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Title	Quantum confinement-induced semimetal-to-semiconductor evolution in large-area ultra-thin PtSe2 films grown at 400 °C
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Supplementary Information

Quantum confinement-induced semimetal-to-semiconductor evolution in large-area ultra-thin $PtSe_2$ films grown at 400 ^{o}C

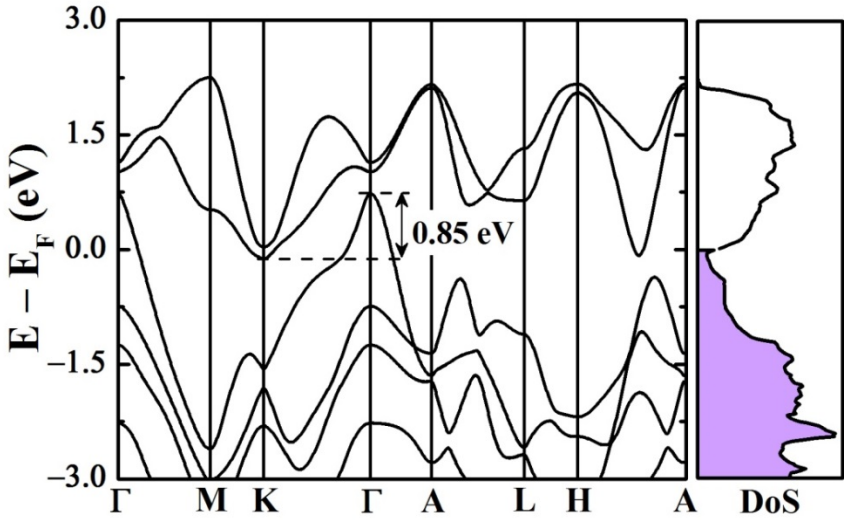
Lida Ansari[1], Scott Monaghan[1], Niall McEvoy[2], Cormac Ó Coileáin[2], Conor P. Cullen[2], Jun Lin[1], Rita Siris[3], Tanja Stimpel-Lindner[3], Kevin Finbarr Burke[1], Gioele Mirabelli[1], Ray Duffy[1], Enrico Caruso[1], Roger E. Nagle[1], Georg S. Duesberg[3], Paul K. Hurley[1], and Farzan Gity[1,*]

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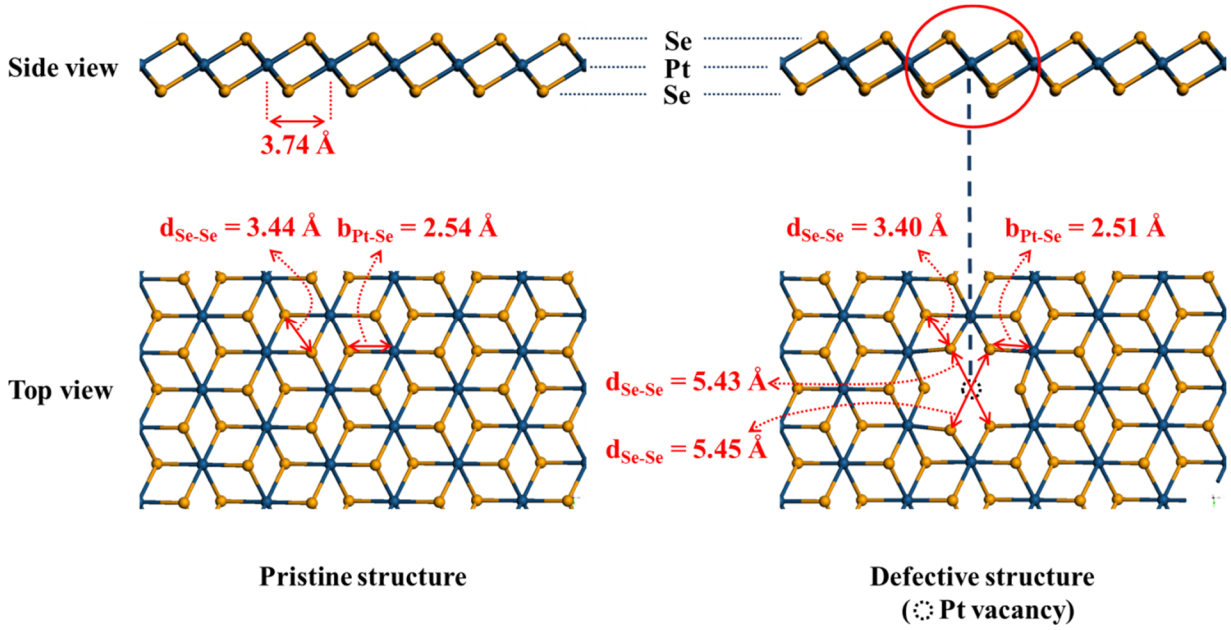
2 Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN) and Advanced Materials and Bioengineering Research (AMBER), School of Chemistry, Trinity College Dublin, Ireland

