Unconventional superconductivity in cuprates, pnictides, and heavy fermions often reaches its optimum value near the quantum critical point (QCP) of a magnetic groundstate, providing a perspective that critical phase fluctuations of the intertwined electronic order drive unconventional superconductivity. However, looking back at conventional superconductors, superconducting (SC) dome is not an unfamiliar feature. It has been observed in Li metal under pressure, doped SrTiO$_3$, gated LaAlO$_3$/SrTiO$_3$ (LAO/STO) interface, pressure tunned Fe metal, and also in $T$Se$_2$ ($T$=Ti, Ta and Nb) families, and more recently in thin flake of MoS$_2$. More interestingly, no evidence of an intertwined electronic order in the SC state is reported in these materials, except in TSe$_2$. The possible role of charge density wave (CDW) in the SC dome in the latter family has also recently been called into question by a pressure dependent x-ray scattering measurement because the QCP of CDW in 1T-TiSe$_2$ lies at a higher pressure than the termination of the SC dome. Therefore the presence of a SC dome with and without an intervening QCP leads to the fundamental question: Can there be an alternative and universal origin of the SC dome which is applicable to all families of superconductors?

We explore the possible role of the momentum dependent density fluctuations (MRDF) in renormalizing the electronic pairing strength and thereby producing optimized SC transition temperature ($T_c$) as a function of doping. Spin and charge fluctuations are among the two dominant electron-electron (EE) correlations which are ubiquitous in weakly to strongly correlated materials, irrespective of the formation of a static electronic order. These fluctuations renormalize the quasiparticle states, which in turn renormalizes the electron-phonon (EP) or more appropriately quasiparticle-phonon coupling strength and vice versa. In this work, we present a self-consistent theory for the combined EE and EP interaction to calculate the electronic self-energy for the band renormalization, the renormalized EP coupling spectral function $\alpha^2 F$, and $T_c$ (see Fig. 1 for these results in MoS$_2$), starting from the materials specific first-principles band structures. We find that the interplay between the EE and EP coupling has a common role in reproducing the SC dome as a function of doping in both MoS$_2$ and TiSe$_2$ samples.

Formalism:- We calculate the electronic self-energy due to...
all three interactions within the MRDF method[14,16]
\[
\Sigma_{mn}(k, \omega) = \frac{1}{\Omega_{BZ}} \sum_{q,\nu} \int_{-\infty}^{\infty} d\omega_p V_{mn}^\nu(q, \omega_p) \Gamma_{mn}^\nu(k, q)
\times \left[ \frac{1 - f^{\nu}_{k-q} + n_p}{\omega + i\delta - \xi^{\nu}_{k-q} - \omega_p} + \frac{f^{\nu}_{k-q} + n_p}{\omega + i\delta - \xi^{\nu}_{k-q} + \omega_p} \right].
\]

Here \(k\) and \(\omega\) are the quasiparticle momentum and frequency, and \(q\) and \(\omega_p\) are the bosonic excitation momentum and frequency, respectively. \(m, n, s, \) and \(t\) are the orbital indices, and \(\nu\) is the quasiparticle band index. \(\Omega_{BZ}\) is the electronic phase space volume. \(f^{\nu}_{k-q}\) and \(n_p\) are the fermion and boson occupation numbers, and \(\xi^{\nu}_{k-q}\) is the corresponding DFT band. The vertex correction \(\Gamma_{mn}^\nu(k, q)\) encodes both the angular and dynamical parts of the vertex, which are combined to obtain \(\Gamma_{mn,s}^\nu(k, q) = \phi_{k-q}^{\nu} \phi_{k}^{\nu} \delta E_{k}^{\nu} (1 - \partial \Sigma_{mn}(k - q, \omega)/\partial \omega)|_0\), where \(\phi\) is the DFT eigenvector. \(V_{mn}^\nu(q, \omega_p)\) is the fluctuation-exchange potential generated by EE and EP interactions. For the EE part, we include both spin and charge fluctuations which give \(V_{mn}^\nu(q, \omega_p) = \langle \eta_i/2 | \hat{U}_{\nu} \hat{\Sigma}^\nu_i(k, \omega_p) \hat{U}_{\nu}^\dagger \rangle_{\text{DFT}}\), where \(i\) stands for spin and charge components with \(\eta_i = 3, 1, \) respectively. \(\hat{U}\) are the Coulomb interaction matrices.[18] defined in the orbital basis, which includes intra-, inter-orbital onsite Coulomb terms, and also Hund’s coupling and pair exchange interactions.[16] \(\hat{\Sigma}\) are the spin and charge many-body susceptibilities computed within the random-phase approximation.[16] For the EP potential, we use \(V_{mn}^\nu(q, \omega_p) = \sum_k |g_{mn}^{\nu}(k, q)|^2 \delta E_{k}^{\nu} \delta_{\eta_1, \eta_2}, \) where \(\omega_{\eta_1}\) are the phonon dispersion for band \(\mu\). The EP coupling matrix-element is \(\delta_{ij}^{\nu}(k, q) = \sum_{\eta_1, \eta_2} g_{ij}^{\nu, \eta_1, \eta_2}(k, q) \delta_{\eta_1, \eta_2} \delta E_{\eta_1}^{\nu} \delta_{\eta_2}^{\nu} \delta_{\eta_1, \eta_2}, \) where the \(k\)-averaged EP scattering amplitude \(g_{ij}^{\nu}\) is deduced from the first-principles calculation.[20] Finally, the self-energy dressed Green’s function becomes \(\check{G}^{-1} = \check{G}_0^{-1} - \hat{\Sigma}\), where \(\Sigma\) is the total self-energy matrix \(\Sigma_{mn} = \Sigma_{mn,s} + \Sigma_{mn,c} + \Sigma_{mn,p}.\) We compute all self-energies self-consistently, until the total self-energy converges, as described in Refs. [14,16,17,21].

