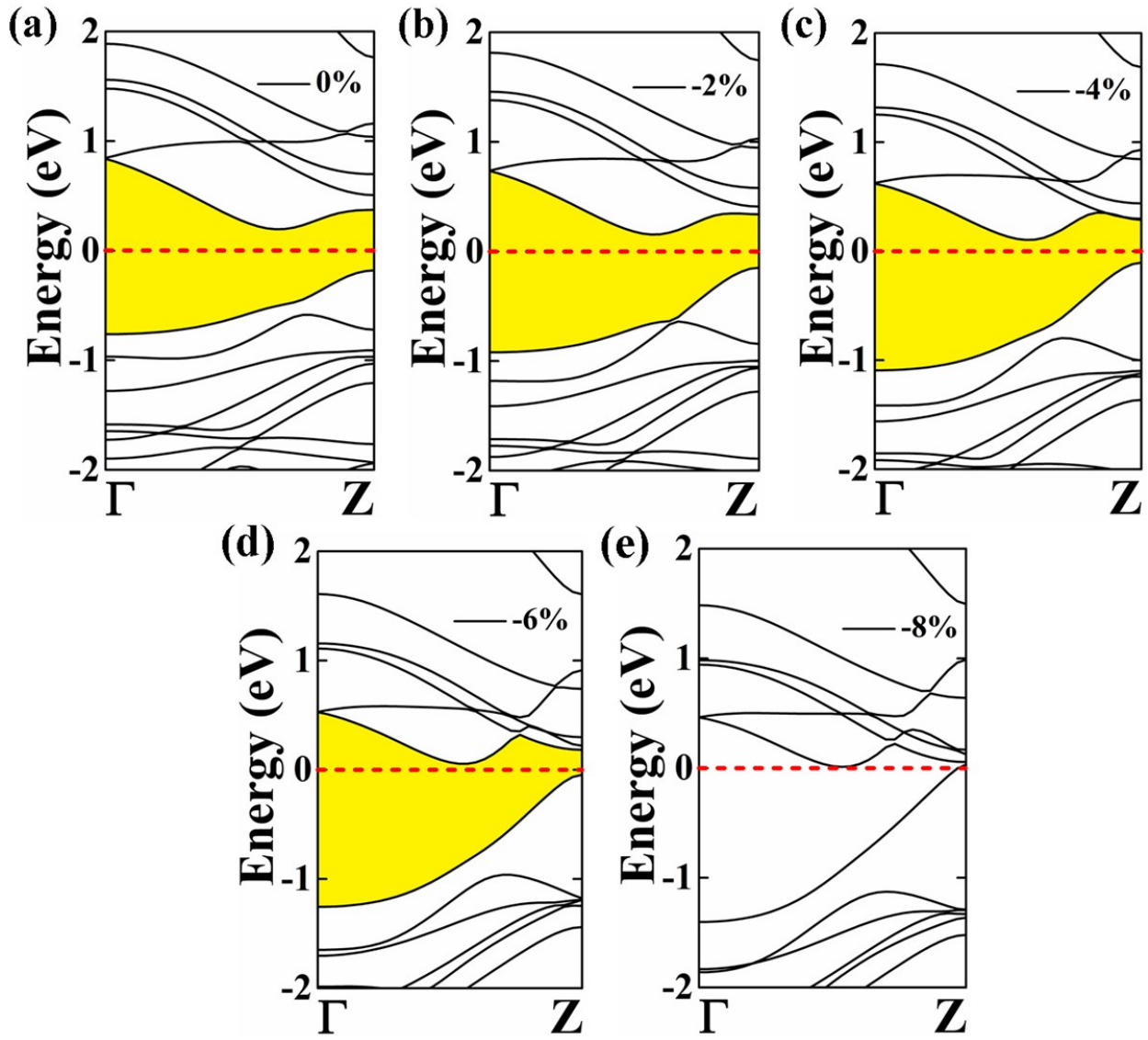

Figure S4: The electronic band structure of penta PdP_2-NW with applied strain. The Fermi level is set at 0K.

