Layered transition metal dichalcogenides (TMDCs) host various electronic, structural, and transport phenomena making them most promising candidates for applications in electronic devices. Among the many novel states, the charge density wave (CDW) phase in these compounds is particularly under scrutiny as it is neighbor to superconductivity in the phase diagrams. In terms of electronic structure, the CDW phase is usually linked to Fermi surface nesting with opening of a gap at specific portion of the Fermi surface connected by the CDW wave vector. In response, atoms move from their original positions forming a superstructure that can be visualized through a scanning tunneling electron microscopy (STM) experiment. Of all TMDCs, 1T-VSe₂ is a special example due to its long wavelength 3D CDW phase in the bulk. It undergoes an incommensurate CDW with 4a x 4a x 3.18c periodic lattice distortion around Tᵣ = 110 K, followed by a second transition to a commensurate CDW state around 80 K. On the other hand, CDW-phase on the electronic structure is anomalously supported by angle resolved photoemission spectroscopy (ARPES) studies. Such as, CDW induced gap has been reported around the M-point of the Fermi surface as a shift of a secondary peak while a spectral intensity suppression at the Fermi level is absent. This appeared to be a well-established way of measuring the CDW induced gap in the bulk 1T-VSe₂ samples. Furthermore, a recent STM study also reported a gap at the Fermi surface which is found to be more pronounced around the Γ-point. However, this observation should not be correlated with the structural transition since the Γ-point is not along the CDW wave vector. The results are even more elusive in the monolayer VSe₂ samples. First, fully gaped Fermi surface claimed to be reported by multiple studies. Such observation is unlikely to be due to the CDW phase because CDW wave vector clearly has no influence in that case. Second, monolayer samples seem to have a larger CDW induced gap (~100 meV) with a higher Tᵣ. On the other hand, experimental band structures do not exhibit any signature of back-bending to support such a large energy gap in contrast to the computational models. Here, we re-evaluate some of the main results reported on 1T-VSe₂ by performing a detailed ARPES experiment and rule out the earlier CDW related claims point by point. The Fermi surface of 1T-VSe₂ contains multiple bands, not previously detected and they have different in-plane and out-plane dispersion. Thereby, the previous observations that are attributed to the CDW phase are due to the lack of resolving these bands. In this regard, the previous theoretical models and experimental observations cannot be assigned to the CDW phase and the impact of structural distortion on the electronic structure requires further characterizations and approaches. But, new observations provide more detailed electronic structure that can guide future studies as well as suggesting the revision of the various other studies regarding electronic properties of 1T-VSe₂.
The experimental electronic structure of 1T-VSe₂ bulk samples is studied by using linear horizontal (LH) and linear vertical (LV) polarized lights in Figure 1(b-e), respectively. In the LH geometry, apparent ellipsoidal electron pockets centered at \(\overline{M}-\overline{\Gamma}\)-points are the main features of the Fermi surface while highly dispersive Se 4p atomic orbitals dominate the zone center (Figure 1d). The corresponding ARPES map along the \(\overline{M}-\overline{\Gamma}-\overline{M'}\) direction exhibits V-3d atomic orbitals with nearly flat dispersion in the vicinity of the \(\overline{\Gamma}\)-point where it overlaps with Se 4p atomic orbitals (Figure 1d). Overall band structure obtained for this particular experimental geometry is consistent with the computed one as well as the earlier ARPES reports [14, 17, 22, 24].

On the other hand, the same band structure taken with LV polarized light reveals differences in details. The zone center exhibits a point like dispersion enabling to study the band structure around the \(\overline{\Gamma}\)-point more precisely. Unlike the single band observed with LH polarized light, three bands called \(\alpha\), \(\beta\), and \(\gamma\) are now resolved around the zone center (Figure 1e). The first two bands are crossing the Fermi level at \(k_\|=-0.37\ \text{Å}^{-1}\) and at \(k_\perp=-0.24\ \text{Å}^{-1}\) while the third band is located just below the Fermi level displaying a flatter dispersion towards \(\overline{\Gamma}\)-point. These additional states are not predicted in the band structure calculation reported here or elsewhere [14, 17, 22, 24]. Implication of the new findings in terms of CDW induced gap is that if a band is located just below the Fermi level, temperature induced lifetime broadening can always lead to a determination of a false gap. This is likely to be the case for a recent STM study that reports a prominent gap in the vicinity of the \(\overline{\Gamma}\)-point [16]. Furthermore, these multiple bands are main characteristics of the material and can be resolved below and above the \(T^*\) showing that they are not due to the structural distortion (Figure 1c and Supplementary Materials Figure S1(a-b)).

By using this new finding, one can reproduce a data appear to host a temperature dependent gap at the Fermi level. The EDCs crossing the \(\alpha\) and \(\beta\) bands at the Fermi level and momentum point across the \(\gamma\) band are given in Figure 1(f) for two temperatures; 10 K (below \(T^*\) and 160 K (above \(T^*\)). Third one has a natural gap since the band is located below the Fermi level and the second one clearly shows no evidence of a CDW gap. However, first one appears to experiencing a shift towards higher binding energy at a lower temperature (marked with blue and red vertical lines in Figure 1(f)). Such shift commonly attributed to the a gap opening in this material [12, 13, 15]. But, spectral intensity at the Fermi level does not show prominent temperature dependence. This apparent shift is due to the \(\beta\) band being located just below the \(\alpha\) band. And, temperature induced lifetime broadening leads them to overlap more in energy. This appears in the band structure as if a band is shifting in energy with temperature. Thereby, lack of the resolving these bands in the earlier studies leads to misinterpreting the experimental data. Indeed, this should have been realized since the vicinity of the \(\overline{\Gamma}\)-point is not along the CDW-wave vector and hence is not expected to be gaped.