3 Institute of Physics, EIT 2, Faculty of Electrical Engineering and Information Technology, Universität der Bundeswehr München, Germany

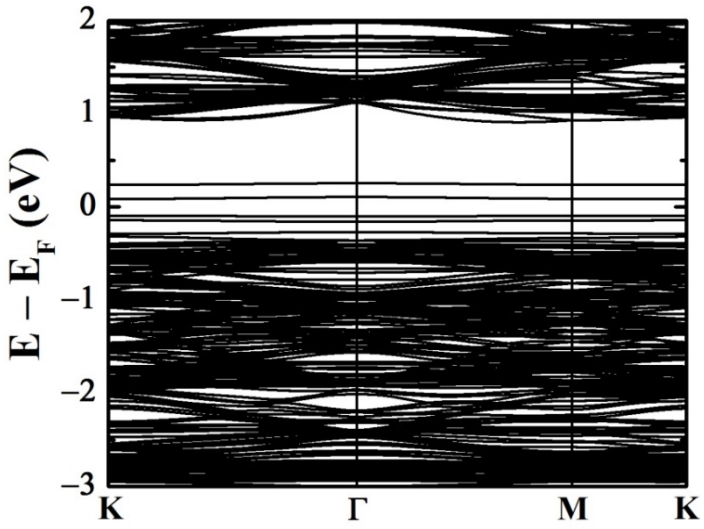
[*] Corresponding author: Farzan.Gity@Tyndall.ie



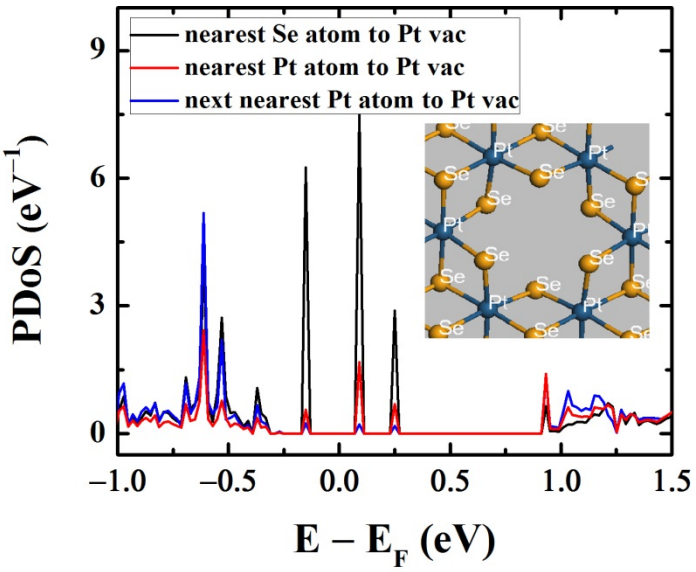
Supplementary Figure 1. Band structure and DoS of "bulk" $PtSe_2$ illustrating the overlap of valence and conduction bands.



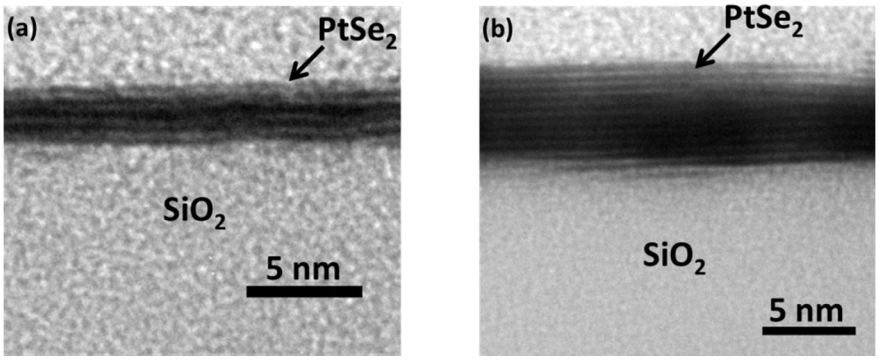
Supplementary Figure 2. Top view (up panel) and side view (down panel) of geometric structures of pristine (left) and defective with Pt vacancy (right) $PtSe_2$ monolayer. Dark blue and orange atoms are Pt and Se atoms, respectively. b, d and ◌ represent bond length, distance and Pt vacancy, respectively.