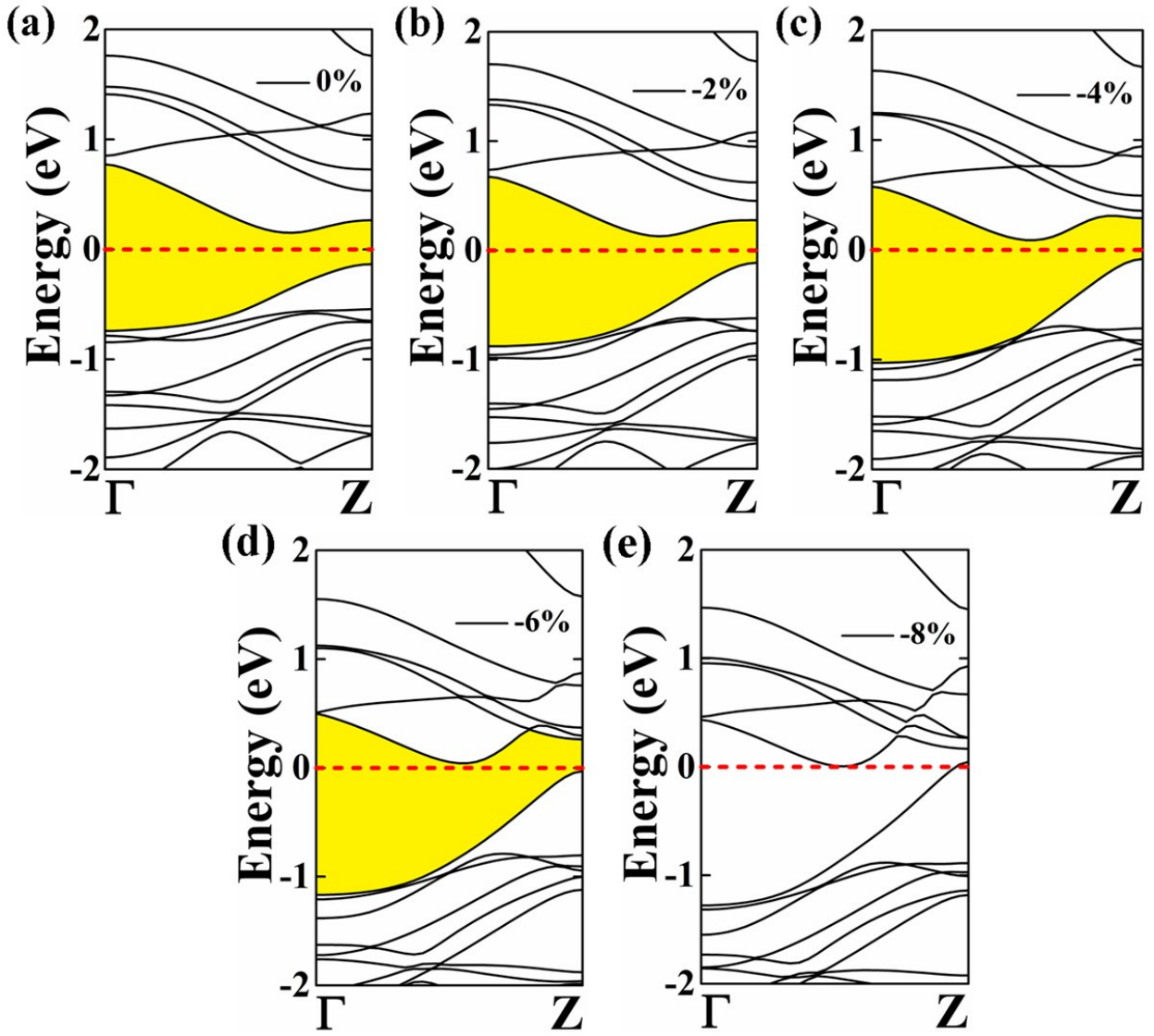

Figure S5: The electronic band structure of penta $PdAs_2$-NW with applied strain. The Fermi level is set at 0K.

