

097502-20212384

补充材料

二维 NiBr_2 单层自旋电子输运以及光电性质研究

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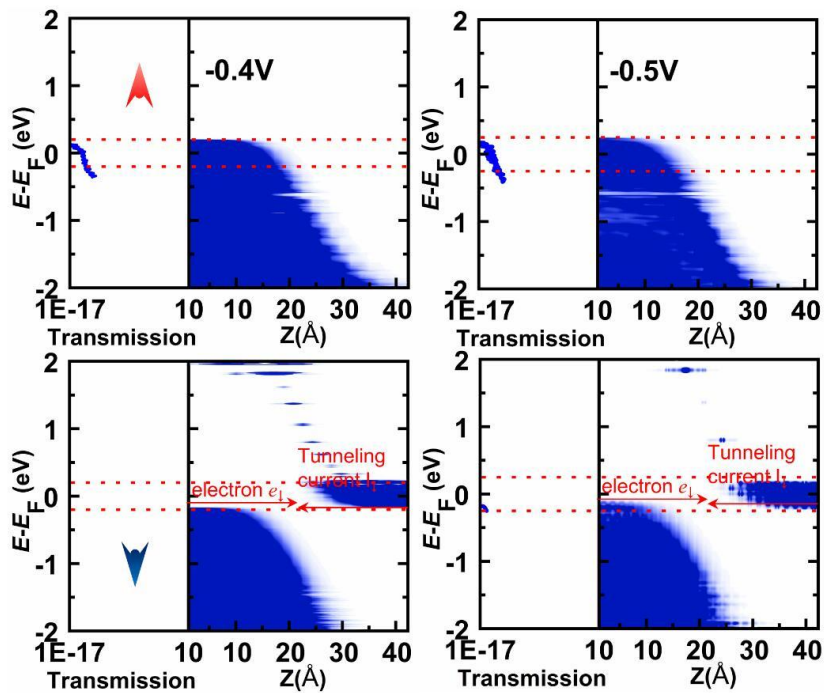


图 S1 Z 型 NiBr_2 单层 PN 结二极管在 -0.4 V 和 -0.5 V 偏置电压下的自旋极化透射谱和投影局域态密度图。

Fig. S1. Spin-resolved transmission spectra $T(E)$ and projected local density of states of Z-type NiBr_2 -ML PN-junction diodes under the biases of -0.4 V and -0.5 V .

