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补充材料：In_2Se_3薄膜的掺杂效应及其纳米带铁电性*

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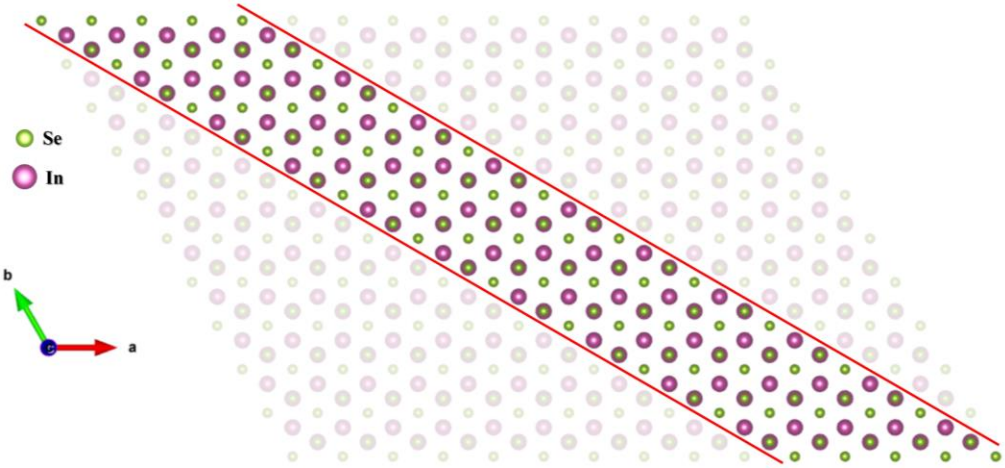

图 S1 In_2Se_3纳米带裁剪示意图

Fig. S1. The simulation model of In_2Se_3 nanoribbon.

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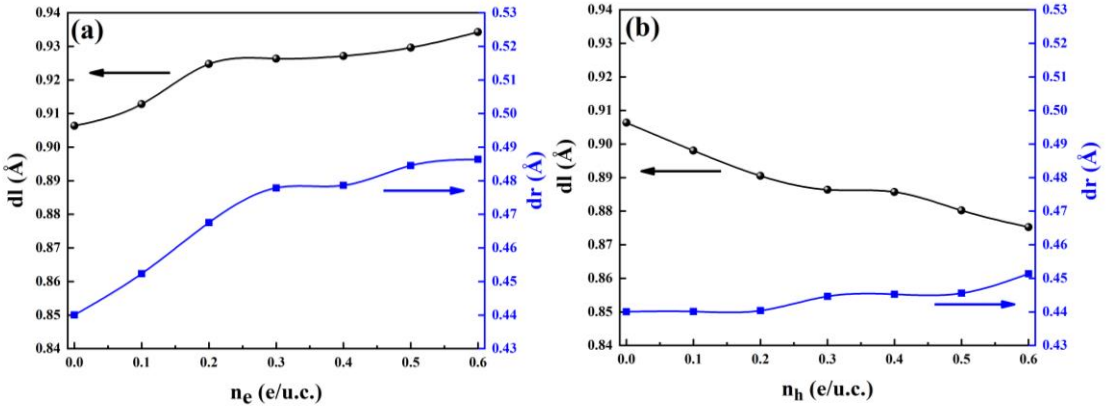

图 S2 In$_2$Se$_3$ 薄膜中 Se2 原子的畸变参数(面内 dl 和面外 dr)随掺杂浓度的变化。(a)电子掺杂，(b)空穴掺杂

Fig. S2. The in-plane distortion **d***l* and out-of-plane distortion dr of Se2 atom in In$_2$Se$_3$ monolayer as a function of doping concentration for the case of (a) electron doping and (b) hole doping.

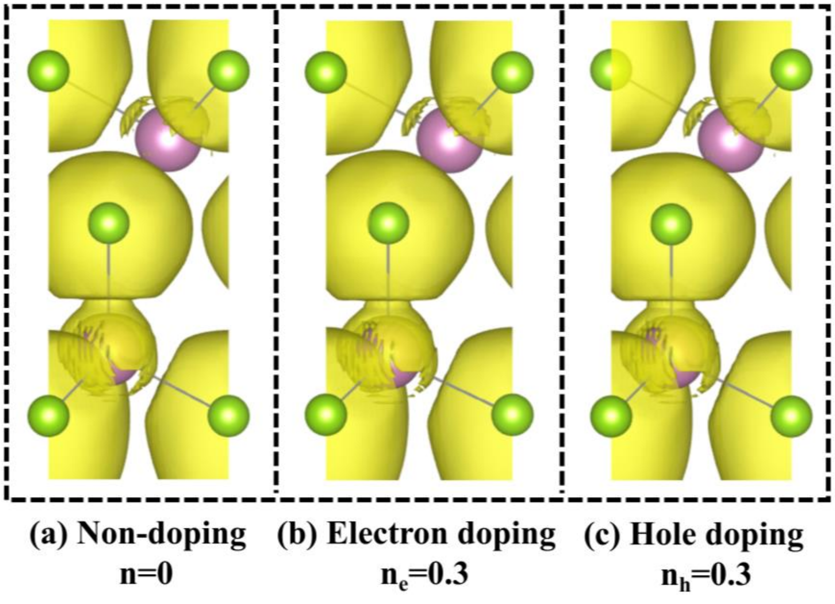
(a) Non-doping
n=0
(b) Electron doping
n_e=0.3
(c) Hole doping
n_h=0.3

