

Electronic Supplementary Informatin (ESI)

Intrinsic Seebeck Coefficients of 2D Polycrystalline PtSe₂ Semiconducting Films through Two-Step Annealing

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1. Parameters used in the COMSOL simulation

Table S1. Material parameters for COMSOL calculation of the temperature distribution

Material	Density [kg/m ³]	Heat capacity at constant pressure [C_p , J/kg·K]	Thermal conductivity [W/m·K]
Sapphire substrate (Al ₂ O ₃)	3,980 ¹	779.15*	40 ¹
PtSe ₂	9,540 ²	201.3 ³	1.62 ()/0.18 (⊥) ⁴
Copper	8,960*	348.8*	392.81*
Bakelite	1,300*	920*	0.2*
Gold	19,276*	128.78*	317.32*
Kapton H	1,420*	758*	0.81*
Thermal grease	2,600*	1,200*	8.5 ⁵

*Values obtained from the COMSOL Material library.

†Interfacial thermal resistance (ITR) between 15-nm-thick PtSe₂ and MoS₂; ITR = 1×10^{-9} K.m²/W.

2. COMSOL settings for calculating the temperature distribution of the PtSe₂ thin films

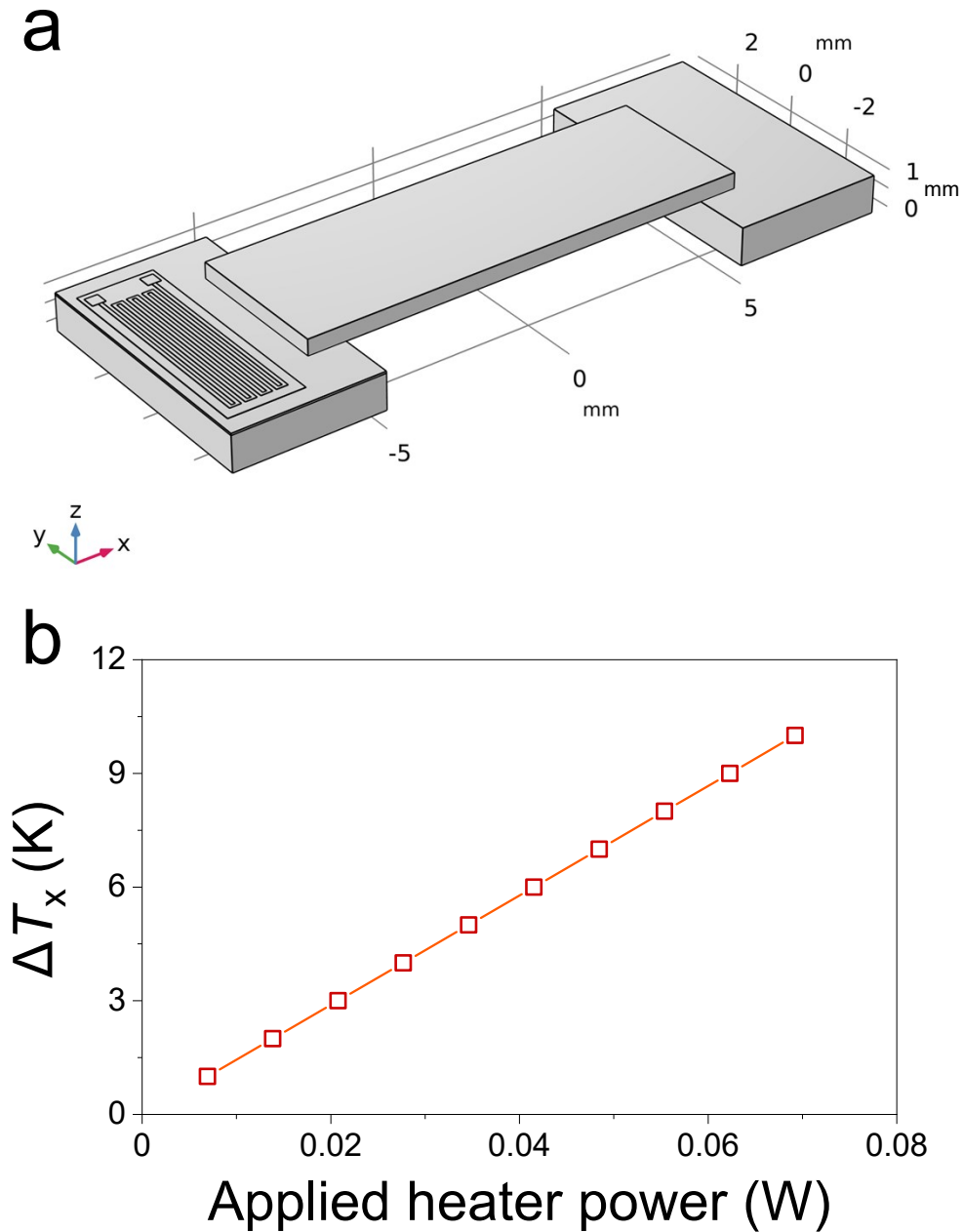


Fig. S1. (a) Geometry setting used to evaluate the in-plane temperature difference of PtSe₂/sapphire substrate. (b) Calculated in-plane temperature difference (ΔT_x) at different applied heater powers.

3. Contact-type difference according to metal electrode

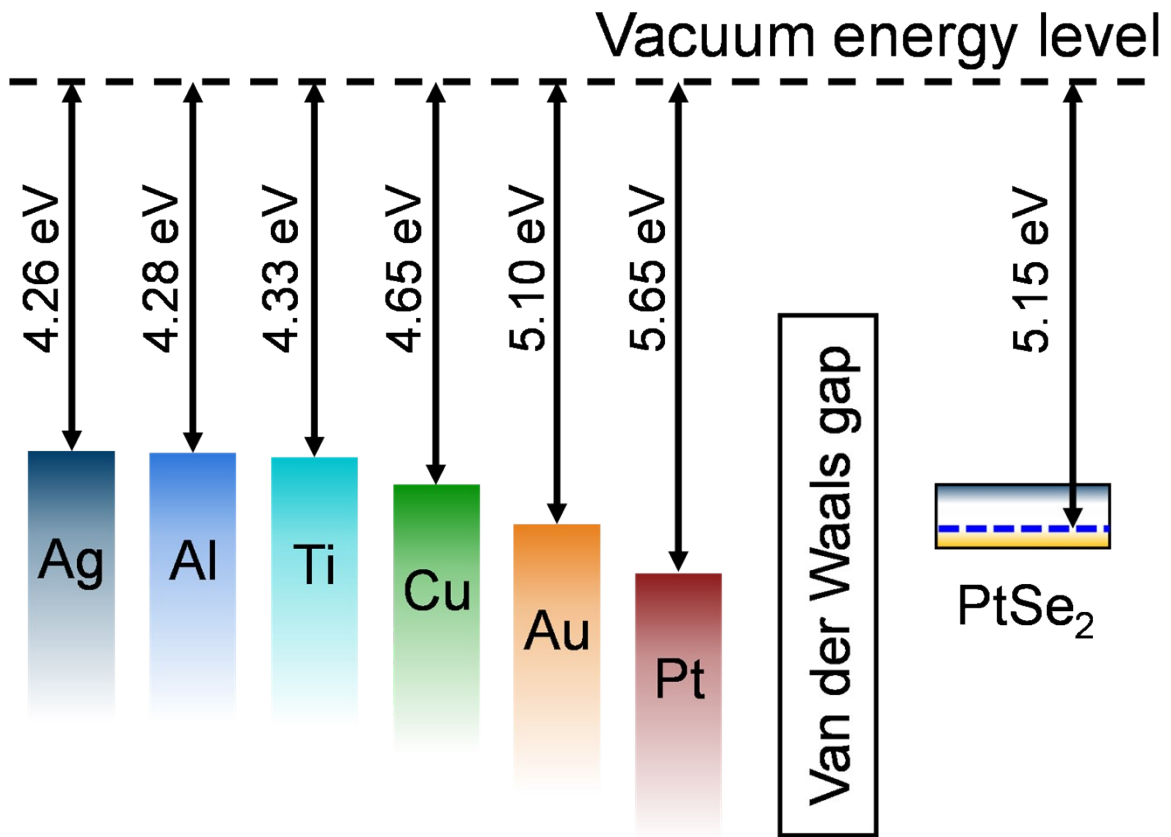


Fig. S2. Comparison between the work functions of the metal electrode and as-grown PtSe₂.