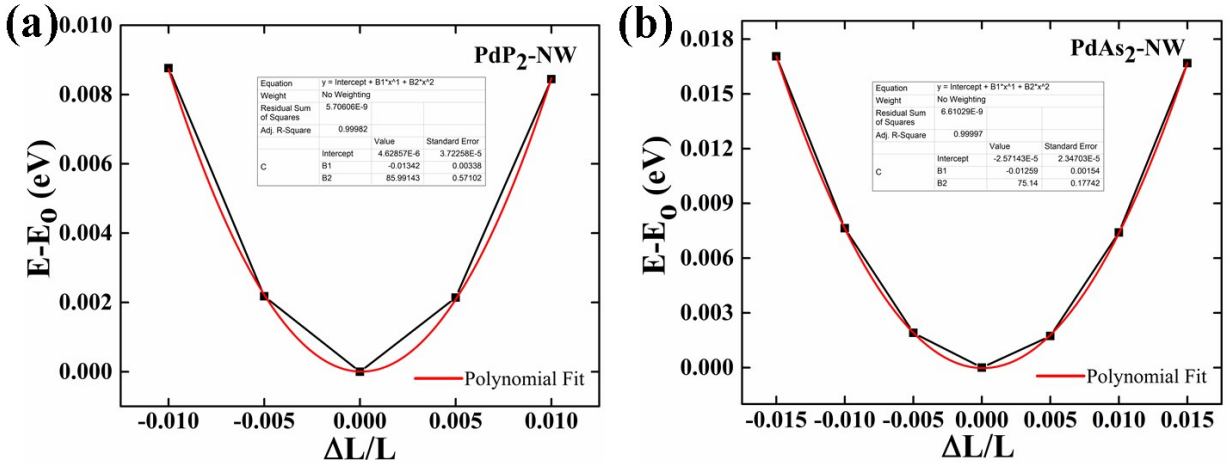

Figure S6: The graph for stiffness constant of (a) PdP_2-NW and (b) $PdAs_2$-NW

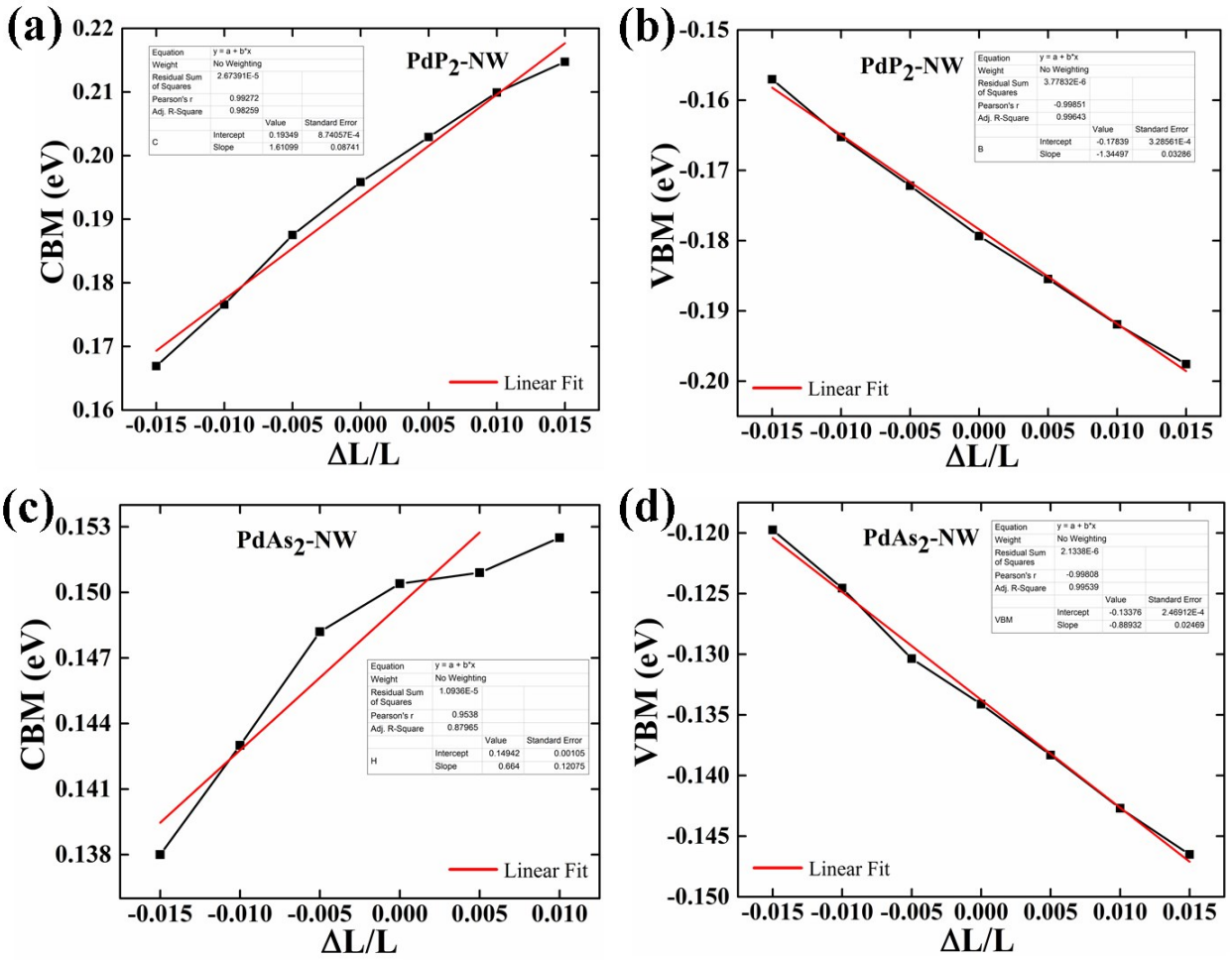

Figure S7: The graph for deformation potential of (a) electrons and (b) holes of PdP_2-NW and (c) electrons and (d) holes of $PdAs_2$-NW

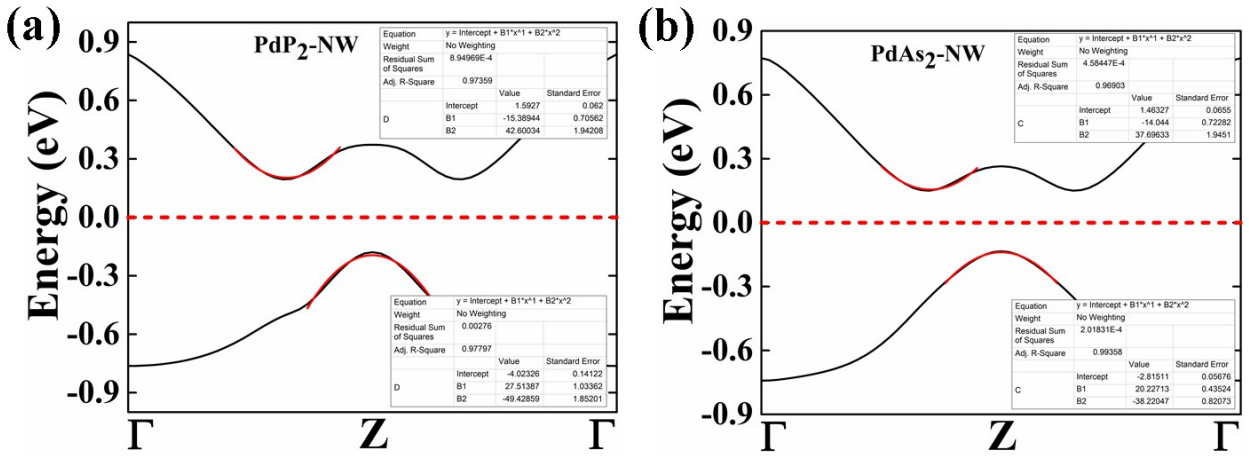

Figure S8: The graph for effective mass calculation of (a) PdP_2-NW and (b) $PdAs_2$-NW