Results: Electronic and phonon bandstructure calculations[17] are carried out using the plane wave DFT package VASP [40] within the local density approximation (LDA) [39]. For MoS\(_2\), SC is observed in a thin flake sample. To simulate thin flake sample, we use band structure for the bilayer MoS\(_2\) (see Fig. 2(a)), because the band structure of monolayer is significantly different from bilayer, but from bilayer to the bulk material, it does not change characteristic.[47,48] Moreover, LDA+GW calculation showed that while the band gap is reduced here, but the actual dispersion does not change characteristically with respect to its LDA one for the conduction band.[17,43] We use a rigid band shift for the LDA dispersion,[26] whereas with self-energy correction, the new Fermi level \((E_F)\) is recalculated self-consistently at each doping. We directly implement the DFT band structure and phonon spectrum into the calculations of self-energy and superconductivity. In the band insulator MoS\(_2\) at \(x=0\), susceptibility is fully gapped below the particle-hole continuum, and thus no significant renormalization arises. At finite doping, as shown for optimal doping \(x=0.1\) in Figs. 2(b-c), several new dynamical excitation channels arise at low-energy, mainly dominated by the intraband transitions across \(E_F\). The spin channel moves to lower energy than the charge one, and possess larger intensity, giving largest contribution to the many-body renormalization effect.

We show the doping evolution of all three correlation functions by computing the \(k\)- and orbital averaged correlation spectrum, commonly known as
\[ \alpha^2 F_i(\omega_p) = 1/\Omega_{\text{BZ}} \sum_{\mathbf{q}} \text{Tr}[\hat{V}_i(\mathbf{q}, \omega_p)], \] for the two electronic correlations. The same for the EP coupling \[ \alpha^2 F_p(\omega_p) = 1/(\Omega_{\text{BZ}} N(0)) \sum_{\mathbf{k},\mathbf{q}} \text{Tr}[\hat{V}_p(\mathbf{q}, \omega_p)] \delta(\xi_{\mathbf{k}}) \delta(\xi_{\mathbf{k}+\mathbf{q}}), \] where \( N(0) \) is the correlated density of states (DOS) at \( E_F \), and the self-energy dressed quasiparticle band is \( \xi_{\mathbf{k}}^{\ast} = \xi_{\mathbf{k}} + \Sigma_{\mathbf{k}}^{\ast}(\xi_{\mathbf{k}}). \]

In Fig. 2(d), the total electronic (spin + charge) \( \alpha^2 F \) is plotted for several dopings. We find several dominant peaks at all dopings, except at \( x = 0 \), whose strength increases with doping, suggesting that the strength of the EE correlation gradually increases with doping. On the other hand, the EP \( \alpha^2 F \), shown in Fig. 2(e), shows maximum intensity at \( x = 0.1 \). Interestingly, the EP \( \alpha^2 F \) without including EE interaction in the electronic spectrum (dashd lines) shows fairly doping independent behavior from underdoped to the optimally doped region. The resulting EP coupling constant, \( \lambda = 2 \int d\omega_p \alpha^2 F_p(\omega_p)/\omega_p \), exhibits a dome feature with doping as shown in the inset to Fig. 1.