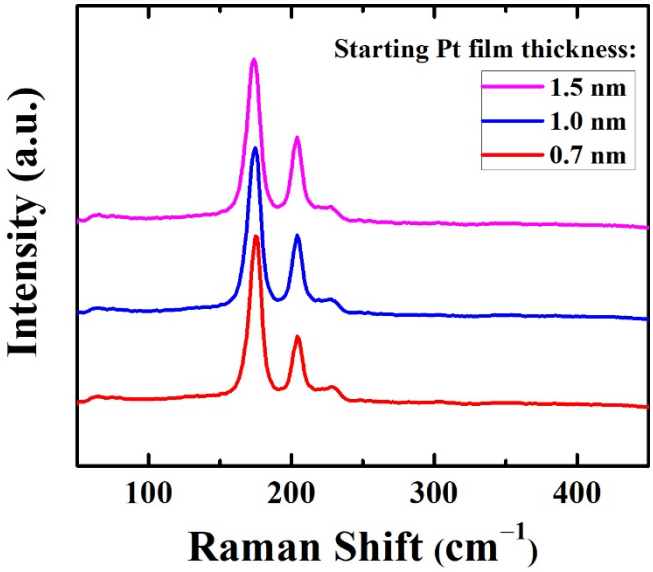
Supplementary Figure 3. Band structure of monolayer $PtSe_2$ supercell with Pt vacancy before unfolding.



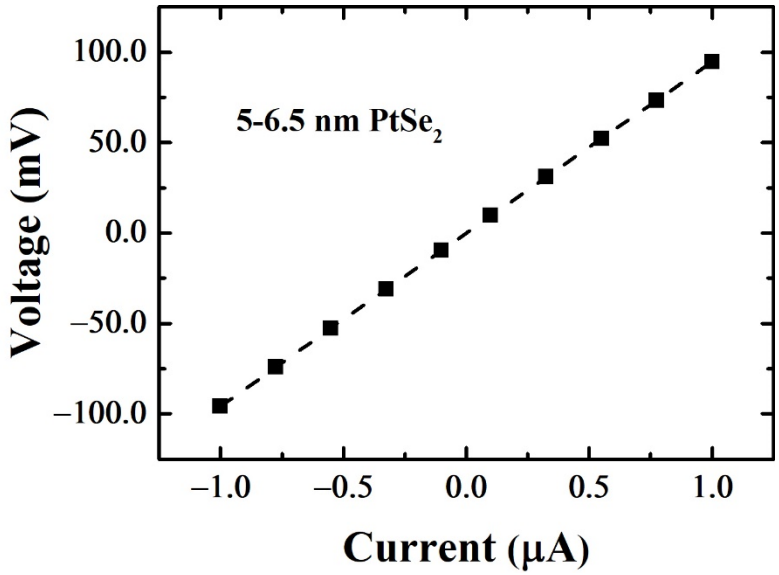
Supplementary Figure 4. Partial density of states (PDoS) of nearest Se and nearest Pt atoms to Pt vacancy compared to PDoS of next nearest Pt atom, showing strong localized nature of the Pt vacancy in $PtSe_2$.



Supplementary Figure 5. Cross-sectional TEM image of transferred (a) 2.5-3 nm, and (b) 5-6.5 nm $PtSe_2$ samples. Scale bar is 5nm.



Supplementary Figure 6. Raman spectra of $PtSe_2$ films made from different starting Pt film thickness showing the characteristic E_g and A_{1g} Raman-active modes for $PtSe_2$. The A_{1g}/E_g intensity ratio increases with increasing layer thickness consistent with previous reports [S1].