Furthermore, the modulation of the color contrast on the electronic structure figures is relied on as a signature of a gap opening at the Fermi level [13, 14]. Here, we repeat a similar experiment. Figure 2(a) presents the Fermi surface that covers the ellipsoidal electron pocket centered at the \(\overline{M}\)-point. Color-contrast is gradually de-
FIG. 2. (a) The Fermi surface is recorded with 93 eV LH polarized lights. (b-c) ARPES maps taken along the dashed black line in (a) and $K - M - K'$, respectively. (d) MDCs were taken at the Fermi level from (b-c). (e) EDCs taken along the dashed black and orange lines in (b-c). Vertical black and orange lines in (e) mark the high intensity points. (f-g) ARPES maps along the $M - M'$ direction taken with 101 eV LH and LV polarized lights, respectively. All data are collected at 10 K.

Increasing towards $M$-point as consistent with the earlier studies. In this regard, one can claim a possible gap opening at the Brillouin zone boundaries. To check if this is the case, a logical experimental approach will be comparing the Fermi edges taken from the different portions of the Fermi surface recorded below $T^*$. In this way, possible experimental errors induced by variable temperature can also be avoided. Thus, ARPES maps taken along the dashed black line in Figure 2(a) and the $K - M - K'$ direction are given in Figure 2(b-c), respectively. Compared to the former one, the latter exhibits lower spectral intensity in the entire band structure rather than only at the Fermi level. Therefore, the apparent spectral intensity does not necessarily represent a gap opening.

The MDCs taken at the Fermi level of Figure 2(b-c) are compared in Figure 2(d) to find out the origin of this spectral intensity modulation. The one along the $K - M - K'$ direction exhibits a broader line shape compared to the other one. Therefore, the lower intensity around $M$ of the Fermi surface is not due to the gap opening but it is caused by a broader electronic structure in momentum space. Furthermore, the EDCs taken along the dashed black line in Figure 2(b) and the dashed orange line in Figure 2(c) are given in Figure 2(e). They exhibit the same Fermi level indicating the absence of an insulating gap. On the other hand, the high intensity points show a difference in the EDCs (vertical orange and black lines in Figure 2(e)). This apparent shift has been considered as well-established experimental signature of the CDW induced gap in VSe$_2$. Indicated existence of multiple bands located in close proximity to each other rather than a gap opening. Therefore, the Fermi surface is expected to be dominated at least two bands in contrast to the previous experiments and computations.

Above argument is experimentally confirmed by analysing the various ARPES maps parallel to $K - M - K'$. Around $M$-point a V-shape band is crossing the Fermi level at $k_z = \pm 0.32 \text{ Å}$ (Figure 3(b)). However, band splitting towards zone center can be seen in Figure 3(c-e) as marked with blue arrows. These additional bands eventually connect with the neighbor electron pockets (Figure 3(f-g)).

Multiple bands can be also probed in the band structure along the $K - M - K'$ with more elaborate approach. Fermi surfaces taken at various photon energies are given in Figure 4(a). In the data, 80 eV and 97 eV photons correspond to $k_z = A$ and $k_z = \Gamma$, respectively, in the Brillouin zone. Ellipsoidal pocket centered at $M$-point shows a strong photon energy dependence and it resembles more like a dog-bone at $k_z = \Gamma$. In addition to this strong spectral feature, second band with a weaker intensity can be also visually observed in some parts of the Fermi surface. These multiple bands can be seen in ARPES maps along $K - M - K'$ as marked with dashed yellow and black lines (Figure 4(b)).

To further support this observation, the MDCs taken at the Fermi level are compared in Figure 4(c). Bands located at $\pm k_z$ with respect to $M$-point exhibit double peak features as indicated with yellow and black fitting lines. Thereby, the V-shape conduction band is indeed formed by two bands as inner and outer ones. Based on Figure 3(b-c), these two bands have distinct $k_z$ disper-
FIG. 4. (a-b) The Fermi surfaces and corresponding ARPES maps along $\overline{K} - \overline{M} - \overline{K}'$ direction. (c) MDCs taken at the Fermi level from each spectrum. Orange and black lines in (c) are the Lorentzian peak fittings and dashed lines in (c) are sum of fittings.

As the outer band is 2D like while the inner one has 3D character and their spectral intensities show an opposite $k_z$ dependence. This has an important implication for the CDW phase of the VSe$_2$. One of the fundamental experimental evidence for the CDW phase was reported to be a warping effect on the Fermi surface along the $k_z$ direction [13, 14, 22]. However, this warping effect is clearly due to the different nature of these multiple bands crossing the Fermi level and not correlated with any type of structural distortion. Indeed, the apparent warping of the band structure is temperature independent (Supplementary Materials SFigure 2). Therefore, earlier observations are due to the lack of resolving multiple bands leading to misinterpretation of the experimental data.

In summary, unlike the earlier studies, we show that the Fermi surface of VSe$_2$ is dominated by multiple bands. By using this, each of the previous observation can be explained and shown to be not related to any structural distortion. These new findings need to be considered in order to understand the correct nature of the CDW phase and find the structural distortion induced modification on the electronic structure. Furthermore, these realization also suggest that the large CDW induced gap of 100 meV in the monolayer VSe$_2$ is questionable [17–19]. This is discussed in the Supplementary Materials SFigure 3 and no gap is deducted around the $\overline{M}$-point that can be associated with CDW phase. Furthermore, the apparent width of the Fermi edge around the $\overline{M}$-point does not change with the temperature in the monolayer case. This indicates that it is dominated by the temperature independent defects such as vacancies which leads misinterpretation of the data. All these new findings need to be considered in the future studies and they are probably the main reason for why the mechanism behind the 3D charge density wave phase in VSe$_2$ has never been understood.

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