In Fig. 3, we present the electronic self-energy and the dressed DOS for MoS\(_2\). The self-energy is presented for the lowest energy band which crosses \( E_F \), and possess largest renormalization. The corresponding \( (k\text{-averaged}) \) mass renormalization factor \( m^*/m_b = (1 - \partial \Sigma(\omega)/\partial \omega)^{-1} \) (where \( m_b \) is the DFT band mass) is shown in Fig. 1. As expected, the electronic \( \Sigma \) is very weak at \( x=0 \). At finite doping, the intra-band excitations provide large mass enhancements, reaching a value above 2 at optimal to overdoped region. The EP contribution, shown in Figs. 3(c-d) remains comparatively weak throughout the phase diagram, however, reaches a maximum value near the optimal doping. Both EE and EP self-energies show strong particle-hole asymmetry due to the semimetallic-like band structure of this system. The imaginary part of the self-energy, \( \Sigma'' \), possesses multiple low-energy peaks, coming from several collective modes in the susceptibility discussed in Fig. 2. Due to causality, the real part of self-energy, \( \Sigma' \) sharply changes slope at energies where \( \Sigma'' \) has peaks.

The self-energy splits the non-interacting DOS into a low-energy quasiparticle peak, and a higher-energy incoherent satellite (or hump) feature as seen in the \( \Sigma \)-dressed DOS in Fig. 3(e). This unique self-energy behavior, creating a peak-dip-hump feature, is also observed in cuprates and actinides superconductors. Although, EP self-energy possess similar energy dependence, however, it fails to create any accountable peak-dip-hump feature in this system due to its weak strength. The spectral weight transfer from the higher energy states to the quasiparticle states at \( E_F \), dictated by the strength of the self-energy effects, can be deduced by the change in DOS between the interacting case (red filled symbol) and non-interacting DOS (blue open circles). This doping dependence of the EE interaction plays a dominant role in creating the dome-like doping dependence of \( T_c \), shown in Fig. 1.

We estimate the value of \( T_c \) from the renormalized EP \( \alpha^2 F \) by using the standard Allen-Dynes formula given in Ref. 28. The so-called Debye frequency, which is modified to a renormalized value as \( \omega_{\text{log}} = \exp [2/\lambda \int d\omega_p \alpha^2 F(\omega_p) \log (\omega_p)/\omega_p], \) does not show any significant doping dependence. Similarly, the renormalized screened Coulomb potential \( \mu^c = \mu^c_0/[1 + \log (U/\omega_{\text{log}})] \) also does not possess any significant doping dependence for the constant value of \( \mu^c_0 \) and onsite Coulomb potential \( U \).

In Fig. 3(a), we present our results of \( T_c \) at optimal to overdoped region. For both materi-
als, using this formula, we find that theoretical estimation of \( T_c \) quantitatively reproduces the experimental dome when both EE and EP interactions are self-consistently included in the renormalization term. When EE interaction is neglected, but the EP self-energy is included in the renormalized \( \alpha^2 F \) spectrum, the calculation overestimates the experimental \( T_c \) in the entire phase diagram (also see calculations of EP coupling induced \( T_c \) in MoS\(_2\) without including its renormalization in Refs. 30 and 31).

Next we study the origin of SC dome in TiSe\(_2\). In Fig. 4(a) we present our results of \( T_c \), calculated for the case...
FIG. 4. (Color online) (a) SC phase diagram of TiSe$_2$. Blue squares are $T_c$, where blue triangles are $T_{\text{CDW}}$ (×10) from Ref. [6]. Red filled and green open circles give computed $T_c$ for the cases of EE+EP, and EP only respectively, but without CDW. Black open circles give $T_c$ when CDW and EE+EP interactions are all self-consistently included. Magenta filled, cyan open and yellow open triangles give the computed mass enhancement for the three cases discussed above. Light blue shading is guide to eyes to the experimental SC dome behavior. (b) DFT band structure in the 3D momentum space (along high-symmetry directions). Different horizontal dashed lines give $E_F$ for $x$=0, 0.04, 0.08 and 0.12 with increasing values. (c) EP coupling constant for the three cases as discussed in (a) with same symbols. (d) DOS at $E_F$ for bare (blue open triangles), with only EP interaction (green open circles), with EE and EP interactions (red filled circles) and with CDW (×4 yellow open circles). Light blue shading is the theoretical $T_c$ in arbitrary unit.

of EP, EE + EP, and with CDW and EE + EP interactions. We include CDW at nesting $Q=$(1/2,1/2) as demonstrated experimentally [12] and the mean-field CDW gap is taken to be $\Delta = 13.4 k_B T_{\text{CDW}}$ at various dopings, which reasonably reproduces the experimental gap [32]. The self-energy properties and the peak-dip-hump feature in the DOS are all characteristically analogous to MoS$_2$. Moreover, in TiSe$_2$ the spin-component dominates the fluctuation strength, and then follows the contributions of charge and phonon terms in order.