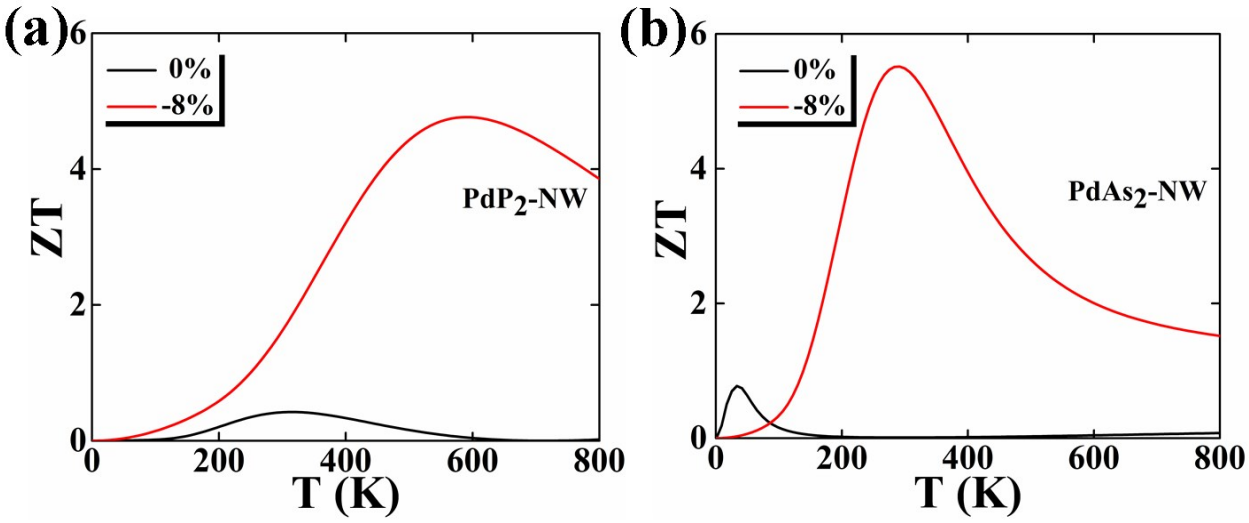

Figure S9: Calculated figure of merit (ZT) of both strained and unstrained (Ɛ= 0% and -8%) for (a) PdP_2-NW and (b) $PdAs_2$-NW as a function of temperature is shown for larger lead. Both lead and scattering region are of the same material. The left and right lead consists of three primitive unit cells. The scattering region is consisting of three primitive cells.