图 S3 In$_2$Se$_3$ 薄膜局域电子密度函数图，(a)未掺杂，(b)电子掺杂 $n_e = 0.3$，(c) 空穴掺杂 $n_h = 0.3$

Fig. S3. Eelectron-Localization-Function of doped In$_2$Se$_3$ monolayers. (a) non-doping, (b) electron doping $n_e = 0.3$, (c) hole doping $n_h = 0.3$.

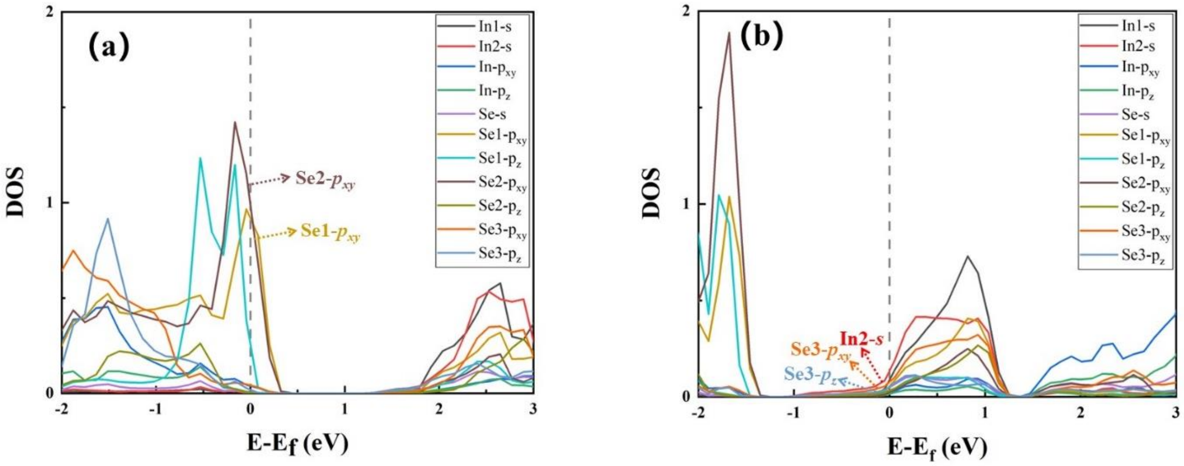

图 S4 掺杂薄膜的电子态密度原子和轨道投影图。（a）空穴掺杂 $n_h = 0.3$（b）电子掺杂 $n_e = 0.3$。

Fig. S4. Projected-DOS of doped In$_2$Se$_3$ monolayers. (a) hole doping $n_h = 0.3$, (b) electron doping $n_e = 0.3$.

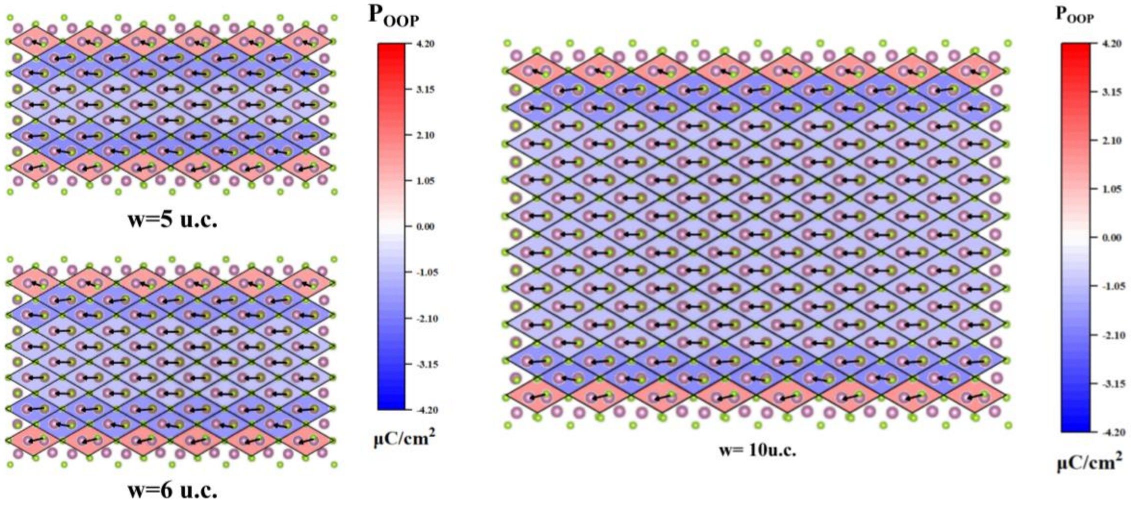

图 S5 纳米带极化分布图（纳米带宽度分别为 5 u.c.、6 u.c.和 10 u.c.），其中平面内极化大小和方向用矢量表示。垂直平面的极化大小用颜色来表示，负号代表极化方向朝下，正号代表极化朝上。

Fig. S5. Distribution of polarization within In$_2$Se$_3$ nanoribbon with different width (w = 5 u.c., 6 u.c., and 10 u.c.), where the magnitude and the direction of P_{IP} are indicated by vector, the magnitude of P_{OOP} is described by different color, and the positive value of P_{OOP} denotes the up direction and negative value denotes the down direction.

