Van der Waals contact between 2D magnetic VSe₂ and transition metals and demonstration of high-performance spin-field-effect transistors

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ABSTRACT This study used density functional theory and the quantum transport method to investigate the interfacial coupling and spin transport of transition metals (TMs) with a Fe, Co, and Ni/2H-VSe₂ hybrid nanostructure. Because the indirect coupling of TM-Se-V led to an obvious reduction of the magnetic moment and the disappearance of the half-metal characteristics of 2H-VSe₂, the expected spin-filtering effect of individual TMs and 2H-VSe₂ deteriorated at the contact region. Nevertheless, all the TM/2H-VSe₂-based dual-probe devices exhibited an interesting bias-dependent spin-injection efficiency with a maximum output spin-polarized current of 666 mA mm⁻¹ in Co/2H-VSe₂. The proposed TM/2H-VSe₂-based spin-field-effect transistor demonstrated outstanding performance. The Ni/2H-VSe₂-based transistor achieved a maximum output spin-polarized current of 3117 mA mm⁻¹ and demonstrated a good switching characteristic of 106 mV dec⁻¹. Importantly, all transistors achieved a widely tunable scale of spin-extraction efficiency ranging consistently between 96% and -92% with gate bias. These results indicate a promising candidate for use in high-performance spintronic devices.

Keywords: VSe₂, contact, DFT, spin-FET

INTRODUCTION

With the gradual slowdown of development in silicon-complementary metal-oxide-semiconductor (CMOS) technology [1], spintronics devices have become key prospective candidates for use in low-power storage and logic device applications due to their outstanding performance [2,3]. Significant increases in storage density have been achieved using classic giant magnetoresistance

and tunnel magnetoresistance [4–6]. More recently, magnetic random access memory devices based on the spin-transfer torque effect have offered additional new opportunities for use in neural computing applications [7,8]. When developing spintronic devices, the smooth surfaces and atomic-level thicknesses of magnetic two-dimensional (2D) materials, such as CrI₃, Fe₃GeTe₂, and VSe₂, enable superior integration and more flexible control [9–12]. In particular, VSe₂ has attracted much attention in the fields of spin-injection control and spin transistors on account of its unique bipolar magnetic properties and essential Curie temperature (*T_c*) of room temperature and above [13]. The experimental synthesis of the metallic phase of monolayer 1T-VSe₂ in 2018 [14] is particularly noteworthy; the 2H phase is predicted to be more stable and possess a much higher *T_c* than the 1T phase [15,16].

Previous studies have demonstrated the use of the gate voltage of the half-metal characteristics of bilayer 2H-VSe₂ [17] to achieve flexible control. Additionally, first-principle calculations based on the non-equilibrium Green's function (NEGF) demonstrated a spin-filtering efficiency of up to 99% in a double-gate transistor consisting entirely of 2H-VSe₂. This shows an excellent potential for application [18].

An enduring research focus in the field of spintronic devices is the realization of efficient spin injection from transitional magnetic metals into semiconductors. For 2D materials, it is possible for the van der Waals (vdW) gap at the metal-semiconductor interface to form a natural tunnel barrier [19], which is favorable for the spin-injection efficiency (SIE) [20,21]. However, the heavy de-

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pendence of spin injection on the orbital hybridization and proximity at the interface [22,23] is widely recognized. The hybridization with the vdW coupling effect at the interfacial region provides new behaviors for 2D materials in terms of proximity effects and spin injection. However, the interfacial characteristics of the metal/2H-VSe₂ interface have not been described, and the SIE has not been investigated. The performance of a spin transistor with a complete metal/2H-VSe₂/metal structure remains unknown.