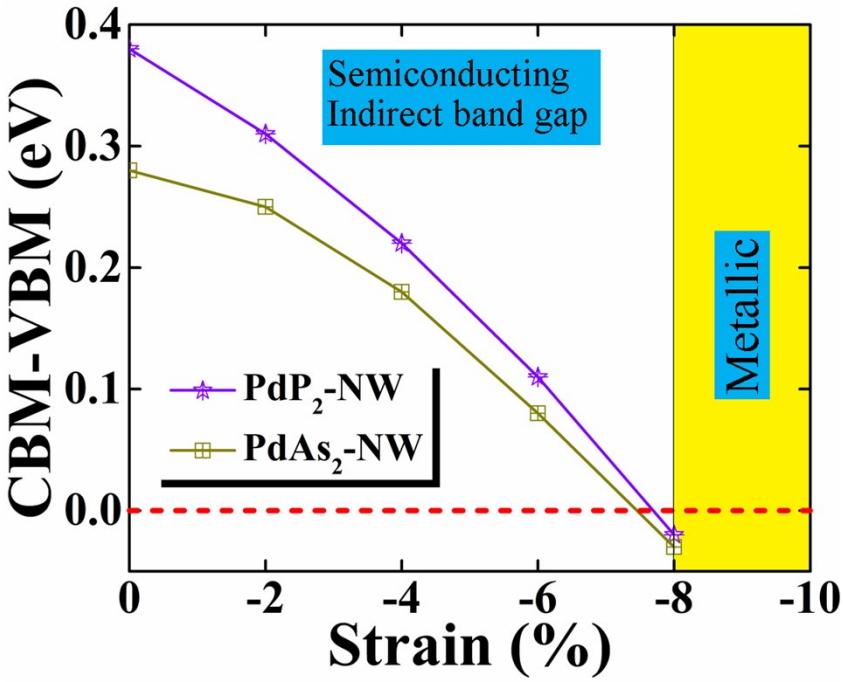

Figure S10: The variation of band gap with applied compressive strain for penta PdP_2 and $PdAs_2$-NW.

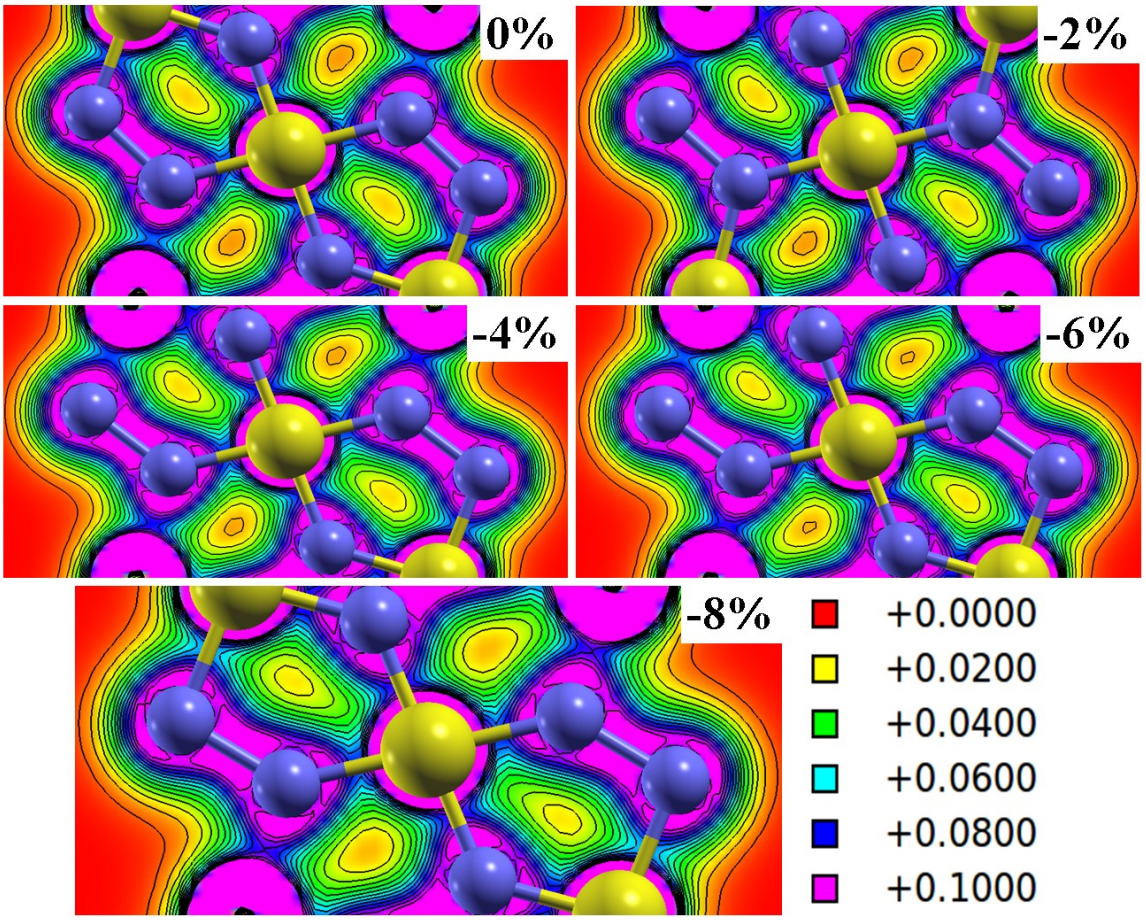

Figure S11: The charge contour plot of PdP_2-NW with applied strain.

