Mottness collapse without metallisation in the domain walls of triangular-lattice Mott insulator 1T-TaS$_2$

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1T-TaS$_2$ is a charge-density-wave (CDW) compound with a Mott-insulating ground state. The metallic state obtained by doping, substitution or pulsed charge injection is characterized by an emergent CDW domain wall network, while single domain walls can be found in the pristine Mott state. Here we study whether and how the single walls become metallic. Tunneling spectroscopy reveals partial suppression of the Mott gap and the presence of in-gap states strongly localized at the domain-wall sites. Using the real-space dynamical mean field theory description of the strongly correlated quantum-paramagnet ground state we show that the local gap suppression follows from the increased hopping along the connected zig-zag chain of lattice sites forming the domain wall, and that full metallisation is preempted by the splitting of the quasiparticle band into bonding and antibonding sub-bands due to the structural dimerization of the wall, explaining the presence of the in-gap states and the low density of states at the Fermi level.

The interplay between superconductivity (SC) and correlated insulating phases, such as Mott insulators and charge density waves (CDW), is one of the central problems in condensed-matter physics. Remarkably, their combination can be found even in simple material systems, such as transition metal dichalcogenide (TMD) van der Waals compound 1T-TaS$_2$. The ground state is a Mott insulator$^1$ with CDW$^2$ and unconventional quantum spin liquid behavior$^3$. Upon Se substitution$^4$, Fe intercalation$^5$, or by applying pressure$^6$ it becomes superconducting, with both CDW and correlated behavior still present. Further control over electronic properties is possible through non-equilibrium charge injection via ultrafast optical or electrical pulses$^7$, which lead to drastic insulator to metastable metal transition. The long-standing hypothesis for metallisation and SC onset is linked to the formation of CDW domain walls, seen in multiple TMDs with different techniques$^8$. Recently, it was challenged experimentally with scanning tunneling spectroscopy (STS)$^9$, which showed the absence of metallisation in certain types of walls. First-principles calculations revealed that atomic reconstruction in the walls may cause the formation of bound states$^{10}$ and band reconstruction$^{11}$, but the correlation effects were left out of scope. Thus, the crucial question of whether the CDW distortion inside the wall can lead to Mottness collapse remains open. In this paper we combine STS and dynamical mean field theory (DMFT) calculations to study the behavior of the Mott gap in CDW domain walls, finding Mottness collapse without metallisation.

In 1T-TaS$_2$, each layer is periodically modulated to form a $\sqrt{13} \times \sqrt{13}$ superlattice of David star deformations$^1$, resulting in a commensurate CDW state with a single half-filled electron band at the Fermi level. The Coulomb repulsion opens a charge gap in this band, resulting in a Mott insulating ground state. The DW is seen as a misfit of the lattices on left and right.

Figure 1. Domain walls in 1T-TaS$_2$. (a) STM topographic image of a single domain wall separating two adjacent CDW domains ($V_{\text{tip}} = -0.8$ V, $I = 100$ pA, $T = 4.2$ K). (b) Schematic diagram of the configuration of David stars near the domain wall: the stars along the wall are brought closer together. The modified center-to-center distances are indicated as $d_1$, $d_2$. (c) Hubbard model description of the domain wall: one-dimensional zig-zag chain with modified hoppings (ratios $r_1$, $r_2$, green line) embedded in a two-dimensional Mott insulator environment. (d) $dI/dV$ map across the domain wall (domain wall A, DW-A, averaged over longitudinal direction). LHB and UHB are lower and upper Hubbard bands, $E_c$ and $E_v$ indicate the additional conducting and valence bands associated with the Ta $d$-shell.

Single CDW domain walls (DWs)$^{17}$ can be found connecting large lattice inhomogeneities in freshly cleaved samples or they remain after the relaxation of the metastable metallic mosaic state created with voltage pulse from the scanning tunneling microscope (STM) tip. We study both examples and find the relevant physics similar.

Topographic STM image, Fig. 1(a), reveals individual David stars as bright spots packed in a triangular lattice. The DW is seen as a misfit of the lattices on left and right.
observed low-energy behavior in the DW. The minimal spectrum, see Fig. 2(a).

Sides: David stars partially overlap and are shifted with respect to each other. Among the twelve possible DW types only a few are observed experimentally: indeed, in the most commonly seen DWs, the stars are drawn closer together, Fig. 1(b), but still retain their shape; see Supplemental Material (SM) for an extended discussion. The DW is very localized, approximately two superlattice constants in extent, so that its core roughly consists of a 1D zig-zag chain of the nearest-neighbor stars, Fig. 1(c).

The tunneling spectra, Fig. 1(d), reveal the apparent Mott gap closing at the DW, while the clear bending of the Hubbard bands outside the DW indicates its charging. The CDW gap is quite robust, except at the very center of the DW. Changes to the Mott gap occur on significantly larger spatial scales, allowing us to decouple the two gaps. The spectral weight is distributed unevenly along the DW (see SM), suggesting finite scattering. Closer inspection of the high-resolution density of states (DOS) in the Mott gap, done on another DW sector, shows two more major features: (i) inside the DW, the DOS is significantly reconstructed and a small non-zero weight appears at the Fermi level, and (ii) in-gap states at -70 mV are present on top of a smooth spectrum, see Fig. 2(a).