This study used density functional theory (DFT) and the quantum transport method to investigate the hybrid structure of transition metals (TMs)/2H-VSe₂, including Fe, Co, and Ni/2H-VSe₂, and their related spin field-effect transistors (spin-FETs). The expected spin-filtering effect from individual magnetic TMs or 2H-VSe₂ was reduced considerably in the hybrid structures due to the indirect coupling of TM-Se-V. However, the TM/2H-VSe₂-based dual-probe devices demonstrated interesting bias-dependent SIE with a maximum spin-polarized current of 666 mA mm⁻¹. The proposed spin-FET not only exhibited a large-scale gate-tunable spin-extraction efficiency (SEE), but also produced an unexpected high-output spin-polarized current.

EXPERIMENTAL SECTION

All calculations were performed within the *ab-initio* theoretical framework. The optimization of the atomic structure and the calculation of bulk characteristics were conducted using the Vienna *Ab-initio* Simulation Package (VASP) [24]. The projected augmented wave method with an energy cutoff of 500 eV was used [25]. The convergence of the electron and ionic steps were 10⁻⁵ eV and 0.01 eV Å⁻¹, respectively. The Perdew-Burke-Ernzerhof (PBE) functional was used as the exchange-correlation functional [26], and the vdW interaction was employed using the DFT-D3 method [27]. The K-mesh densities were 4 and 15 Å for static and density-of-states (DOS) calculations, respectively. To provide more detail, a smearing width of 0.05 eV was adopted in the DOS calculation, and both ferromagnetic (FM) and anti-ferromagnetic (AFM) couplings between TMs and 2H-VSe₂ were considered in the spin-polarized calculations. Systems with an initial set of FM or AFM couplings always converged to the same ground state with a deterioration of the half-metal characteristic of 2H-VSe₂. The Hubbard-U term was not used in the calculations for two reasons. The first is that when considering the TMs-2H-VSe₂ hybridization, although parameters from pristine 2H-VSe₂ can be fitted, the on-site interaction of the d-

orbital from the TM in the hybrid structure is unclear. Some very recent investigations on contact between TMs and magnetic 2D materials have used the PBE functional [28,29]. The second reason is that typically, 2D-material-based devices have a high unintentional doping level, which tends to decrease the bandgap [30]. Therefore, the PBE functional provides reliable results [31], and it can be used in the transport calculation of magnetic 2D materials [32,33].

The QuantumATK software package and the non-equilibrium green's function (NEGF) method were used for all the transport calculations in this study [34], and a double-zeta polarized basis set with a cutoff of 160 Ry was employed. The K-mesh densities for the periodic and transport directions were 4 and 150 Å, respectively. The Fermi-Dirac smearing scheme with a broadening of 1200 K was used to integrate Kohn-Sham eigenvectors and provide an improved convergence.

RESULTS AND DISCUSSION

Interfacial characteristics of TM/VSe₂ hybrid structures

To maintain the characteristics of 2H-VSe₂, the interface models of the TM/2H-VSe₂ hybrid were constructed by straining the metal only. Table 1 presents the lattice parameters and the mean mismatch of each system. The lattice matching of Co and Ni/2H-VSe₂ is excellent, and the mismatch of ~0.55% suggests an outstanding potential for use in device fabrication. Although Fe exhibits a mismatch of 3.05%, it is still below 5%. Fig. 1 contains the side and top views of the TM/2H-VSe₂ systems after fully atomic relaxation. The atomic structure of 2H-VSe₂ in the pristine form is well preserved in all three systems, which suggests that the TM-2H-VSe₂ hybridization has little influence on the surface morphology of the semiconductor.

The spin-resolved band structure of the pristine phase of 2H-VSe₂ was calculated to obtain its half-metal characteristics (Fig. S1). Then, the electronic structure of the TM/2H-VSe₂ systems was evaluated by the spin-resolved DOS. To achieve each element's contribution, the DOS were projected individually to the orbitals of the first layer

Table 1 Lattice parameters and the mean mismatch of TM/2H-VSe₂ hybrid structures

TM/2H-VSe ₂	<i>a</i> (Å)	<i>b</i> (Å)	Mismatch (%)
Fe/2H-VSe ₂	5.779	10.009	3.05
Co/2H-VSe ₂	6.673	11.557	0.54
Ni/2H-VSe ₂	6.673	11.557	0.58