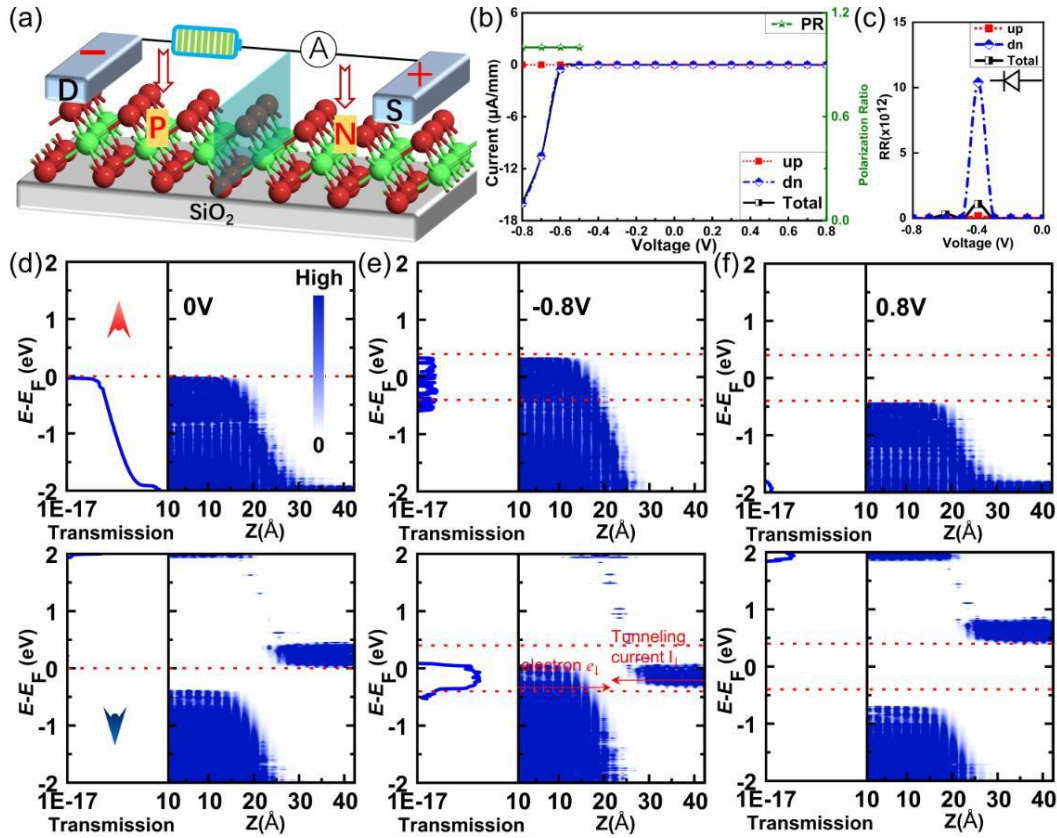


图 S2 NiBr₂ 单层 PN 结二极管的自旋输运性质 (a) NiBr₂ 单层 PN 结二极管示意图; (b) A 型 NiBr₂ 单层 PN 结二极管的偏置电压-电流和极化率曲线; (c) A 型 NiBr₂ 单层 PN 结二极管的整流比曲线; (d)–(f) 在 0, -0.8 和 0.8 V 偏置电压下的自旋极化透射谱(左侧)和投影局域态密度图(右侧), 其中上图对应自旋向上态, 下图对应自旋向下态. 图(d)中的颜色卡显示了 (d)–(f) 中的数据从 0 (白色) 到高 (蓝色)

Fig. S2. Spin-resolved transport properties of PN-junction diodes of NiBr₂-ML: (a) Schematic of the PN-junction diodes of NiBr₂-ML. (b) *I*-*V* and polarization ratio (PR) curves of A-type PN-junction diode of NiBr₂-ML; (c) rectifying ratio curve of A-type PN-junction diode of NiBr₂-ML; (d)–(f) spin-resolved transmission spectra *T*(*E*) and projected local density of states under the biases of 0, -0.8, and 0.8 V, where the top panel and bottom panel correspond to spin-up and spin-down state, respectively. The colorbar shows the data from 0 (white) to high (blue).

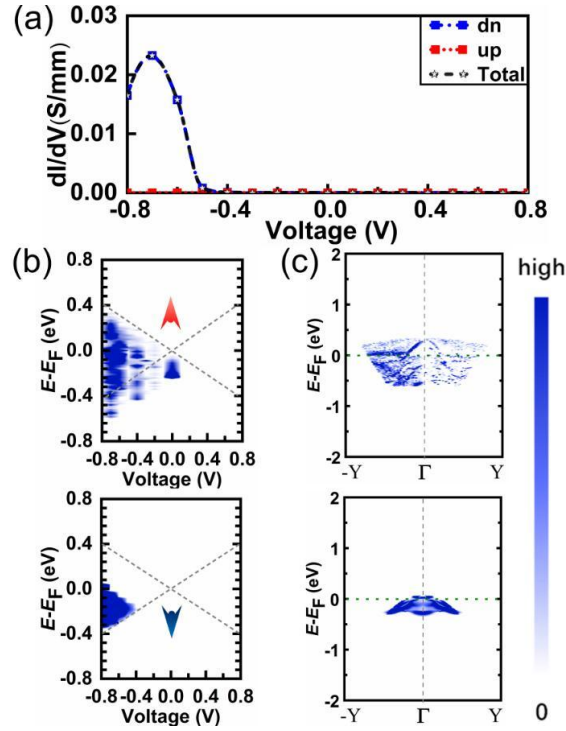


图 S3 NiBr₂ 单层 PN 结二极管的器件特性 (a) A 型 NiBr₂ 单层 PN 结二极管的微分电导曲线; (b) 偏压相关的自旋向上和自旋向下态的电子透射谱; (c) -0.8 V 偏压时 k 空间相关的自旋电子透射系数 $T(E,k)$. 颜色图显示了从 0 (白色) 到高 (蓝色) 的图 (b) 和 (c) 数据, 其中上图对应自旋向上态, 下图对应自旋向下态

Fig. S3. Device properties of the PN-junction diodes of NiBr₂-ML: (a) Difference conductance curves of A-type PN-junction diodes of NiBr₂-ML; (b) bias-dependent transmission spectra for the spin-up and spin-down states; (c) k -dependent transmission coefficients $T(E,k)$ at -0.8 V. The colormap shows the $T(E,k)$ from 0 (white) to high (blue). Top and bottom panel in (b) and (c) correspond to spin-up and spin-down state, respectively.