表S1：纳米带(w = 1 u.c.)中各原子波恩有效电荷

Table S1. Born effective charges for the nanoribbon (w = 1 u.c.)

Atom	Q_x	Q_y	Q_z
Se1	-1.96	-0.37	-0.37
Se2	-2.17	-0.41	-0.63
Se3	-1.04	-0.43	-0.93
Se4	-1.64	-0.28	-0.32
Se5	-2.34	-0.14	-1.07
Se6	-1.39	-0.40	-0.39
Se7	-1.04	-0.43	-0.93
Se8	-2.17	-0.41	-0.63
Se9	-1.96	-0.37	-0.37
In1	2.35	0.56	1.03
In2	2.33	0.54	0.82
In3	3.33	0.44	0.68
In4	3.04	0.60	1.26
In5	2.33	0.54	0.82
In6	2.35	0.56	1.03

表S2: 纳米带(w = 2 u.c.)中各原子波恩有效电荷

Table S2. Born effective charges for the nanoribbon (w = 2 u.c.)

Atom	Q_x	Q_y	Q_z
Se1	-1.12	-0.40	-0.64
Se2	-2.20	-0.47	-0.34
Se3	-2.06	-0.52	-0.35
Se4	-2.18	-0.62	-0.24
Se5	-2.06	-0.67	-0.24
Se6	-2.28	-0.29	-0.69
Se7	-2.62	-0.70	-0.28
Se8	-1.81	-0.40	-0.62
Se9	-2.66	-0.71	-0.29
Se10	-2.28	-0.30	-0.69
Se11	-2.06	-0.67	-0.24
Se12	-2.18	-0.62	-0.24
Se13	-2.06	-0.52	-0.35
Se14	-2.20	-0.47	-0.34
Se15	-1.12	-0.40	-0.64
In1	2.55	1.43	2.53
In2	2.53	1.03	0.65
In3	3.42	0.50	0.62
In4	3.56	0.48	0.58
In5	3.37	0.51	0.62
In6	3.38	0.42	0.55
In7	3.56	0.48	0.58
In8	3.42	0.50	0.62
In9	2.53	1.03	0.65
In10	2.55	1.41	0.66

表S3：纳米带(w = 3 u.c.)中各原子波恩有效电荷

Table S3. Born effective charges for the nanoribbon (w =3 u.c.)

Atom	Q_x	Q_y	Q_z
Se1	-1.13	-0.27	-0.62
Se2	-2.09	-0.33	-0.34
Se3	-2.23	-0.40	-0.34
Se4	-2.28	-0.40	-0.70
Se5	-2.12	-0.98	-0.23
Se6	-2.22	-1.04	-0.23
Se7	-1.95	-0.62	-0.60
Se8	-2.54	-1.04	-0.27
Se9	-2.56	-1.04	-0.26
Se10	-2.15	-0.70	-0.57
Se11	-2.43	-1.06	-0.23
Se12	-2.36	-1.12	-0.22
Se13	-2.54	-1.04	-0.27
Se14	-2.56	-1.04	-0.26
Se15	-1.95	-0.62	-0.60
Se16	-2.22	-1.03	-0.23
Se17	-2.12	-0.99	-0.23
Se18	-2.28	-0.40	-0.70
Se19	-2.23	-0.40	-0.34
Se20	-2.09	-0.33	-0.34
Se21	-1.13	-0.27	-0.62
In1	2.61	3.38	0.63
In2	2.61	1.60	0.63
In3	3.38	0.68	0.59
In4	3.53	0.60	0.62
In5	3.44	0.45	0.54
In6	3.44	0.42	0.54
In7	3.54	0.47	0.56
In8	3.60	0.41	0.51
In9	3.44	0.41	0.54
In10	3.44	0.44	0.54
In11	3.53	0.55	0.62
In12	3.38	0.68	0.59
In13	2.61	1.64	0.63
In14	2.61	3.37	0.63

表 S4: 薄膜中各原子波恩有效电荷

Table S4. Born effective charges for the In_2Se_3 monolayer

Atom	Q_x	Q_y	Q_z
Se1	-2.53	-2.73	-0.23
Se2	-1.79	-1.02	-0.55
Se3	-2.56	-2.82	-0.22
In1	3.42	3.27	0.50
In2	3.46	3.30	0.51