**CONDENSED MATTER PHYSICS**

**Monolayer 1T-NbSe\(_2\) as a 2D-correlated magnetic insulator**

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Monolayer group V transition metal dichalcogenides in their 1T phase have recently emerged as a platform to investigate rich phases of matter, such as spin liquid and ferromagnetism, resulting from strong electron correlations. Newly emerging 1T-NbSe\(_2\) has inspired theoretical investigations predicting collective phenomena such as charge transfer gap and ferromagnetism in two dimensions; however, the experimental evidence is still lacking. Here, by controlling the molecular beam epitaxy growth parameters, we demonstrate the successful growth of high-quality single-phase 1T-NbSe\(_2\). By combining scanning tunneling microscopy/spectroscopy and ab initio calculations, we show that this system is a charge transfer insulator with the upper Hubbard band located above the valence band maximum. To demonstrate the electron correlation resulted magnetic property, we create a vertical 1T/2H NbSe\(_2\) heterostructure, and we find unambiguous evidence of exchange interactions between the localized magnetic moments in 1T phase and the metallic/superconducting phase exemplified by Kondo resonances and Yu-Shiba-Rusinov–like bound states.

**INTRODUCTION**

Strong electron correlations underpin many unique phases of quantum matter, including unconventional superconductivity (1, 2), correlated insulator (3–6), magnetism (7, 8), spin liquids (8), and Wigner crystals (6, 9, 10). Recently, 1T phase group V transition metal dichalcogenides (TMDs) (MX\(_2\), with M = V, Nb, Ta; and X = S, Se) have emerged as an interesting platform to explore the charge transfer nature (9–11), magnetic properties (12–14), and magnetic insulator (15–17), in particular, Mott insulating state (17), charge density wave (CDW) (18–21), and magnetism (22–25), especially in the monolayer regime where electron screening is reduced. Among these exotic quantum phases, several outstanding questions remain; for example, (i) whether the insulating gap character is of Mott-Hubbard gap or charge transfer gap needs to be clarified; (ii) the associated magnetic property remain either under heavy debate, such as the ferromagnetism in 1T-VSe\(_2\) (23–25), or not experimentally verified, such as the quantum spin liquid state in 1T-TaSe\(_2\) (22).

Newly emerging is the 1T phase NbSe\(_2\) that does not occur naturally in bulk crystals (26), but it was found that monolayer 1T-NbSe\(_2\) can exist during molecular beam epitaxy (MBE) growth on graphene substrate (27). This discovery has stimulated many theoretical interests to explore whether correlated electronic phenomena exist in this phase. The calculations revealed that the correlated gap is of charge transfer nature (28–30), contrary to the previous assumed Mott-Hubbard gap (27, 31). Moreover, it is revealed that the interplay of a CDW and strong electron correlation could lead to the existence of ferromagnetism in monolayer 1T-NbSe\(_2\) (28, 29). These prior predictions make monolayer 1T-NbSe\(_2\) a unique platform to explore correlation-driven magnetic insulating states.

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Here, we report the controlled growth of pure 1T-NbSe\(_2\), pure 1H-NbSe\(_2\), and their mixed phases in the monolayer regime by fine-tuning the MBE parameters. We probe the electronic structure of monolayer 1T-NbSe\(_2\) using scanning tunneling microscopy/spectroscopy (STM/STS). By combining our spectroscopic data with Hubbard-corrected density functional theory (DFT) calculations, we show that the gap is of charge transfer nature. The localized upper Hubbard band (UHB) is located above the valence band maximum (VBM) and the lower Hubbard band (LHB) is found to merge with the valence band. Detailed orbital textures as a function of energy are mapped out and compare favorably with our theoretical calculations, demonstrating the energy-dependent spatial wave function distribution, especially the localization of UHB. We also find that the localized Hubbard band can be easily destroyed by point defects, indicating the fragility of UHB under disorder. To probe the magnetic states in 1T-NbSe\(_2\), we create a vertical heterostructure composed of monolayer 1T-NbSe\(_2\) on top of metallic/superconducting 2H-NbSe\(_2\). Our STS measurements on this heterostructure reveal Kondo resonances (32, 33) and Yu-Shiba-Rusinov (YSR)–like bound states (34–37), which are clear fingerprints of the exchange interaction between localized magnetic moments in 1T-NbSe\(_2\) and the electrons/Cooper pairs in 2H-NbSe\(_2\). In addition, the spatial modulation of Kondo peak amplitude correlates with the calculated spin density across the David star CDW, thus providing direct and unambiguous evidence for the existence of large localized magnetic moments driven by electron correlations.