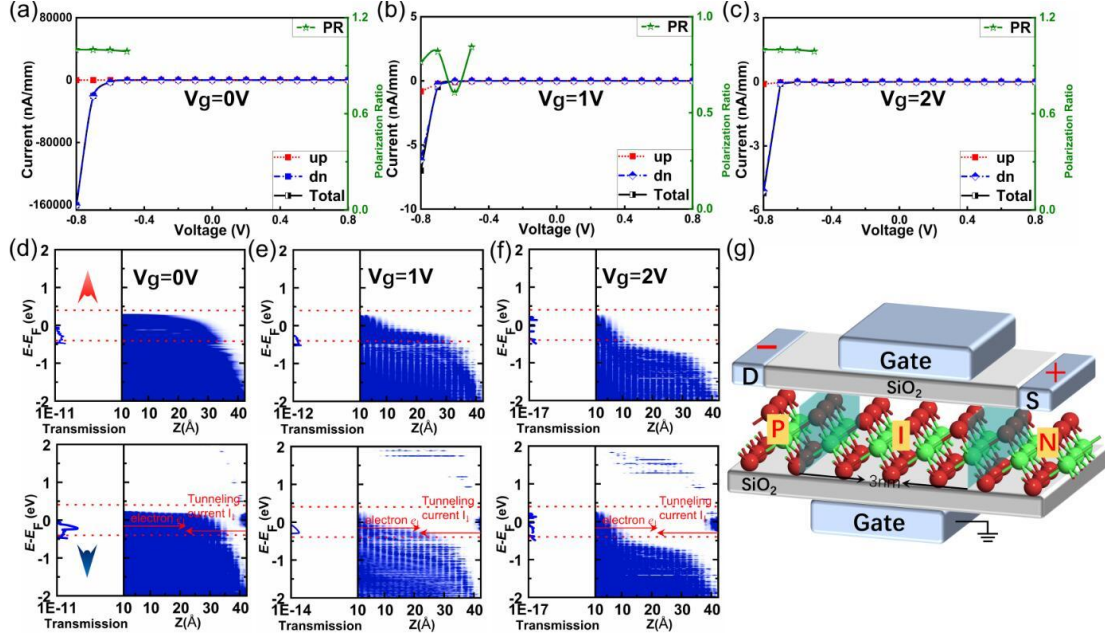


图 S4 A 型 $NiBr_2$ 单层 PIN 结场效应晶体管在不同栅压下的运输特性 (a)–(c) 0, 1 和 2 V 栅极电压下自旋向上和自旋向下的偏置电流和自旋极化率曲线; (d)–(f) 在 0, 1 和 2 V 栅极电压下的自旋极化透射谱和投影局域态密度图, 其中上图对应自旋向上态, 下图对应自旋向下态; (g) $NiBr_2$ 单层 PIN 结场效应晶体管示意图

Fig. S4. Transport properties of A-type $NiBr_2$ -ML PIN-junction field-effect transistors (FET) under different gate voltages: (a)–(c) I - V and polarization ratio curves under the gate voltages of 0, 1, and 2 V, respectively; (d)–(f) spin-resolved transmission spectra $T(E)$ and projected local density of states under the biases of 0, 1, and 2 V, where top and bottom panel correspond to spin-up and spin-down state, respectively; (g) schematic of the $NiBr_2$ -ML FET.