Figure 1 (a–c) Top and (d–f) side (profile) views of the TM/2H-VSe₂ hybrid systems. The letters “a” and “b” represent the x and y directions, respectively, of the lattice parameters.

of TM, V, and Se, respectively. The results are presented in Fig. 2a–c. It is observed that the interfacial coupling in the majority and minority spin channels is mainly induced by the TM and the outermost Se atoms. A strong hybridization occurs between the 3d orbitals of the TM with the 4p states of Se, which in all systems ranges between -8 and -5 eV. Although there is no direct hybridization between the TM and V atoms, the TM–Se coupling leads to rehybridization between the 3d and 4p states from V and Se, respectively. Accordingly, all of the electron states at the Fermi level are completely metalized, leading to the disappearance of the half-metal characteristic of 2H-VSe₂. The determination of the magnetic moment of V reveals an obvious reduction in the magnetic moment after the formation of the hybrid systems. The magnetic moment of Fe/2H-VSe₂ is reduced from 1.0 to 0.15 $\mu\text{B atom}^{-1}$. The reduction is much evident for the other two systems at 0.98 and 0.88 $\mu\text{B atom}^{-1}$ for Co/2H-VSe₂ and Ni/2H-VSe₂, respectively.

To understand the global reduction of the magnetic moment, the charge density difference, which was obtained by subtracting the charge of the hybrid TM/2H-VSe₂ from that of the freestanding TM and the 2H-VSe₂ monolayer, and the valence electron density distributions were calculated. Fig. 2d–f present the plane-averaged results for Fe/2H-VSe₂, Co/2H-VSe₂, and Ni/2H-VSe₂, respectively. It is clear that all systems experience a transfer

of majority and minority spin electrons along the opposite direction at the 2H-VSe₂ region. In 2H-VSe₂, the interfacial coupling effect tends to decrease the majority spin electrons and increase the minority spin electrons, which reduces the magnetic moment. There is a similar evolution in the spin-charge variations at the sides of the TM, albeit at a reduced scale. These consistent evolutions indicate that the charge transfer between the TM and the 2H-VSe₂ is not restricted to the same spin channel. However, a spin-charge redistribution occurs, which decreases the spin-polarization of the system. Similar charge rearrangements have been reported previously, e.g., when N adsorbs on the surface of magnetic MnPc, electrons transfer from the Mn atoms to the N atom. The considerable electron redistribution between the different spin configurations leads to a reduction in the number of spin states [35]. Furthermore, the fluctuation clearly weakens in the outermost two layers, suggesting that the vdW coupling is localized mainly between the 2H-VSe₂ and the second layer of the TM. Additionally, the different transfers between the two spin channels create an observable spin-dependent interfacial coupling in all three hybrid structures.

The highest peak value difference of $0.022 \text{ \AA}^{-3}$ is exhibited by Fe/2H-VSe₂. This spin-dependent interfacial coupling is also evident in the valence electron density distribution. Both the electron density and the interfacial

Figure 2 (a–c) Spin-resolved DOS of Fe/2H-VSe₂, Co/2H-VSe₂, and Ni/2H-VSe₂, respectively. (d–f) Spin-resolved difference charge (upper panel) and valence electron (lower panel) density distribution for each TM/2H-VSe₂ system.

coupling distance for Fe/2H-VSe₂ show clear differences. Compared with the majority spin channel, the minority spin provides a longer interfacial coupling distance with a lower valence electron density.

