

**Supplementary Materials for**  
**Pressure-enhanced Optoelectronic Properties in Two-dimensional**  
**Metal Phosphorus Trichalcogenides Semiconductor SnPSe<sub>3</sub>**

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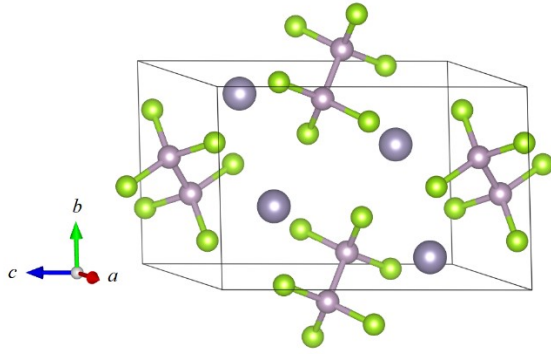


Fig. S1. Schematic crystal structure of SnPSe<sub>3</sub> at ambient conditions. Sn, P, and Se are represented by gray, purple, and green spheres, respectively.

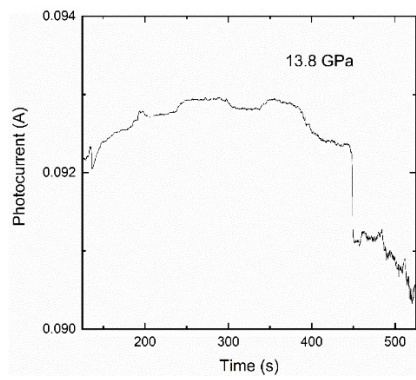


Fig. S2. Photocurrent of SnPSe<sub>3</sub> at 13.8 GPa.

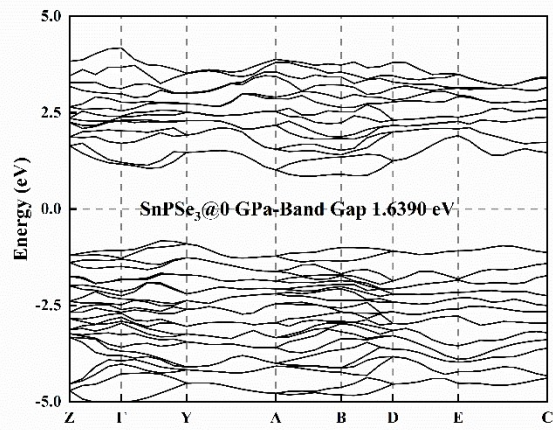


Fig. S3. The calculated band gap of SnPSe<sub>3</sub> at 0 GPa via using HSE method.

Table S1. Calculated Bader charges of Sn, P, and Se in SnPSe<sub>3</sub> at 0 and 10 GPa.

	0 GPa					10 GPa			
	No.	X	Y	Z	CHARGE (e)	X	Y	Z	CHARGE (e)
Sn	1	-0.1624	2.8617	7.2413	13.056	-0.1539	2.9119	6.7996	13.0602
	2	0.3331	4.7513	2.3245	13.056	0.3595	4.4338	2.309	13.0602
	3	-2.9566	6.6682	7.1074	13.056	-2.7492	6.5847	6.8478	13.0603
	4	3.1273	0.9448	2.4584	13.056	2.9548	0.7609	2.2608	13.0603
P	5	-0.2721	0.8839	4.1181	4.615	-0.3563	0.7885	3.9476	4.6934
	6	0.4428	6.7291	5.4477	4.6108	0.5619	6.5571	5.161	4.6848
	7	3.7325	4.6904	0.6648	4.6107	3.6707	4.4613	0.6223	4.6848
	8	-3.5618	2.9226	8.901	4.615	-3.465	2.8843	8.4864	4.6934
Se	9	0.8721	0.0769	7.2987	6.4451	0.9081	0.1594	7.1115	6.4022
	10	-0.7014	7.5361	2.2671	6.4451	-0.7024	7.1862	1.9971	6.4022
	11	-3.991	3.8834	7.05	6.4451	-3.8112	3.8322	6.5359	6.4022
	12	4.1617	3.7296	2.5158	6.4451	4.0168	3.5134	2.5727	6.4022
	13	2.2434	6.1559	0.5156	6.4295	2.1089	5.9883	0.4562	6.4408
	14	-2.0728	1.4571	9.0502	6.4295	-1.9033	1.3573	8.6524	6.4408
	15	1.2169	2.3494	4.2673	6.4295	1.2055	2.3155	4.1136	6.4408
	16	-1.0462	5.2636	5.2985	6.4295	-0.9998	5.0301	4.995	6.4408
	17	-0.9858	5.2956	9.1353	6.4565	-0.7464	5.2067	8.6679	6.4076
	18	1.1565	2.3174	0.4305	6.4565	0.952	2.1389	0.4407	6.4076
	19	-2.1331	1.4891	5.2134	6.4565	-2.1567	1.5339	4.9795	6.4076
	20	2.3038	6.1239	4.3524	6.4565	2.3623	5.8117	4.1292	6.4076