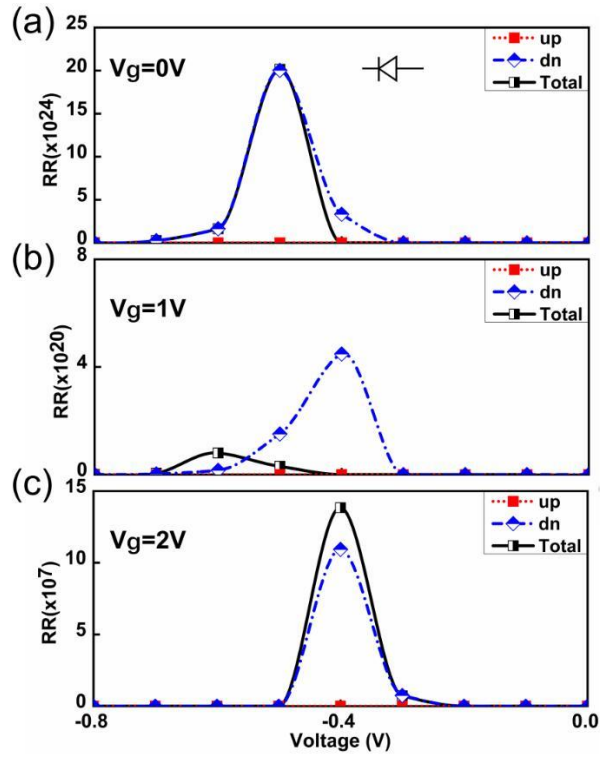


图 S5 在不同栅极电压下, A 型 NiBr₂ 单层 PIN 结场效应晶体管的自旋向上(up)、自旋向下(dn)及总的(Total)整流比曲线 (a) $V_g = 0 \text{ V}$; (b) $V_g = 1 \text{ V}$; (c) $V_g = 2 \text{ V}$

Fig. S5. Spin-up, spin-down, total rectifying ratio curves of A-type NiBr₂-ML PIN-junction FET under different gate voltages: (a) $V_g = 0 \text{ V}$; (b) $V_g = 1 \text{ V}$; (c) $V_g = 2 \text{ V}$.

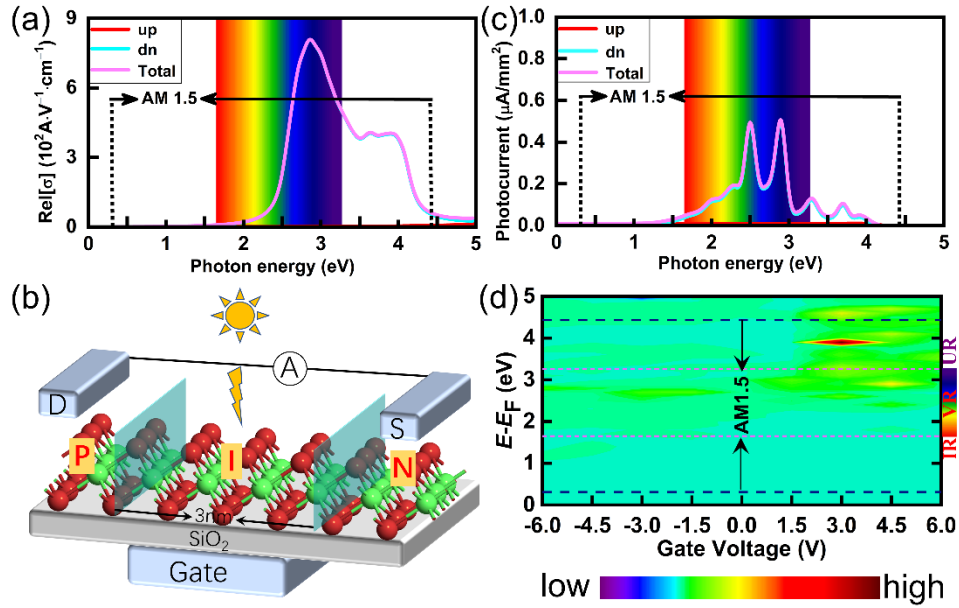


图 S6 NiBr₂ 单层的光电特性 (a) NiBr₂ 单层的光电导率，七彩光谱背景色为可见光区；(b) NiBr₂ 单层的 PIN 结光电晶体管示意图；(c) A 型 NiBr₂ 单层的 PIN 结光电晶体管在 0 V 偏压(无电源)下的自旋光电流密度；(d) 0 V 偏压时不同栅极电压下的 A 型 NiBr₂ 单层的 PIN 结光电晶体管光电流谱. IR, VR, UR 分别指红外区、可见光区、紫外区

Fig. 6. Photoelectric properties of the NiBr₂-ML. (a) Optical-conductivity of NiBr₂-ML. The embedded spectrum pattern displays the visible region. (b) Schematic of the PIN-junction phototransistor of NiBr₂-ML. (c) Spin-resolved photocurrent density of the A-type PIN-junction phototransistor of NiBr₂-ML under zero bias (without power). (d) Gate-dependent photocurrent spectra of the A-type phototransistor of NiBr₂-ML under zero bias. IR, VR, and UR refer to the infrared, visible, and ultraviolet region, respectively.