We now construct an effective model to understand the observed low-energy behavior in the DW. The minimal model for the Mott state in TaS$_2$ is the single-band Hubbard model on a triangular lattice at half filling [29, 30, 33, 37]:

$$H = \sum_{<ij>,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{\sigma} \epsilon_i n_{i\sigma} + \sum_i U_i n_{i\uparrow} n_{i\downarrow},$$

where $i,j$ are site indices, $\sigma = \uparrow, \downarrow$ is spin, $c_{i\sigma}^\dagger$ are electron creation operators, $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ are the local electron-occupation operators, $t_{ij}$ are the hopping constants between nearest-neighbors, $\epsilon_i$ are the on-site potentials, and $U_i$ are the Hubbard repulsion parameters. Down to the lowest temperatures, TaS$_2$ does not order magnetically [6, 9]. A simple approximation to describe this experimentally observed paramagnetic Mott insulating state, theoretically predicted to exist in a range of $U$ between the paramagnetic metal and the 120° Neél ordered state [38, 39], is the DMFT [29, 40]. This approach can be generalized to the inhomogeneous case [41–50]. Here we assume the DW lattice structure to be predetermined and fixed, and we focus on the effects of such a deformation on the electronic degrees of freedom.

The modified separation between the stars in the DW is reflected in a change of the corresponding hopping constants $t_{ij}$ due to a different overlap of the corresponding Wannier wavefunctions; see the adjacent black and red stars in Fig. 1(b), represented by the green line in Fig. 1(c). The rescale factor for the hopping constants will be denoted as $r$. (In unperturbed bulk $t_{ij} \equiv t$, while $t_{ij} = rt$ for $i, j$ belonging to the DW.) The superlattice deformation along the DW has a longitudinal component leading to a period-2 modulation of $r$ along the DW (the values will be denoted by $r_1$ and $r_2$). Next, we allow for a modification of the on-site energies $\epsilon_i$ resulting from the deformation of the stars. The additional on-site potential at the DW sites will be denoted as $\delta$. For simplicity we assume that the Hubbard constants remain uniform, $\bar{U}_i \equiv U$. We set $U = 4D$, where $2D = 9t$ is the bandwidth of the triangular-lattice DOS. We fix the chemical potential in the centre of the bulk Mott gap. We now study the effects of the inhomogeneity on the local DOS (LDOS) using the real-space DMFT approach as described in SM. The main result is that in the DW the Mott state collapses if at least one of $r_1, r_2$ is large enough, due to an increase in the kinetic energy of the DW subsystem, however the resulting state has a low Fermi-level LDOS for $r_1 \neq r_2$ due to the splitting of the quasiparticle band into bonding and antibonding subbands which tends to open a (pseudo)-gap.

In 1T-TaS$_2$, the lattice geometry effects are particularly important: The zig-zag nature of the lattice distortion makes the DW a connected linear system embedded in a bulk Mott insulator sheet. The homogeneous Hubbard model undergoes Mott metal-insulator (MIT) transitions of two types [33, 40, 51]: interaction/bandwidth-driven (Hubbard repulsion $U$ overcomes the kinetic energy proportional to hopping) or doping-driven (for sufficiently large $U$ the electron repulsion approaches half-filling). If the system lacks translation invariance, the MIT can also take place in a subsystem, e.g. on a surface, at an interface,
or in a domain-wall [41,45]. In TaS$_2$, the DW sub-system metallises if $r_1 = r_2$ or $r$ becomes large (bandwidth-driven MIT) or if $\delta$ becomes large (doping-driven MIT), see Fig. 3(a).

The “local charge gap” is reduced inside the DW. This is due to the enhanced hopping $r$ that increases the effective bandwidth so that local LHB and UHB become broader, while the band centers shift only little. Because of the particle-hole asymmetry in the triangular lattice, the top of LHB and the bottom of UHB have quite different shapes and the upper edge of the LHB moves towards the Fermi level with increasing $r$ faster than the bottom edge of the UHB. For high enough $r = r_1 = r_2$, the DW goes through a MIT and it metallizes: A quasiparticle (QP) band emerges inside the Mott gap, Fig. 3(b), so that the Fermi-level local LDOS jumps to a finite value, Fig. 3(a).