TiSe$_2$ is a three-dimensional system with considerable dispersion along the $k_z$ direction as shown in Fig. 4(b). Therefore, the correlation effect is reduced here compared to MoS$_2$, as evident in the lower mass renormalization seen in Fig. 4(a). As a result, the values of EP coupling constant and $T_c$ with and without including EE interaction are closer to each other in this system. However, the presence of CDW enhances the EP coupling constant above $\lambda > 2$ at the optimal doping, as shown in Fig. 4(c), in which the Migdal theorem is violated [33]. We find that CDW overestimates $T_c$ by about 10-20 times. On the basis of this reasoning, we conclude that CDW and SC are competing in TiSe$_2$. Our finding is consistent with the conclusions of the x-ray scattering data in 1T-TiSe$_2$ systems [12], and also with a DFT calculation [34]. Moreover, in QCP induced unconventional superconductors, a linear-in-$T$ dependence of resistivity is observed at the SC dome, which is attributed to non-Fermi liquid behavior. But in TiSe$_2$, the resistivity data continues to exhibit quadratic $T$ dependence throughout the entire SC dome [6] pointing against the existence of a QCP.

With the same interaction parameters which give good estimation of $T_c$, [35] we also get mass renormalization in good accord with experiments in both systems. For MoS$_2$, we find $m'/m_b \sim 2 - 2.5$ in the optimal to overdoped region. The corresponding experimental value, deduced by ARPES [36] with respect to a simple parabolic band, is $\sim 2.4$ for the hole band. Again for TiSe$_2$, we estimate the experimental mass renormalization by comparing ARPES data [37] with the DFT band, and find an average value for two low-lying bands is $m'/m_b \sim 1.74$, which is close to our result of 1.8 - 2.

Conclusion: The main conclusion of this work is that the EP coupling constant is substantially modified by the dynamical EE interactions, which are, in general, tunable via external parameters such as doping, pressure, magnetic field, and others. While the examples are demonstrated here for two families of conventional superconductors, generalization to other forms of electron-boson coupling, such as spin-fluctuation or polaron mediated superconductivity is rather straightforward. Doping a Mott insulator usually weakens the EE correlation strength as seen in cuprates [14]. On the other hand, as demonstrated here, doping enhances EE interactions in the band insulator. In both Mott and band insulators, superconductivity seemingly emerges when the EE interaction strength falls into the intermediate coupling region where sufficient spectral weight is transferred to the quasiparticle states near $E_F$ from the higher energy ‘incoherent’ hump (s) via coupling to dominant spin and charge fluctuations [14] [38]. We find that when these EE interactions are taken into account in the EP (or, more appropriately, quasiparticle-phonon) coupling, its strength and $T_c$ are significantly changed and acquires doping dependence. Taken together, our study suggests that as a method of controlling the quasiparticle-boson coupling to optimize $T_c$, EE interactions may play the common role in creating the SC dome behavior in both conventional and unconventional superconductors.

The work is facilitated by the computer clusters at the Graphene Research Center at the National University of Singapore.
Electronic structure calculations are carried out using density functional theory (DFT) within the local density approximations (LDA) in the Ceperley-Alder parameterization [39] for exchange-correlation functional as implemented in Viena Abinitio Simulation Package (VASP) [40]. Projected augmented-wave (PAW) [41] pseudopotentials are used to describe core electrons. The conjugate gradient method is used to obtain relaxed geometries. Both atomic positions and cell parameters are allowed to relax, until the forces on each atom are less than 1 meV/Å. The relaxed lattice parameters are: \(a = 3.121 \, \text{Å} \) for MoS\(_2\); \(a = 3.437 \, \text{Å} \) and \(c/a = 1.693 \) for TiSe\(_2\). The kinetic energy cutoff is fixed at 650 eV. \(\Gamma\) centered \(k\)-mesh grids of \(14 \times 14 \times 1\) and \(14 \times 14 \times 8\) are used in the self-consistent calculations for MoS\(_2\) and TiSe\(_2\), respectively. Note that we did not consider any van der Waals (vdW) correction in our calculations, as the previous vDW+DFT calculations show that bilayer MoS\(_2\) exhibits an indirect gap between the \(\Gamma\) to K direction, which contradicts GW calculations [42][43]. However our calculated LDA band structure correctly describes this feature. Spin-orbit correction (SOC) is included in the band structure calculations. We note that for bilayer MoS\(_2\), the SOC is significantly reduced due to the presence of the inversion symmetry [44]. Furthermore, in order to study the lattice dynamics, force constants are calculated for 3\(\times\)3\(\times\)1 and 3\(\times\)3\(\times\)2 super-cell of MoS\(_2\) and TiSe\(_2\), respectively within the framework of density functional perturbation theory [45] using the VASP code. Subsequently, phonon dispersions are calculated using Phonopy package [46].

