Supporting Information

Observation of anisotropic magnetoresistance in layered nonmagnetic semiconducting $PdSe_2$

Rui Zhu,[1#] Zhibin Gao,[4,1#] Qijie Liang[5,1], Junxiong Hu,[1] Jian-Sheng Wang[1], Cheng-Wei Qiu,[3] Andrew Thye Shen Wee[1,2,*]*

[1]Department of Physics, National University of Singapore, 2 Science Drive 3, Singapore 117551, Singapore

[2]Centre for Advanced 2D Materials and Graphene Research Centre, National University of Singapore, 6 Science Drive 2, Singapore 117546, Singapore

[3]Department of Electrical and Computer Engineering, National University of Singapore, 4 Engineering Drive 3, Singapore 117583, Singapore

[4]State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an 710049, China

5 Songshan Lake Materials Laboratory, Songshan Lake Mat Lab, Dongguan 523808, Guangdong, China

Corresponding email: phyweets@nus.edu.sg; liangqijie@sslab.org.cn

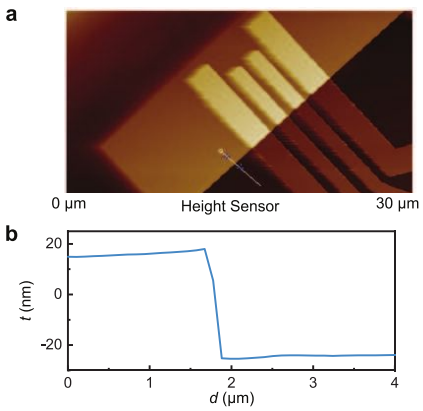

Figure S1 AFM image of exfoliated $PdSe_2$ flake and corresponding thickness spectra.

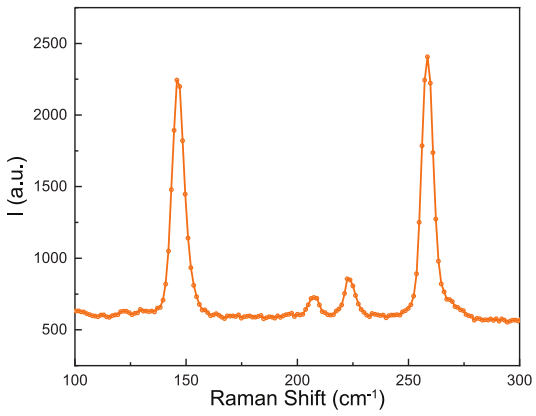

Figure S2 Raman Spectra of exfoliated 38 nm $PdSe_2$ flake.

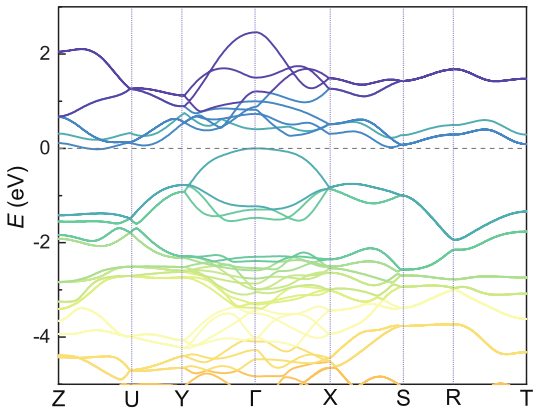

Figure S3 Calculated electronic band structure of bulk $PdSe_2$ with 0 eV bandgap using PBE-SCAN+rVV10 functionals and its lattice constants. The Fermi level is set at the maximum of the valence band.

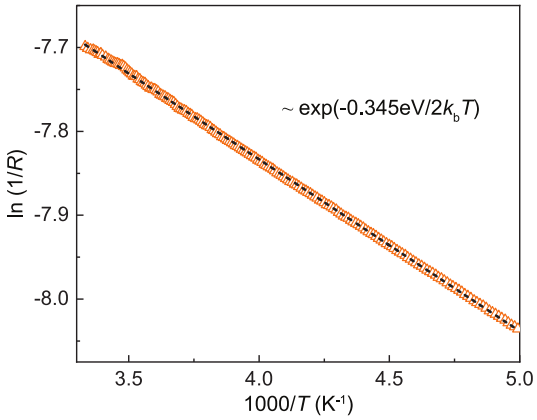

Figure S4 $ln\frac{1}{R}$ versus $\frac{1000}{T}$ fitted by $\frac{1}{R} \propto \exp\left(\frac{-E_g}{2kT}\right)$.