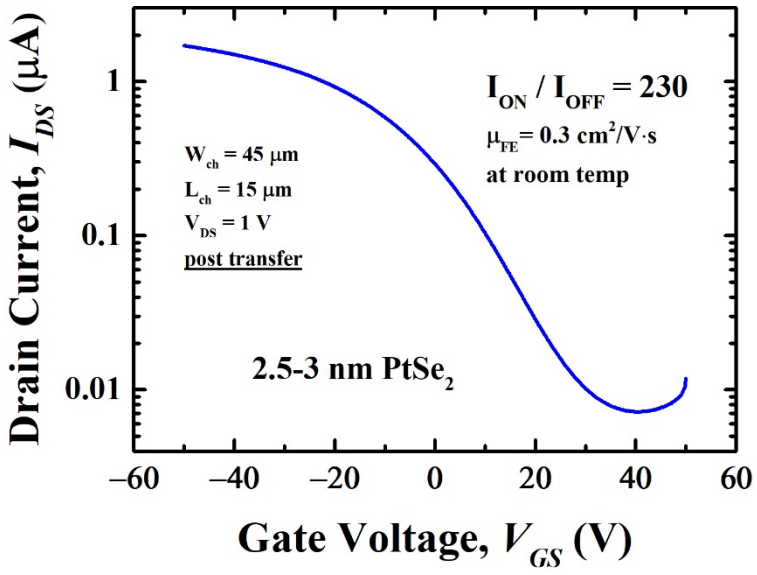
Supplementary Figure 7. Typical two-point IV characteristic of a 5-6.5 nm $PtSe_2$ film indicating good Ohmic contacts. Linear behaviour was found for all samples.

Supplementary Table 1. Hall-effect results of two different batches of $PtSe_2$ samples grown separately with 3-month interval by e-beam evaporation of Pt film on Si/SiO_2, followed by TAC process at 400 °C, confirming the reproducibility of the process.

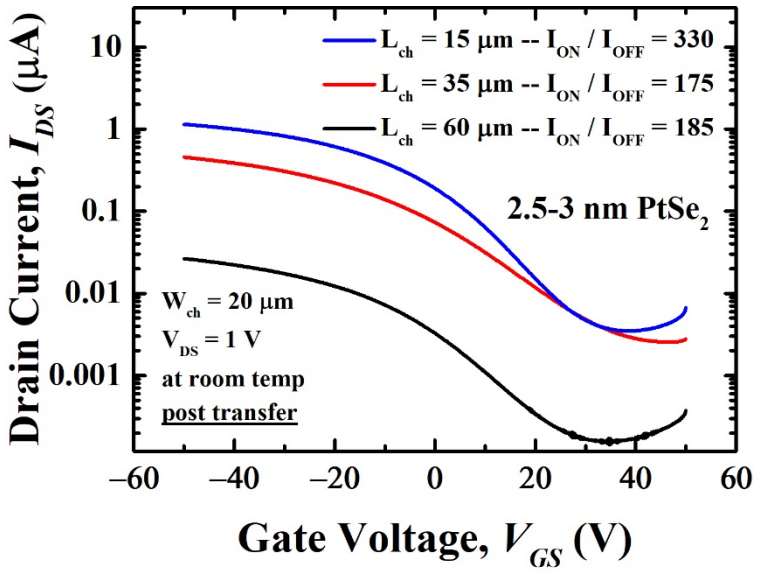
Starting Pt film nominal thickness	1 nm Pt	1 nm Pt
Carrier Type	*P*	*P*
Hall mobility ($cm^2/V.s$)	5.6	5.3
Sheet resistivity (Ω/sq)	$2.1x10^4$	$2.7x10^4$
Sheet carrier concentration (cm^{-2})	$5.4x10^{13}$	$4.3x10^{13}$

Supplementary Table 2. Hall-effect results of three batches of $PtSe_2$ samples grown by e-beam evaporation of Pt film on sapphire, followed by TAC process 400 °C showing very consistent results compared to Si/SiO_2 substrate.