**RESULTS**

**MBE growth and electronic structure of monolayer 1T-NbSe\(_2\)**

Bulk NbSe\(_2\) does not occur naturally in the 1T polymorph. Using MBE, we can achieve controlled growth of the 1T and 1H polymorphs of monolayer NbSe\(_2\) (Fig. 1, A and B) on both graphite and graphene substrates by changing the growth temperature and the Se-to-Nb flux ratio. Figure 1C shows the parameter space used to control the growth of monolayer NbSe\(_2\) on highly oriented pyrolytic graphite (HOPG) substrates. Note that in this parameter space, the
ties. A √ \sqrt{13} \times \sqrt{13} David star CDW is observed on 1T-NbSe 2 (Fig. 1G) in direct comparison between calculations and experiments allows us to identify the Γ point energy of the UHB and LHB, as indicated in Fig. 2 (B and E). Although the calculated bandgap is slightly larger than in the experiments (by ~0.1 eV), the calculated DOS shows good agreement with the experimental spectrum. The fact that UHB and LHB are spin-polarized and well separated from the Fermi level suggests the existence of a net magnetic moment and potential magnetic order. We will come back to this point in the section "Localized magnetic moment".

**Orbital texture mapping of 1T-NbSe 2**

We further probe the energy-dependent orbital textures to reveal the spatial wave function distribution, especially the localization of UHB, and compare the results with our calculations. We use a constant height mode to map the dI/dV image (Fig. 3, A to F). Previously, illustrated in Fig. 2C. The strong electron correlation opens a charge gap in the original half-filled band. The band pushed above the Fermi level is labeled as UHB, and the one below the Fermi level is labeled as LHB. The LHB is pushed low enough that it hybridizes with the valence band continuum. Note that these observations directly differ from the previous reported 0.4-eV gap in a Mott-Hubbard insulator scenario (27).

This interpretation is consistent with our DFT + U calculations. Shown in Fig. 2D is the band structure calculated with U = 2.95 eV. (See fig. S2 for the discussion of U value chosen.) In the calculation, the energy is referenced to the VBM with the UHB and LHB highlight in red and their spins in opposite directions. The UHB is nearly isolated and flat with a bandwidth of only 25 meV, while the LHB falls within the valence band continuum thus demonstrating the charge transfer character of this system. In addition, a few pronounced spectral peak features seen in the dI/dV spectrum (Fig. 2B) are also captured in the calculated DOS (Fig. 2E). A careful comparison between calculations and experiments allows us to identify the Γ point energy of the UHB and LHB, as indicated in Fig. 2 (B and E). Although the calculated bandgap is slightly larger than in the experiments (by ~0.1 eV), the calculated DOS shows good agreement with the experimental spectrum. The fact that UHB and LHB are spin-polarized and well separated from the Fermi level suggests the existence of a net magnetic moment and potential magnetic order. We will come back to this point in the section "Localized magnetic moment".

![Fig. 1. Growth parameter and structural characterization of monolayer NbSe 2.](image)

**Fig. 1. Growth parameter and structural characterization of monolayer NbSe 2.** (A and B) Schematic illustrations of 1T and 2H polymorphs of monolayer NbSe 2. The Nb (Se) atoms are shown in blue (yellow). The magenta lines in (A) outline the √ \sqrt{13} \times \sqrt{13} David star CDW in the 1T phase. (C) Growth parameter space for 1T and 1H NbSe 2 as a function of growth temperature and the Se-to-Nb flux ratio. Se-to-Nb flux ratio is varied under constant Se vapor pressure. (D) The reflection high-energy electron diffraction pattern of monolayer NbSe 2 on bilayer graphene/SiC substrate. (E and F) Large-scale topographic images of NbSe 2 flakes. (E) Single 1T phase on HOPG substrate. (F) Coexisting 1T and 1H phases on graphene substrate. (G and H) STM images of 1T-NbSe 2 and 1H-NbSe 2. The √ \sqrt{13} \times \sqrt{13} David star CDW unit cell is marked in (G); the 3×3 CDW unit cell is marked in (H).
Fig. 2. Charge transfer insulator nature of 1T-NbSe₂.
(A) Atomic-resolution topographic image of 1T-NbSe₂. The area enclosed by the blue dashed-dotted square is enlarged with an enhanced color contrast. The 1T-NbSe₂ lattice model superimposed on top is aligned with the atomic sites, and the white dashed arrows show the rotation of the CDW relative to the lattice. (B) dI/dV STS spectrum of 1T-NbSe₂. The UHB is above the insulating gap and relatively isolated from the conduction band continuum; the LHB is below the VBM and merged with the valence band continuum, as marked by the black arrows. DOS, density of states; a.u., arbitrary units. (C) Schematic illustration of energy levels for charge transfer insulator driven by electron correlation U. The green band represents the valence band continuum. (D) Calculated band structure of 1T-NbSe₂ in the $\sqrt{13} \times \sqrt{13}$ CDW ground state. The dashed and solid lines represent up and down spin bands, respectively. The UHB and LHB are highlighted in red. (E) Calculated DOS. The black arrows indicate the $\Gamma$ point energy of UHB and LHB.