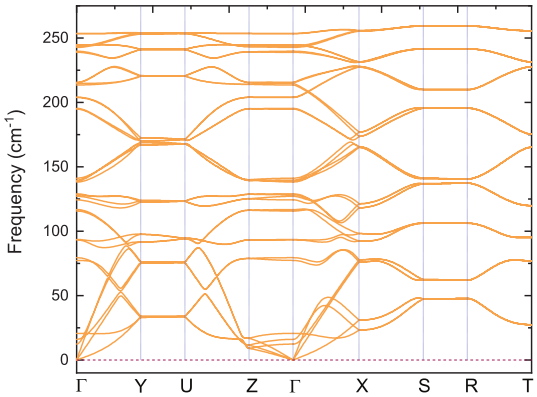

Figure S5 Calculated phonon dispersion of bulk $PdSe_2$. All phonon modes are free from the imaginary frequencies, indicating the dynamical stability.

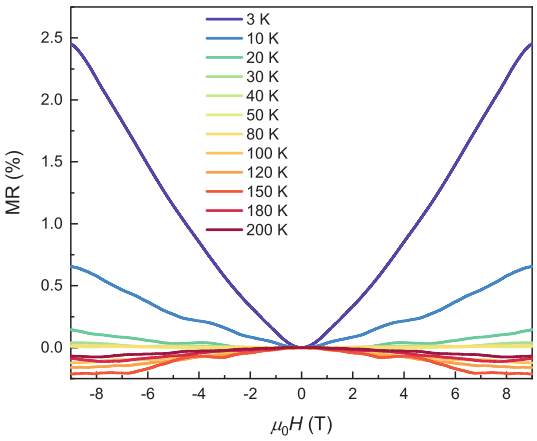

Figure S6 Linear MR along b-axis at various temperatures from 3 K to 300 K.

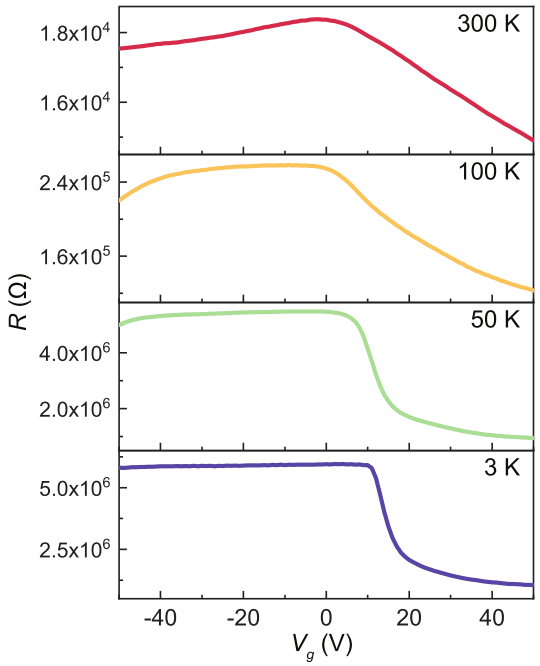

Figure S7 Gate voltage dependence of resistance under zero magnetic field at various temperatures from 3 K to 300 K.

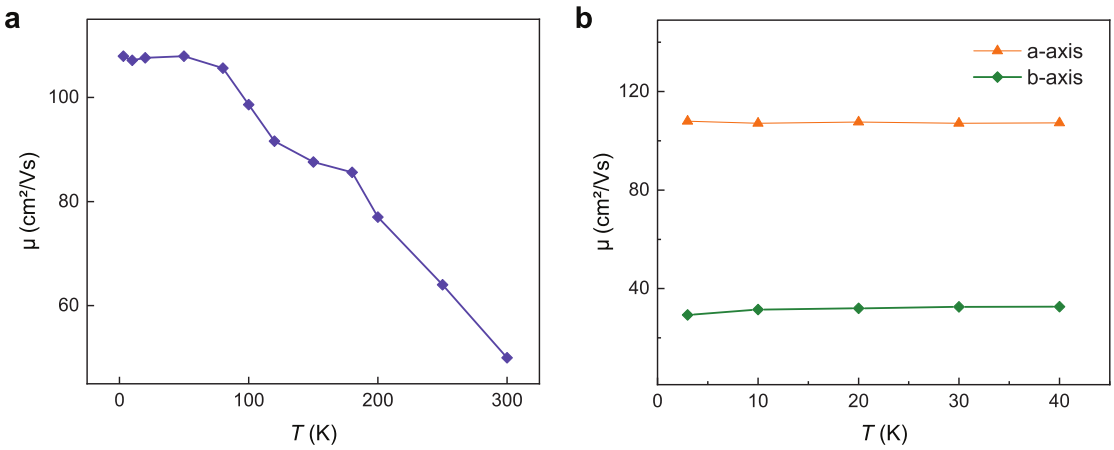

Figure S8 a, measured electron mobility for a-axis as a function of temperature from 3 K to 300 K. b, electron mobility for a-axis and b-axis from 3 K to 40 K.