As mentioned in the main text, the band structure for monolayer and bilayer MoS\(_2\) has significant differences. [47][48] In monolayer system, both the conduction band bottom and the valence band top lie at the \(\Gamma\) point. In bilayer system, the bottom of the conduction band shifts to somewhere in between the \(\Gamma\) to K points, and the top of the valence band moves to the \(\Gamma\) point. However, from bilayer to the bulk system, the band structure does not change significantly. Therefore, given that the experiment is performed on a thin flake of MoS\(_2\) sample, we use the band structure for the bilayer system.

The band dispersion between LDA and LDA+GW calculation does not change characteristically [43][48] which means the doping dependence of the density of states would also be similar for both cases at the expense of a constant energy shift. Therefore, our many body and \(T_c\) calculations would yield similar results for the LDA and LDA+GW band structure inputs.

**APPENDIX**

**DENSITY FUNCTION THEORY CALCULATION**

Electronic structure calculations are carried out using density functional theory (DFT) within the local density approximations (LDA) in the Ceperley-Alder parameterization [39] for exchange-correlation functional as implemented in Viena Abinitio Simulation Package (VASP) [40]. Projected augmented-wave (PAW) [41] pseudopotentials are used to describe core electrons. The conjugate gradient method is used to obtain relaxed geometries. Both atomic positions and cell parameters are allowed to relax, until the forces on each atom are less than 1 meV/Å. The relaxed lattice parameters are: \(a = 3.121 \, \text{Å} \) for MoS\(_2\); \(a = 3.437 \, \text{Å} \) and \(c/a = 1.693 \) for TiSe\(_2\). The kinetic energy cutoff is fixed at 650 eV. \(\Gamma\) centered \(k\)-mesh grids of \(14 \times 14 \times 1\) and \(14 \times 14 \times 8\) are used in the self-consistent calculations for MoS\(_2\) and TiSe\(_2\), respectively. Note that we did not consider any van der Waals (vdW) correction in our calculations, as the previous vdw+DFT calculations show that bilayer MoS\(_2\) exhibits an indirect gap between the \(\Gamma\) to K direction, which contradicts GW calculations [42][43]. However our calculated LDA band structure correctly describes this feature. Spin-orbit correction (SOC) is included in the band structure calculations. We note that for bilayer MoS\(_2\), the SOC is significantly reduced due to the presence of the inversion symmetry [44]. Furthermore, in order to study the lattice dynamics, force constants are calculated for 3\(\times\)3\(\times\)1 and 3\(\times\)3\(\times\)2 super-cell of MoS\(_2\) and TiSe\(_2\), respectively within the framework of density functional perturbation theory [45] using the VASP code. Subsequently, phonon dispersions are calculated using Phonopy package [46].

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The band dispersion between LDA and LDA+GW calculation does not change characteristically [43][48] which means the doping dependence of the density of states would also be similar for both cases at the expense of a constant energy shift.

**MOMENTUM RESOLVED DENSITY FLUCTUATION (MRDF) THEORY**

The VASP band structure information is directly implemented within our momentum resolved density fluctuation (MRDF) code. The single-particle Green’s function is defined as \(\tilde{G}_I(k, i\omega_n) = (i\omega_n \tilde{1} - \tilde{H})^{-1}\), where \(i\omega_n\) is the Matsubara frequency for the fermions, and \(\tilde{H}\) is the non-interacting Hamiltonian constructed by downfolding the DFT bands into the low-energy energy levels. The explicit form of \(\tilde{G}\) is then obtained as

\[
G_{mn}(k, i\omega_n) = \sum_{\nu} \phi_{km}^{\nu} \phi_{km}^{\nu \dagger} (i\omega_n - \xi_{k}^{\nu}).
\]

Here \(\phi_{km}^{\nu}\) is the eigenstate for the \(\nu\)th band (\(\xi_{k}^{\nu}\)), projected onto the \(m\)th orbital. The non-interacting density fluctuation susceptibility in the particle-hole channel represents joint density of states (JDOS), which can be calculated by convoluting the corresponding Green’s function over the entire Brillouin zone (BZ) to obtain (spin and charge bare susceptibility are the same in the paramagnetic ground state) [49]:

\[
\chi_{0,mn}(q, \omega_p) = -\frac{1}{\Omega_{\text{BZ}}^2} \sum_{k,n} G_{mn}(k, i\omega_n) \times G_{st}(k + q, i\omega_n + \omega_p),
\]

where \(\beta = 1/k_B T\), and \(k_B\) is the Boltzmann constant and \(T\) is temperature. After performing the Matsubara summation over the fermionic frequency \(\omega_n\) and taking analytical continuation to the real frequency as \(\omega_n \rightarrow \omega + i\delta\), we get

\[
\chi_{0,mn}(q, \omega_p) = -\frac{1}{\Omega_{\text{BZ}}^2} \sum_{k,v,r} \phi_{k+q,v}^{\nu} \phi_{k+q,v}^{\nu \dagger} \phi_{k,v}^{\nu} \phi_{k,v}^{\nu \dagger} \times f_{\omega_p}^v - f_{\omega_p}^{\nu v} \omega_p + i\delta - \xi_{k}^{\nu} + \xi_{k+q}^{\nu}. \quad (4)
\]