Spin transport of TM/VSe₂-based dual-probe devices

The current–voltage characteristics of a dual-probe device were proposed to evaluate its spin-related transport properties. The SIE is defined as

$$\text{SIE} = \frac{\left(|I_{\text{majority spin}}| - |I_{\text{minority spin}}| \right)}{\left(|I_{\text{majority spin}}| + |I_{\text{minority spin}}| \right)},$$

and the current–voltage curves were calculated, as presented in Fig. 3a–c. The insets contain the side views of the dual-probe device, which mainly focuses on the interfacial region by minimizing the length between the TM and the 2H-VSe₂. In the forward bias range, the SIEs in Fe/2H-VSe₂ and Co/2H-VSe₂ achieve good maximum levels of 75.7% and 79.4%, respectively. However, Ni/2H-VSe₂ has a relatively low SIE of 61.3%. In all three systems, outstanding majority spin currents are observed with maximums of 534, 666, and 455 mA mm^{−1} for Fe/2H-VSe₂, Co/2H-VSe₂, and Ni/2H-VSe₂, respectively.

Interestingly, in the reverse bias range, the SIE values of the three systems are very close at −88.4%, −86.9%, and −84.4% for Fe/2H-VSe₂, Co/2H-VSe₂, and Ni/2H-VSe₂, respectively. The negative values indicate that the minority spin current becomes higher than that of the majority spin, and the comparable results suggest that 2H-VSe₂ dominates the transport at the cathode.

Furthermore, both the majority and minority spin currents exhibit clear diode-like volt-ampere characteristics. Because TM/2H-VSe₂ systems are not intentionally doped with p- or n-type, this diode-like characteristic is derived from the interface between the metal and the semiconductor, i.e., in all systems, a Schottky barrier (SB) is formed for both the majority and minority spin transport. However, as the TM/2H-VSe₂ interfaces are metalized for both spin channels, the formation of the SB remains unclear.

The transmission spectrum at the zero bias of each system was calculated to clarify SB formation, SIE evolution, and current–voltage characteristics (Fig. 3d). It can be seen that both the majority and minority spin possess a transmission gap, which corresponds well to the half-metal band structure of 2H-VSe₂. Therefore, the complete rehybridization between V and Se at the contact

Figure 3 Current–voltage characteristics and the SIE of (a) Fe/2H-VSe₂, (b) Co/2H-VSe₂, and (c) Ni/2H-VSe₂, respectively. The insets are the side views of the dual-probe devices. (d) Spin-resolved transmission spectra of all systems at 0 V.

region should result in the formation of the SB at the interface between the contact region and the cathode.

Additionally, Fe/2H-VSe₂ has lower transmission coefficients than either Co/2H-VSe₂ or Ni/2H-VSe₂ across nearly the entire range. This explains why the current of Fe/2H-VSe₂ (presented in Fig. 3a) is lower than in the other two systems. Furthermore, the bias windows in the transmission spectrum help to clarify the SIE. When the device is under a finite bias, a bias window emerges at the Fermi level and extends to include the valid transmission. In the majority spin channel, the transmission barrier of Co/2H-VSe₂ is slightly lower than that of Ni/2H-VSe₂ at 0.015 eV. Meanwhile, the barriers in the minority spin channel are almost identical. Accordingly, the higher transmission of Co/2H-VSe₂ in the majority spin channel leads to higher SIE in the positive bias range.

The spin-resolved projected local DOS (PLDOS) of all devices at a bias of 0 V was calculated to better understand the spin-polarized transport (see Figs S2–S4 for the results). All devices exhibit the formation of a spin-dependent SB at the TM–2H-VSe₂ interfaces. Under finite bias, the majority and minority spin currents are transported *via* the valence and conduction bands of 2H-VSe₂, respectively. An increase in bias can lead to more valence band states in the transmission window, which results in

an increased SIE.

The well preserved half-metal characteristics in the cathode facilitate the bias-dependent evolution of SIE in all the TM/2H-VSe₂ devices. Inspired by the tunable SIE, it is anticipated that an effective gate potential on 2H-VSe₂ can result in increased flexibility for the manipulation of spin currents. Therefore, a monolayer 2H-VSe₂-based spin-FET is proposed.