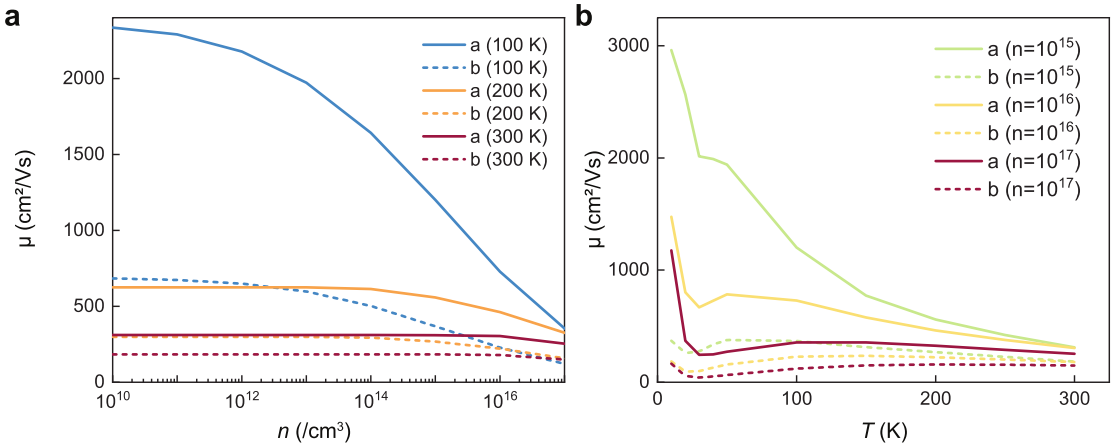

Figure S9 a, calculated electron mobility as a function of electron concentration without boundary effect. b, temperature-dependent electron mobility with various electron concentration for a-axis and b-axis without boundary effect which means we only consider acoustic deformation potential scattering and polar optical phonon scattering.

Functionals/Lattice constants	**a-axis**	**b-axis**	**c-axis**
	angstrom	angstrom	angstrom
Experimental data	5.7457	5.8679	7.6946
LDA	6.0866	6.119	6.0963
LDA-D2	6.0315	6.0618	6.0376
LDA-D3	-	-	-
LDA-DF2	6.003	6.1444	8.3721
LDA-optB86b	6.2027	6.2519	6.203
LDA-optB88	5.94926	6.02628	7.19619
PBE	5.77889	5.9335	8.68174
PBE-D2	6.1871	6.2346	6.1712

PBE-D3	6.19025	6.24115	6.18027
PBE-DF2	6.01165	6.15096	8.3432
PBE-optB86b	6.20987	6.25489	6.2083
PBE-optB88	5.95954	6.0343	7.1772
PBEsol	6.1368	6.1818	6.141
PBEsol-D2	6.07844	6.1149	6.0803
PBEsol-D3	6.08639	6.11878	6.09385
PBEsol-DF2	6.0116	6.15096	8.3432
PBEsol-optB86b	6.20987	6.25489	6.20832
PBEsol-optB88	5.95954	6.0343	7.1772
LDA-SCAN+rVV10	5.7351	5.8611	7.7466
PBE-SCAN+rVV10	5.7419	5.8667	7.7307

Table S1 Comparison of calculated lattice constants under different functionals. The experimental data comes from the X-ray diffraction measurement[1].

101.14333	11.64908	8.88653	0	0	0
11.64908	146.8856	6.17761	0	0	0
8.88653	6.17761	6.75079	0	0	0
0	0	0	43.05149	0	0
0	0	0	0	1.58601	0
0	0	0	0	0	2.68592

Table S2 Elastic constant matrix.

high frequency dielectric matrix		
16.196737	0	0
0	16.51295	0
0	0	6.36932
the static dielectric matrix		
17.566914	0	0
0	17.99658	0
0	0	6.39056

Table S3 the static dielectric matrix, and high-frequency dielectric matrix.

Reference

1. Soulard, C.; Rocquefelte, X.; Petit, P. E.; Evain, M.; Jobic, S.; Itié, J. P.; Munsch, P.; Koo, H. J.; Whangbo, M. H. Experimental and Theoretical Investigation on the Relative Stability of the PdS_2- and Pyrite-Type Structures of $PdSe_2$. *Inorg. Chem.* **2004**, *43* (6), 1943–1949.