Fig. 3. Orbital texture mapping of 1T-NbSe₂. (A to F) Constant-height dI/dV images of 1T-NbSe₂ at different biases showing energy-dependent orbital textures. The calculated charge density distributions are overlaid on the left half of each dI/dV image. Extended information on DFT-calculated maximum and minimum charge densities can be found in table S1. Energies at which calculations are performed: (A) $E_{\text{VBM}} - 0.25$ eV; (B) $E_{\text{VBM}} - 0.65$ eV; (C) $E_{\text{UHB}}$; (D) $E_{\text{UHB}} + 0.25$ eV; (E) $E_{\text{UHB}} + 0.45$ eV; (F) $E_{\text{UHB}} + 0.7$ eV. $E_{\text{VBM}}$ and $E_{\text{UHB}}$ refer to the energies of VBM and UHB, respectively.

this mode has been shown to reflect the orbital texture better than the constant current dI/dV image (38, 39) because constant current dI/dV mode is subjected to a convolution effect due to the modulation of absolute tip-to-sample distance. A detailed comparison and discussion between these two modes can be found in fig. S3. The calculated charge density distribution is superimposed to the STM image (Fig. 3, A to F) and is consistent with the experimental map. Among the valence band, the orbital textures show similar features;
thus, we only show two energies here (Fig. 3 A and B). The $dI/dV$ images follow the symmetry of the David star CDW with most charge density concentrated on the center of each star (Fig. 3 A and B). A richer orbital texture is found in the conduction band. The orbital texture corresponding to the UHB energy (Fig. 3C) is strongly localized around the central Nb atom. This localization is consistent with the very small bandwidth of the UHB (Fig. 2D). At higher energies, the orbital texture appears to be smeared out (Fig. 3D), and it gradually evolves to become delocalized, forming mesh structures and connecting with other David stars (Fig. 3, E and F), in line with the dispersive nature expected of states in the conduction band continuum. Good agreement in the orbital texture mapping and the theoretical calculation over an extended energy range strongly support the conclusion that the gap is of charge transfer nature, as predicted by the theory. Note that this conclusion differs from a recent report (31).

The fragility of UHB at local defect positions

To gain more insight into the properties of the Hubbard band and its localized charge distribution, we investigate the impact of point defects. Shown in Fig. 4A are two defects most commonly observed and naturally formed in 1T-NbSe$_2$. We label these defects as type I and type II on the basis of the morphology of their associated CDW. The type I defect appears as a weakened CDW spot, while the type II defect appears as a missing CDW spot. In direct contrast to the $dI/dV$ spectra on pristine 1T-NbSe$_2$ (Figs. 4B and 2B), the $dI/dV$ spectra on type I and type II defects (Fig. 4, C and D) miss the UHB feature. As a result, the insulating gap at these defects’ positions is much wider, reaching up to about 0.45 eV. As previously reported, the most commonly formed defects in TMDs are either a metal atom vacancy or a chalcogen atom vacancy (40). From the discussion in Figs. 2 and 3, we know that the UHB is strongly localized on the central Nb atom of the David star in pristine 1T-NbSe$_2$; therefore, we hypothesize that a missing David star feature may be associated with a missing central Nb atom. We theoretically choose a Nb atom vacancy model (see fig. S5 for more details) to simulate type II defects. The calculated DOS of this model (Fig. 4E) shows the disappearance of the UHB, consistent with our experimental observation. While a more thorough exploration of point defects in 1T-NbSe$_2$ is warranted, this model confirms the crucial role of the central Nb atom. Putting together the information gathered so far on pristine and defective 1T-NbSe$_2$, we demonstrate the significance of the crystallinity and infer that the David star is crucially linked with the spin-polarized electron density around the central Nb atom and is very sensitive to the local bonding environment.