Performance of TM/VSe₂-based spin-FET

Fig. 4 presents the device configurations of all systems. The channel length was 5 nm, and double gates with an effective oxide thickness of 0.5 nm were adopted at the channel region for improved electrostatic control. This is in accordance with the scaling of CMOS technology. To achieve a realistic scale, the drain and source were extended using a 1-nm length of TM (approx.). The transfer characteristics, which denote current (I_{DS}) as a function of gate voltage (V_{GS}), were calculated using a voltage drop of 0.1 V between the drain and the source (V_{DS}). The results are presented in Fig. 5. First, it is evident that Fe/2H-VSe₂ has a lower maximum current than Co/2H-VSe₂ and Ni/2H-VSe₂ for both its majority and minority spin carriers. This is due to the higher resistivity of Fe compared with the other TM. A similar performance is demonstrated by both Co/2H-VSe₂ and Ni/2H-VSe₂ for the majority spin

Figure 4 Profile view of the TM/2H-VSe₂ transistors. The channel length was 5 nm. The TM extension regions were introduced between the electrode and the contact region.

Figure 5 (a–c) Transfer characteristics of the TM/2H-VSe₂ transistors at a V_{DS} of 0.1 V. (d) The SEE of the TM/2H-VSe₂ transistors.

current of about 1100 mA mm^{-1} at -1.4 V , while the performance of Ni/2H-VSe₂ is slightly better for the minority spin current of 3117 mA mm^{-1} at 1.4 V . These ultra-high levels indicate that both devices have excellent spin-current-driving capability, which is significant for application in fast spin-based devices.

Second, the transition speeds between the off (low current) and on (high current) states of the devices were evaluated by extracting the sub-threshold slope (SS). The similar performance of all systems in terms of majority and minority spin currents indicates that SS is dependent mainly on 2H-VSe₂. The remarkable switching char-

acteristic of $\sim 100 \text{ mV dec}^{-1}$ achieved for the minority spin current approaches that of a recently reported 2D vdW tunnel transistor and an III-V-based Fin-FET [36,37].

Third, the SEE, which is redefined from the SIE for the output spin current, was calculated. Fig. 5d shows the results. It is interesting to note that the evolution of SEE as a function of V_{GS} is similar in all the TM/2H-VSe₂-based devices. This indicates that the status of 2H-VSe₂ at the channel region is the main determiner of SEE. At high V_{GS} in particular, the entire SEE converges to a much closer value to that of ultra-high polarization, which denotes the production of an almost purely polarized current in the 2H-VSe₂ channel. Significantly, the SEE ranges dramatically between 96% and -92% with gate control. The ultra-high SEE of >90% provides excellent potential for application in spintronic devices.

The PLDOS of a device can help clarify the gate-tunable SEE mechanism in the TM/2H-VSe₂-based spin-FET. Fig. 6 shows the results of the Ni/2H-VSe₂-based spin-FET as an example, and the PLDOS of the TM/2H-VSe₂ spin-FET at a V_{GS} of 0 V and a V_{DS} of 0.1 V is presented in Figs S5–S7. Compared with the relatively small difference in DOS between the two spin channels in the Ni/2H-VSe₂ hybrid regions, a considerable difference is evident between the source and drain regions; this indicates the strong spin-polarized electronic structure of Ni metal. Of further interest is that the DOS of the majority spin is lower than that of the minority spin in the

bias window. Therefore, the variations in SEE among spin-FETs with a low V_{GS} (Fig. 5d) can be attributed to the different interfacial spin polarizations in the transmission window.

Additionally, it is clear that the gate potential offers considerable scope for tuning the position of band edges. For the majority spin channel, the transmission window of 0.1 V is entirely below the valence band maximum at a V_{GS} of -1 V, leading to a high-level majority spin current. However, at a V_{GS} of 1 V, there is an obvious downward shift in the band edges of 2H-VSe₂ by the gate potential, completely burying the transmission window in the bandgap. Therefore, the transport becomes limited with little tunneling current. In the minority spin channel, the half-metal characteristic results in a simultaneous shifting of the band edges with the gate potential. At a V_{GS} of 1 V, the transmission window is entirely above the conduction band minimum, leading to a high level of minority spin current. At a V_{GS} of -1 V, the transmission window is within the bandgap, resulting in a low minority spin tunneling current. It is clear that the transmission of spin current in the spin-FET can be extensively manipulated by the positions of the band edges relative to the bias window. There is a similar evolution of the SEE in all the TM/2H-VSe₂-based transistors, which can be controlled flexibly by the gate bias.