The interacting density-density correlation functions are computed within the random phase approximation which includes multiband components of the electronic interaction including intra- and inter-orbital Coulomb interactions, \(U\) and \(V\), as well as Hund’s coupling \(J_H\), and pair-exchange term \(J':

\[
H_{\text{int}} = \sum_{k1-k1} \left[ U \sum_{m} c_{k1,m\uparrow}^\dagger c_{k1,m\downarrow} c_{k2,m\uparrow} c_{k2,m\downarrow} + \sum_{m<n,r} \left( V \sum_{k1,mr} c_{k1,m\sigma}^\dagger c_{k1,n\sigma} c_{k1,mr} c_{k1,n\sigma} + (V - J_H) c_{k1,m\sigma}^\dagger c_{k1,n\sigma} c_{k1,m\sigma} c_{k1,n\sigma} + J' c_{k1,m\sigma}^\dagger c_{k1,n\sigma} c_{k1,m\sigma} c_{k1,n\sigma} + h.c. \right) \right].
\]

\[ (5) \]
Here $c_{\sigma,m}^\dagger$ is the creation (annihilation) operator for an orbital $m$ at crystal momentum $k$, with spin $\sigma = \uparrow$ or $\downarrow$, where $\bar{\sigma}$ corresponds to opposite spin of $\sigma$. In the multi-orbital spinor, the above interacting Hamiltonian can be collected in an interaction tensor $\tilde{U}_{s/c}$, where the subscripts $s, c$ stand for spin and charge density fluctuations. The nonzero components of the matrices $\tilde{U}_s$ and $\tilde{U}_c$ are given as:\textsuperscript{49, 50}

$$
\tilde{U}_{s,rmn} = U, \quad \tilde{U}_{s,pmn} = \frac{1}{2} J_H, \\
\tilde{U}_{s,rmn} = \frac{1}{4} J_H + V, \quad \tilde{U}_{s,rmn} = J', \\
\tilde{U}_{c,rmn} = U, \quad \tilde{U}_{c,pmn} = 2V, \\
\tilde{U}_{c,rmn} = \frac{3}{4} J_H - V, \quad \tilde{U}_{c,pmn} = J'.
$$

(6)

Of course, it is implicit that all the interaction parameters are orbital dependent. Within the RPA, spin and charge channels become decoupled. The collective many-body corrections of the density-fluctuation spectrum can be written in matrix representation: $\tilde{\chi}_{s/c} = \tilde{\chi}^0 [1 \pm \tilde{U}_{s/c}(\tilde{\chi}^0)]^{-1}$, for spin and charge densities, respectively. $\tilde{\chi}^0$ matrix is consist of components $\chi^0_{mn}$ with the same basis in which the interactions $\tilde{U}_{s/c}$ are defined above.

As mentioned in the main text, the interaction parameters $(U, V, J_H, J')$ are not estimated individually. Rather, we estimate the components of the $\tilde{U}_{s/c}$ within the Kanamori criterion $\tilde{U}_{s,c} \leq \max[\tilde{U}_{s,c}(\tilde{\chi}^0)]^{-1}$ and set the values at the optimal doping for each system. The interaction matrix for charge component are set to be $\tilde{U}_c = \tilde{U}_s$. The interaction values are assumed to be doping independent, but material dependent. The largest interaction we find is $\sim 2$ eV for both materials. The momentum-resolved spin and charge density fluctuations are shown in supplementary Fig.\textsuperscript{5}.

Finally, the full momentum resolved density fluctuation (MRDF) exchange potentials for the electronic state are computed as

$$
V^\eta_{mn}(\mathbf{k}, \omega_p) = \frac{\eta \hbar}{16} \left[ \tilde{U}_{s,c} \tilde{\chi}^0_s(\mathbf{k}, \omega_p) \right]_{mn}^\eta, \quad (7)
$$

where $\eta$ stands for spin and charge components, $\eta = 3, 1$ for the spin and charge channels, respectively.