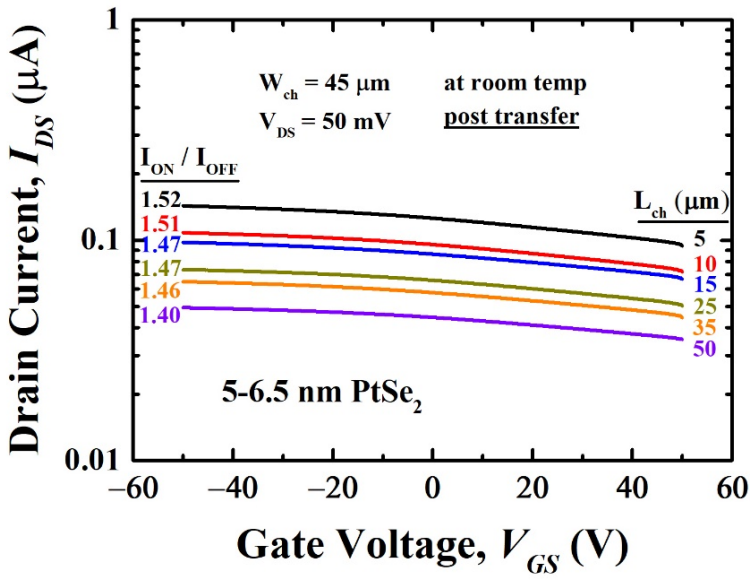
Starting Pt film nominal thickness	0.5 nm Pt	0.7 nm Pt	1 nm Pt	2 nm Pt
Carrier Type	*P*	*P*	*P*	*P*
Hall mobility ($cm^2/V.s$)	1.0	4.2	5.0	7.2
Sheet resistivity (Ω/sq)	$4.2x10^5$	$5.6x10^4$	$2.6x10^4$	$6.1x10^{13}$
Sheet carrier concentration (cm^{-2})	$1.5x10^{13}$	$2.7x10^{13}$	$4.8x10^{13}$	$1.4x10^{14}$


Drain Current, I_{DS} (μA)
1
0.1
0.01
I_{ON} / I_{OFF} = 230
μ_{FE}= 0.3 cm²/V·s
at room temp
W_{ch} = 45 μm
L_{ch} = 15 μm
V_{DS} = 1 V
post transfer
2.5-3 nm $PtSe_2$
–60
–40
–20
0
20
40
60
Gate Voltage, V_{GS} (V)

(a)

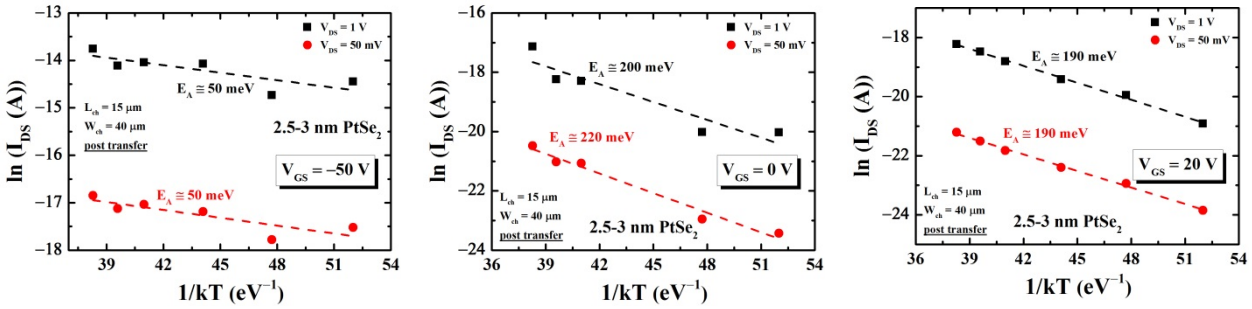

Drain Current, I_{DS} (μA)
10
1
0.1
0.01
0.001
L_{ch} = 15 μm -- I_{ON} / I_{OFF} = 330
L_{ch} = 35 μm -- I_{ON} / I_{OFF} = 175
L_{ch} = 60 μm -- I_{ON} / I_{OFF} = 185
2.5-3 nm $PtSe_2$
W_{ch} = 20 μm
V_{DS} = 1 V
at room temp
post transfer
–60
–40
–20
0
20
40
60
Gate Voltage, V_{GS} (V)

(b)

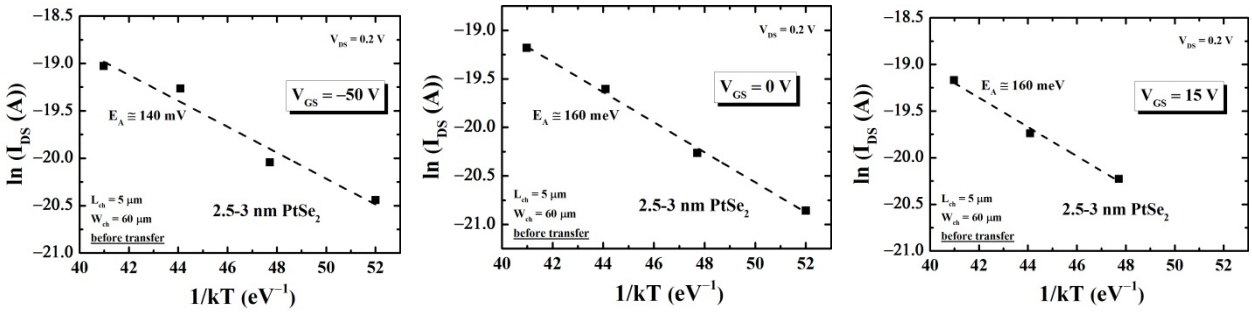


(c)