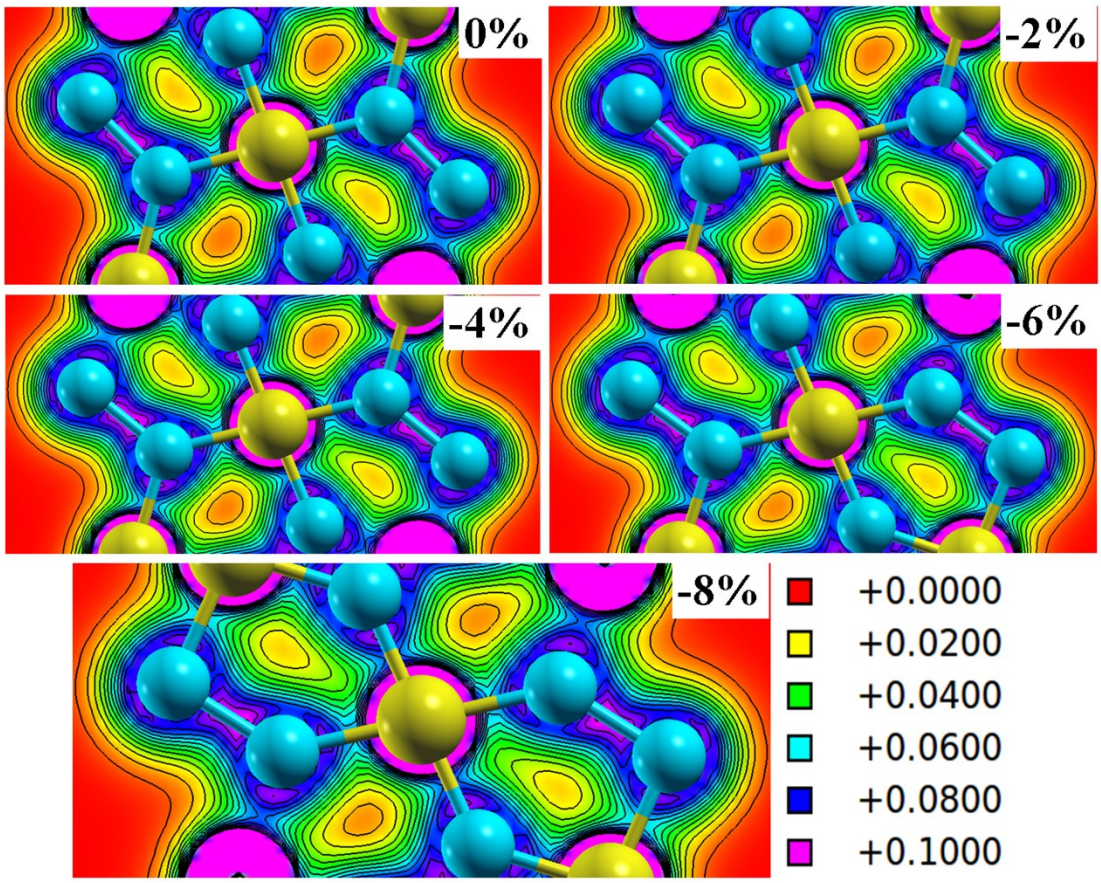

Figure S12: The charge contour plot of $PdAs_2$-NW with applied strain.

References:

(1) Yuan, H.; Li, Z.; Yang, J. Atomically Thin Semiconducting Penta-PdP2 and PdAs2 with Ultrahigh Carrier Mobility. *J. Mater. Chem. C* **2018**, *6* (34), 9055–9059. https://doi.org/10.1039/C8TC03368D.