CONCLUSIONS

In conclusion, this study systematically investigated the

Figure 6 Spin-resolved PLDOS of a Ni/2H-VSe₂ transistor at a V_{DS} of 0.1 V with a V_{GS} of (a, b) 1 V and (c, d) -1 V, respectively. The color bar indicates the level of the electron density of the state.

spin-resolved electronic structure and carrier transport of TM/2H-VSe₂ under the vdW coupling effect. The vdW effects between the TM and the 2H-VSe₂ at the interfacial regions yield an indirect coupling of TM-Se-V. This can alter the electronic structure at the interfacial region with a universal reduction of the magnetic moment. Additionally, the SIE of TM/2H-VSe₂ was found to be significantly different from ordinary TMs/semiconductors. All of the TM/2H-VSe₂ systems exhibited consistent bias-dependent SIE evolution due to the domination of the half-metal characteristic of 2H-VSe₂. In particular, Co/2H-VSe₂ demonstrated the highest level of 79.4% in the positive bias with a simultaneous highest majority spin current of 666 mA mm⁻¹. Inspired by the bias-tunable SIE, a TM/2H-VSe₂-based spin-FET was proposed, which demonstrated excellent performance in terms of output current and SEE. The Co/2H-VSe₂ and Ni/2H-VSe₂-based spin-FETs exhibited outstanding current-driving capability with switching characteristics. Spin-polarized output currents of 2550 and 3117 mA mm⁻¹ with an SS of 108 and 106 mV dec⁻¹ were achieved for Co/2H-VSe₂ and Ni/2H-VSe₂, respectively. The SEE can be heavily and continuously tuned from 96% to -92% with gate bias. This study not only provides a deep insight into TM electrode contacts for the 2D magnetic half-metal 2H-VSe₂, but also demonstrates a high-performance spin-FET that sheds light on the way to future spintronic devices.

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Author contributions Zhu J and Zhang J proposed the idea and performed the calculations. Chen X, Shang W, Ning J and Wang D participated in this work and analyzed the data. Hao Y supervised the project.

Conflict of interest The authors declare that they have no conflict of interest.

Supplementary information Supporting data are available in the online version of the paper.

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二维磁性 VSe_2 与过渡金属的范德华接触及其高性能自旋场效应晶体管研究

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摘要 本文利用密度泛函理论和量子输运方法研究了过渡金属(TM): Fe、Co、Ni/ 2H-VSe_2 杂化纳米结构的界面耦合和自旋输运特性。由于TM-Se-V的间接耦合作用导致体系的磁矩明显减小且 2H-VSe_2 半金属特性消失, 所以预期的独立过渡金属、 VSe_2 的自旋过滤效果在接触区域变差。尽管如此, 所有基于TM/ 2H-VSe_2 的双端口器件仍呈现出一种有趣的偏压依赖自旋注入效率(SIE), 其中Co/ 2H-VSe_2 获得了非常可观的自旋输出电流: 高达 666 mA mm^{-1} 。进一步提出的基于过渡金属/ 2H-VSe_2 的自旋场效应晶体管表现出出色的性能。在基于Ni/ 2H-VSe_2 的晶体管中实现了非常高的自旋极化电流, 高达 3117 mA mm^{-1} , 器件同时还具有 106 mV dec^{-1} 的开关特性。更为重要的是, 所有晶体管在栅压的调控下, 实现了自旋抽取效率(SEE)从96%到-92%连续可调, 这些结果表明该器件有望应用于高性能自旋电子器件。