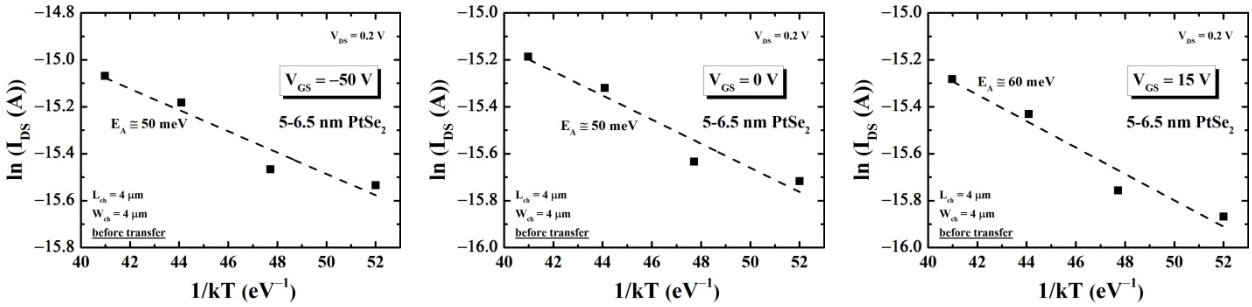
Supplementary Figure 8. (a) Transfer characteristic of the same device as shown in Fig. 4(b), in semi-log scale. Transfer characteristic of the back-gated FET devices with $PtSe_2$ channel thickness of (b) 2.5-3 nm, and (c) 5-6.5 nm, in semi-log scale.



(a)

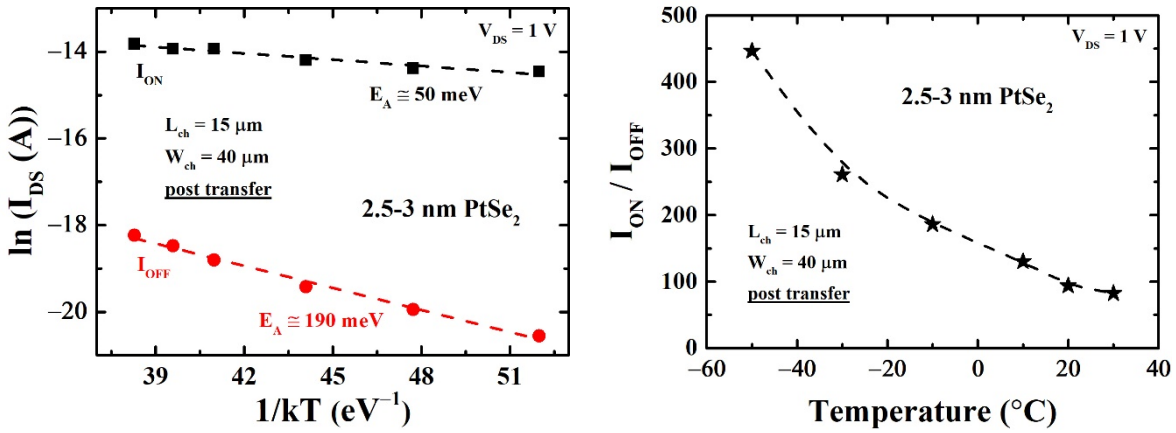


(b)



(c)

Supplementary Figure 9. Activation energy (E_A) extracted from temperature-dependent measurements for (a) 2.5-3 nm $PtSe_2$ sample transferred onto unprocessed Si/SiO_2 substrate, (b) 2.5-3 nm $PtSe_2$ sample on as-grown substrate, and (c) 5-6.5 nm $PtSe_2$ sample on as-grown substrate.



Supplementary Figure 10. Variation of (left) I_{ON} and I_{OFF}, and (right) I_{ON}/I_{OFF} ratio with temperature for a typical device (W_{ch} = 40 µm and L_{ch} = 15 µm) with 2.5-3 nm $PtSe_2$ channel thickness. E_A is activation energy.

References

[S1] O'Brien, M. et al. Raman characterization of platinum diselenide thin films. *2D Mater.* **3**, 021004 (2016).