Localized magnetic moment

Our spin-polarized DFT calculation has a free energy that is 57 meV per David star lower than the spin-nonpolarized case, indicating a magnetic ground state. To explore the localized magnetic moments in 1T-NbSe$_2$, we couple them with an itinerant electron bath by creating 1T-NbSe$_2$/2H-NbSe$_2$ vertical heterostructures following the approach of Bischoff et al. (41). A schematic illustration is shown in Fig. 5A, and the STM image of the heterostructure is shown in

![Fig. 4. The fragility of UHB at local defect positions. (A) Two types of common defects in 1T-NbSe$_2$. Type I defects label weakened CDW spot. Type II defects label missing CDW spot. (B to D) Typical $dI/dV$ spectra taken at pristine CDW and type I and type II defects. In contrast to pristine CDW, $dI/dV$ spectra on type I and type II defects show missing UHB. (E) Calculated DOS for Nb vacancy model (orange lines) and pristine CDW (black lines). The dash and solid lines represent the up and down spin bands, respectively. The spin-polarized UHB appears in the pristine CDW but is missing in the Nb vacancy model.](image-url)
Fig. 5B. Detailed information of the 1T/2H heterostructure including the formation mechanism can be found in fig. S6. The coupling between the conduction electrons in 2H-NbSe$_2$ and the magnetic moment in 1T-NbSe$_2$ was manifested by the Kondo effect. (B) STM image on the heterostructure surface showing the CDW of 1T-NbSe$_2$. (C) False-color images of dI/dV spectra taken along the red line in (B). A periodic modulation of the Kondo peak amplitude was observed, and the two maxima marked by the red and black arrows correspond to the CDW centers. (D) Calculated spin density distribution in unit of $a_0^3$, where $a_0$ is the Bohr radius. The red and black arrows mark the CDW centers. (E) Selected dI/dV spectra from (C) (index numbers #4, #7, and #10). Their positions are marked in (B) with the corresponding colors. (F) dI/dV spectra with finer energy resolution on the heterostructure surface demonstrate the coexistence of YSR bound state and the Kondo resonance (red and dark blue lines); $\varepsilon_b$ labels the binding energy of the YSR states. For comparison, the dark yellow line plots the dI/dV spectrum taken on pristine bulk 2H-NbSe$_2$, which exhibits superconductivity; $\Delta$ labels the superconducting gap.

Fig. 5. Localized magnetic moment in 1T-NbSe$_2$. (A) Schematics of vertical heterostructure formed by monolayer 1T-NbSe$_2$ on bulk 2H-NbSe$_2$. The height profile in red represents the 1T-NbSe$_2$ CDW. Each unit cell carries a net magnetic moment illustrated by a white arrow, and their directions are artificially set to be parallel. The coupling between the conduction electrons in 2H-NbSe$_2$ and the magnetic moment in 1T-NbSe$_2$ was manifested by the Kondo effect. (B) STM image on the heterostructure surface showing the CDW of 1T-NbSe$_2$. (C) False-color images of dI/dV spectra taken along the red line in (B). A periodic modulation of the Kondo peak amplitude was observed, and the two maxima marked by the red and black arrows correspond to the CDW centers. (D) Calculated spin density distribution in unit of $a_0^3$, where $a_0$ is the Bohr radius. The red and black arrows mark the CDW centers. (E) Selected dI/dV spectra from (C) (index numbers #4, #7, and #10). Their positions are marked in (B) with the corresponding colors. (F) dI/dV spectra with finer energy resolution on the heterostructure surface demonstrate the coexistence of YSR bound state and the Kondo resonance (red and dark blue lines); $\varepsilon_b$ labels the binding energy of the YSR states. For comparison, the dark yellow line plots the dI/dV spectrum taken on pristine bulk 2H-NbSe$_2$, which exhibits superconductivity; $\Delta$ labels the superconducting gap.