The electron-phonon coupling effect is calculated similarly. Here, we use

$$
V^\eta_{mn,p}(\mathbf{k}, \omega_p) = \sum_{\mathbf{q},\mu} \left| g^\mu_p(\mathbf{k}, \mathbf{q}) \right|^2 |g^\nu_{s}^{\mu}(\mathbf{k}, \mathbf{q})| \delta(\omega_p - \omega_{q\mu}), \quad (8)
$$

where $\omega_{q\mu}$ is the phonon dispersion for band $\mu$, and the subscript 'p' stands for the EP term. The EP coupling matrix-element is $g^\mu_p(\mathbf{k}, \mathbf{q}) = \sum_{\alpha} g^\mu_{q\alpha} \delta^\nu_{q\alpha} \delta^\rho_{q\alpha} h_{\mathbf{k}+\mathbf{q}+\mathbf{q}},$ where the momentum averaged EP scattering amplitude $g_{\mathbf{k}+\mathbf{q}+\mathbf{q}}$ is deduced from the first-principles calculation.

The feedback effect of the many-body MRDF potential on the electronic spectrum is then calculated via self-energy calculation as demonstrated in Eq. (1) of the main text. Full self-consistency requires the bare Green’s function $G_0$ in the supplementary Eq. (2) to be replaced with the self-energy dressed $\tilde{G}^{-1}(\mathbf{k}, \omega) = \tilde{G}_0^{-1}(\mathbf{k}, \omega) - \tilde{\Sigma}(\mathbf{k}, \omega)$, where the total self-energy tensor is $\tilde{\Sigma}(\mathbf{k}, \omega) = \tilde{\Sigma}_s(\mathbf{k}, \omega) + \tilde{\Sigma}_c(\mathbf{k}, \omega) + \tilde{\Sigma}_p(\mathbf{k}, \omega)$. This procedure is numerically expensive, especially in the multiband systems and when full momentum dependence is retained. Therefore, we adopt a modified self-consistency scheme, where we expand the real part of the total self-energy tensor as $\tilde{\Sigma}_r(\mathbf{k}, \omega) = (1 - \tilde{Z}_k - \omega)\tilde{\Sigma}_s(\mathbf{k}, \omega)$ in the low-energy region $|\omega| < 0.2 - 0.3$ eV in the present materials]. The resulting self-energy dressed quasiparticle dispersions $\tilde{\xi}_w(\mathbf{k}) = Z_\mathbf{k}^\omega(\mathbf{k})$ are used in Eqs. (2)-(8), which keep all the formalism unchanged with respect to the momentum resolved orbital selective quasiparticle renormalization factor $Z_k$. The vertex correction $\Gamma$ defined in the main text is also calculated self-consistently at all cycles.

**QUASIPARTICLE-PHONON COUPLING AND SUPERCONDUCTING TRANSITION TEMPERATURE**

In the systems where the interaction strength is of the order of the bandwidth, i.e., the kinetic and potential energies are of the same order, various instabilities develop. Different materials having different lattice structure and Fermi surface topology are prone to different forms of instabilities, among which leading contributions usually arise from the superconductivity and density wave fluctuations in the spin, charge and lattice sectors. These instabilities often lead to an incoherent, or a gapped Fermi surface at the expense of superconductivity and/or a static density wave (s).

Therefore, even for conventional superconductors, especially for the $d$-electronic systems, such correlated electronic structure or quasiparticle spectrum can lead to substantial modification of the electron-phonon coupling constant, as originally proposed by Eliashberg.\textsuperscript{54} The same effect also lead to a violation of the Migdal’s theorem.\textsuperscript{53} We treat this problem using a quasi-perturbation method in which the non-interacting electron and phonon dispersions are computed via DFT framework. Then the EP coupling vertex is calculated self-consistently in which the electronic state is dressed with both EE (density fluctuations) and EP coupling. The quasiparticle-phonon coupling density of states (DOS) or the so-called $\alpha^2 F$ is calculated as

$$
\alpha^2 F_p(\omega_p) = \frac{1}{\Omega_{BZ} \bar{N}(0)} \sum_{\mathbf{q},\nu} \text{Tr} \left[ \tilde{V}_p(\mathbf{q}, \omega_p) \tilde{\chi}_s(\nu) \tilde{\chi}_c(\nu) \right], \quad (9)
$$

where $\bar{N}(0)$ is the correlated electronic DOS at the Fermi level, and the self-energy dressed quasiparticle band is $\tilde{\xi}_w = \tilde{\xi}_w + \tilde{\Sigma}_s(\tilde{\xi}_w)$, and $V_p$ is defined in Eq. (8) but with self-energy correction. Therefore, the SC transition temperature becomes