4. Calculated PDOS for layers IV–VI

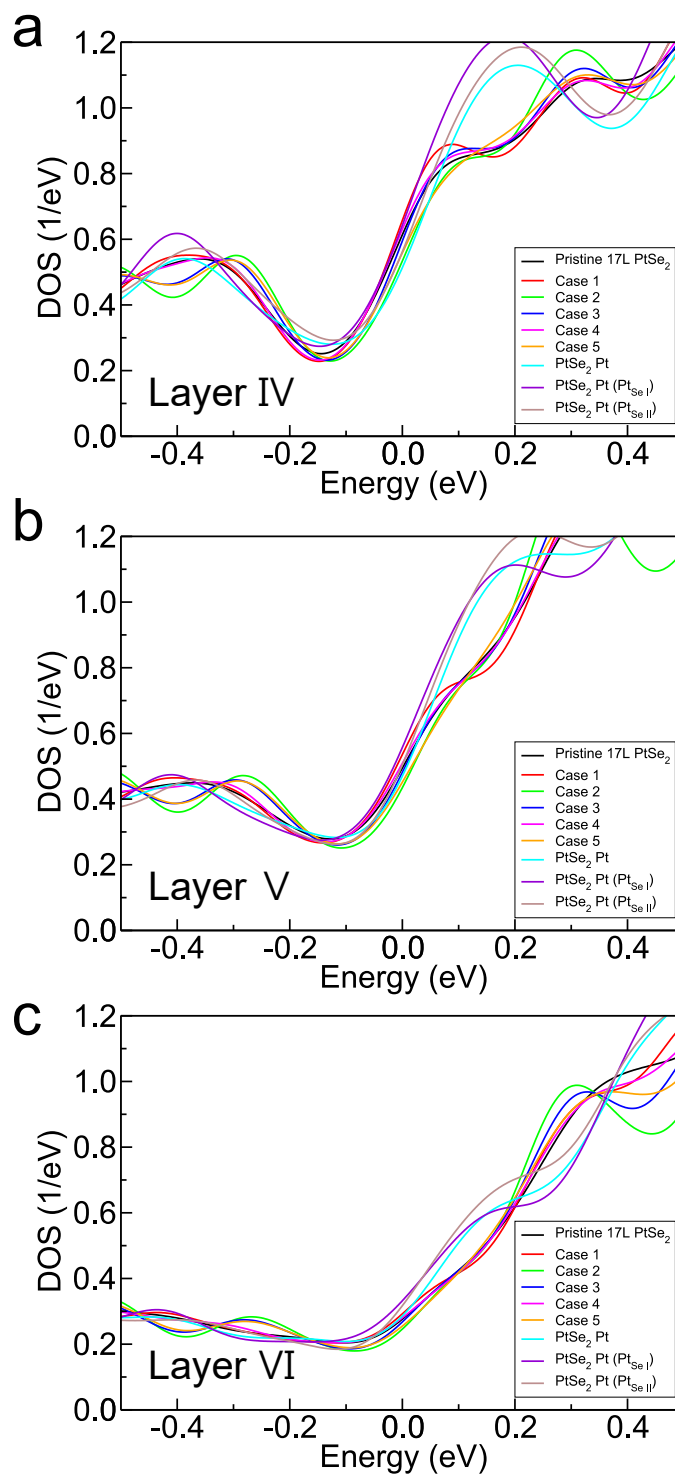


Fig. S3. Calculated PDOS of PtSe₂ and Pt/PtSe₂ for different layers: (a) IV layer, (b) V layer, and (c) VI layer.

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