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Fig. 5F, we show two representative spectra acquired on the 1T phase, along with the superconducting gap observed on the neighboring 2H phase. In the 1T region, multiple YSR-like bound states appear superimposed to the Kondo resonance background, thus demonstrating the interplay between Kondo physics and superconductivity (37, 43–45). Note that the broader Kondo width compared to the bound state binding energy indicates a regime of “spin-screen” (37, 46, 47), in which Kondo resonance and bound state coexist. Extended discussion can be found in the Supplementary Materials. While the binding energies of these bound states and the electron-hole spectral weight asymmetry depend on the microscopic details of the exchange interaction, Coulomb repulsion, and superconducting pairing (43, 48–50) and certainly deserve a separate investigation, our current measurements provide additional strong evidence for the localized magnetic moments in 1T-NbSe₂.

DISCUSSION

In this work, we have achieved a controlled growth of monolayer single-phase 1T-NbSe₂ on both graphite and bilayer graphene/SiC substrates, and we demonstrated that this new system is a charge transfer insulator. We find a nondispersive UHB associated with the central Nb atom of the Davidson star resulting from the $\sqrt{13} \times \sqrt{13}$ CDW reconstruction, and we show that this feature is very sensitive to the local bonding environment, demonstrating the essential role of crystallinity when revealing its intrinsic property. Further experiments such as in situ atomic force microscopy are needed to address more specific characters of defects. By fabricating insulator/superconductor heterostructures of 1T and 2H NbSe₂, we provide direct and unambiguous evidence for localized magnetic moments via the observation of Kondo resonances and YSR-like bound states. Note that the interlayer coupling between the 1T and 2H NbSe₂ may alter the inter-David star exchange interaction, and as a result, the long-range magnetic order in the 1T/2H NbSe₂ may be different from a suspended monolayer 1T-NbSe₂; thus, further investigations are needed to conclude whether long-range magnetic order exists in the monolayer 1T-NbSe₂. Having demonstrated the controlled growth and orbital texture mapping of pure phases of 1T-NbSe₂ and 2H-NbSe₂ as well as their mixed phases and heterostructures, we believe that NbSe₂ now offers a uniquely versatile platform to investigate the interplay of charge, spin, and lattice degrees of freedoms in two dimensions, as well as to advance our understanding of magnetism and superconductivity in atomically thin crystals.

MATERIALS AND METHODS

Sample growth and STM/STS measurements

Monolayer 1T-NbSe₂ was grown in a home-built MBE chamber with base pressure at $\sim 10^{-10}$ torr. High-purity Nb (99.99%) and high-purity Se (99.999%) were evaporated from an e-beam evaporator and a standard Knudsen cell, respectively. The flux ratio was determined using crystal monitor. Samples were transferred from MBE into STM, base pressure $\sim 10^{-11}$ torr, through a transfer vessel, base pressure $\sim 10^{-10}$ torr, to maintain the perfect crystallinity of the film. STM/STS measurements were conducted at 4.3 K except for the measurements of Kondo and YSR bound states, which were performed at 0.35 K. The W tip was prepared by an electrochemically etched W tip treated with in situ electron beam cleaning. STM $dI/dV$ spectra were measured using a standard lock-in technique with feedback loop off, whose modulation frequency is 490 Hz. Constant height $dI/dV$ mappings were performed with feedback loop open.

DFT calculations

DFT calculations are performed in the Quantum ESPRESSO software package (51). The Perdew-Burke-Ernzerhof (PBE) exchange correlation function is used to approximate the exchange and correlation energy (52). Nb and Se self relativistic optimally norm-conserving Vanderbilt pseudopotentials from the PseudoDojo repository are used (53). On-site correlation on the Nb-4d states is treated by performing DFT + U calculations including spin polarization (54). A plane wave energy cutoff of 120 rydberg (Ry), a charge density cutoff of 480 Ry, a $\Gamma$-centered $4 \times 4 \times 1$ k-point integration grid, and 20 Å of vacuum are used to converge the total energy of the cell. The $\sqrt{13} \times \sqrt{13}$ CDW phase unit cell of 1T-NbSe₂ is generated by distorting the Nb atoms toward their respective David star centers and relaxing the forces on each atom to below $1 \times 10^{-7}$ Ry/bohr. Densities of states, orbital textures, and the spin-charge density are calculated non-self consistently on a $16 \times 16 \times 1$ Gamma-centered k-point integration grid. Gaussian broadening factors of 50 and 25 meV are used in Figs. 2E and 4E, respectively.

SUPPLEMENTARY MATERIALS

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