$$
T_c = \frac{\omega_{\text{gap}}}{1.2 k_B} \exp \left( - \frac{1.04(1 + \lambda)}{\lambda - \mu^* (1 + 0.62 \lambda)} \right), \quad (10)
$$
where the traditional Debye frequency is replaced by\[56\]
\[
\omega_{\text{log}} = \exp\left(\frac{2}{\lambda} \int d\omega_p \log \omega_p \frac{\alpha^2 F_p(\omega_p)}{\omega_p}\right).
\]
and the EP coupling strength for the Cooper pair is
\[
\lambda = 2 \int d\omega_p \frac{\alpha^2 F_p(\omega_p)}{\omega_p}.
\]
Note that the EP coupling in the SC channel, \(\lambda\), is different from the EP coupling constant for the single quasiparticles \(\lambda_{\text{QP}} = Z^{-1} - 1\), where \(Z^{-1} = 1 - (\partial \Sigma / \partial \omega)_{\omega=0}\), that one often obtains from the quasiparticle self-energy.\[57\]
The Coulomb pseudopotential \(\mu^*\) is often taken as a parameter, and set to be 0.1 as standard value, however, the evolution of it in correlated system and as a function of doping can be estimated as
\[
\mu^* = \frac{\mu_0}{1 + \mu_0^* \log \left(\frac{\omega_{\text{log}}}{\omega_{\text{log}}^0}\right)},
\]
where the renormalized Coulomb interaction is \(\tilde{U} = U/(1+\lambda)\). The doping dependent values of \(\omega_{\text{log}}\) and \(\mu^*\) are shown in the supplementary Fig.8 for both materials.

### ADDITIONAL RESULTS

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\[
\omega_{\text{log}} = \exp\left(\frac{1}{\lambda} \int d\omega_p \log \omega_p \frac{\alpha^2 F_p(\omega_p)}{\omega_p}\right).
\]
FIG. 5. Imaginary parts of the spin and charge susceptibilities for various representative cases. (a)-(b) In the band insulating state of MoS$_2$, both spin and charge susceptibilities are gapped inside the particle-hole continuum. No collective excitation develops inside the spin gap in a band insulator, unlike in a magnetic insulator where a spin-wave dispersion (Goldstone mode) arises inside the particle-hole continuum due to symmetry breaking (see e.g., Fig. 6 of Ref. [58]). (c)-(d) At finite doping, in the metallic state, various intra-band transitions turn on and give rise to low-energy modes. Some of the modes extend to $\omega_p \to 0$. The spin channels are moved to lower in energy than the charge counterpart due to the many body correction within the random-phase approximation. These low-energy modes are responsible for the increase of renormalization effect at finite doping. (e)-(f) Zoomed in view of the same data shown in (c), and (d), respectively. (g)-(h), Same data, but for TiSe$_2$ at its optimal doping. Due to the presence of many bands in the low-energy spectrum, the density fluctuation channels exhibit several modes. The results for TiSe$_2$ are plotted in the log-scale for clarity, while that for MoS$_2$ are plotted in linear scale. (i)-(j), Zoomed in view of their corresponding upper panels. All results are shown by summing over all band contributions.

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FIG. 6. Analysis of various self-energy properties for MoS$_2$. (a)-(b) Momentum dependence of the real and imaginary parts of total self-energy at optimal doping for the band which crosses the Fermi level. (c)-(d) Various components of the total self-energy at the same doping. As mentioned in the main text, the largest contribution stems from the spin channel. (e) The mass enhancement $m^*/m_b = 1/Z$ at the Fermi level for the highest renormalized band (nearest to the Fermi level) as a function of doping. As shown in Fig. 1 in the main text, the phonon part (black dots) exhibit a dome-like feature centering the optimal doping, while spin and charge contributions increase gradually with doping. As the phonon-contribution decreases in the overdoped region, the spin-contribution rises sharply.

FIG. 7. Analysis of various self-energy properties for TiSe$_2$. (a)-(b) The momentum dependence of the self-energy is reduced in this system than in MoS$_2$. The three-dimensionality of the self-energy is also weak. (c)-(d) As in MoS$_2$, the spin-density fluctuation is also dominant in TiSe$_2$. The CDW results are shown for $x = 0.05$. (e) The mass renormalization at the Fermi-level as a function of doping. The phonon and charge contributions are very similar as a function of doping. In the CDW state, the renormalization is dominant for the undoped case, and then decreases monotonically with doping. All results are presented for one of the two bands in the low-energy spectrum in which the renormalization effect is strongest.
FIG. 8. Doping dependence of renormalized $\omega_{\log}$ and $\mu^*$. As demonstrated in the main text, both these features remain fairly doping independent, and do not exhibit any apparent anomaly at the optimal doping. More interestingly, the values are almost identical for EP and EE+EP cases, demonstrating that these features do not contribute to the formation of SC dome in these systems.