The QP band has a highly asymmetric internal structure with a sharp maximum $M$ in the occupied part of the spectrum (the maximum is not pinned to the Fermi level) and an extended flat plateau $P$ in the unoccupied part, see Fig. 4(d), right panel. In addition, in the range $r \lesssim 2.5$ we find a weak secondary peak $S$ (see SM for its interpretation). Information about the in-gap states can be extracted from the momentum-resolved (partially Fourier transformed) spectral function $A_{k,i}(\omega)$, where $k$ is the longitudinal momentum in the DW direction, while $i$ is the index of the DW site in the transverse direction. An overview is shown in Fig. 4(c), and a close-up to the QP band in Fig. 4(d). The dominant features ($M$ and $P$) in the structure of the QP band are due to the one-dimensional nature of the DW which is a 1D zig-zag chain with nearest and next-nearest neighbour hopping constants differing by a factor of $r$. The band dispersion for such a non-interacting tight-binding model with $r = 2.4$ indeed matches the QP dispersion, Fig. 4(d).

Surprisingly, the boundary bandwidth-driven MIT is first order even at zero temperature, unlike the bulk MIT. We find a sizeable region with coexisting DMFT solutions: with increasing $r$, the insulating solution metalizes at $r_{c,2}$, while with decreasing $r$ the metallic solution becomes insulating at $r_{c,1} < r < r_{c,2}$. The insulating solution is stable in the entire coexistence region, $r_{c,1} < r < r_{c,2}$, Fig. 4(b). As a consequence, the bandwidth-driven transition from the insulating state happens at the moment when the Hubbard band (here LHB) touches the chemical potential, similar to the scenario for the disappearance of the metastable insulating DMFT solution in the bulk case. We note, how-
ever, that for $r > r_{c,2}$ the LHB becomes clearly separated from the quasiparticle (QP) peak, i.e., at $r = r_{c,2}$ the LDOS changes discontinuously. The doping-driven boundary Mott transition also proceeds by the mechanism of LHB crossing the chemical potential, but the QP peak is pinned to the top of the LHB right after the transition (see SM for more details).

The superlattice deformation at the DW corresponds to an increase of hopping that can easily attain values of $r \approx 3$ or 4 (see SM for estimates corresponding to common DW types). One would thus generically expect to observe a strong metallisation and a prominent peak at (or close to) the Fermi level. In reality, however, the DW is naturally dimerized so that $r_1 \neq r_2$. For most DW types $r_1$ and $r_2$ can indeed be quite different. The Mott phase collapses at the DW if the kinetic energy of the 1D subsystem is high enough. For this to occur, it is sufficient for one of $r_1, r_2$ to be large, even if the 1D subsystem in isolation from the triangular-lattice bulk would actually be gapped (a band insulator). The alternation of hoppings gives rise to molecular orbitals localized on the nearby sites forming dimers, thereby splitting the QP band into bonding and anti-bonding subbands. The resulting spectrum has a prominent peak in the occupied part of the spectrum ($\omega < 0$) and a gap-like strong suppression of DOS around the Fermi level, see Figs. 2(b) and 3(c).

The major observations from the tunneling spectra can thus be consistently understood within this model. In the DW core, two effects dominate: reconstruction of spectra, and emergence of the bound state. If the in-gap resonance is disregarded, it can still be observed that the Mott gap is smaller and the DOS distribution is smeared - the behavior reproduced by the intra-DW change of hopping. The in-gap DOS peak at negative bias results from the QP band splitting. The features in the unoccupied part of the spectrum are most likely pushed toward the UHB and are largely submerged into it. We also observe a small yet clearly non-zero value of Fermi-level LDOS inside the DW, which results from the subband spectral tails of the split QP band. The spatial distribution of the Fermi level LDOS and the bound state LDOS are indeed quite similar, see Fig. 2(c), which confirms their common origin. Finally, the band bending outside the DW is effectively reproduced with the local potential. Its role in metallization is unpronounced inside the DW, even when UHB is brought very close to the Fermi level (see SM).

We thus conclude that the structural change in an isolated DW does not yield a good metal in spite of the Mottness collapse. The same result can be extrapolated to the DWs in the hidden state, which have an even larger structural distortion [17, 20]. Optical or electrical pulses can, however, affect the orbital structure [56] or cause redistribution of electrons in the Brillouin zone, and lead to metallization independently of the density and the type of DWs. Finally, we mention the possibility that the superconductivity in these compounds is unrelated to the DWs, and that upon doping, the SC state emerges directly from the quantum spin liquid state, thus 1T-TaS$_2$ might be an unconventional resonanting-valence-bound superconductor.

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[1] E. Tosatti and P. Fazekas, “On the nature of the low-temperature phase of 1T-TaS$_2$,” J. de Physique Colloques 37 (C4), 165 (1976).
[2] P. Fazekas and E. Tosatti, “Electrical, structural and magnetic properties of pure and doped 1T-TaS$_2$,” Philos. Mag. B 39, 229 (1979).
[3] P. Fazekas and E. Tosatti, “Charge carrier localization in pure and doped 1T-TaS$_2$,” Physica B 99, 183 (1980).
[4] R. E. Thomson, U. Walter, E. Ganz, J. Clarke, A. Zettl, P. Rauch, and F. J. DiSalvo, “Local charge-density-wave structure in 1T-TaS$_2$ determined by scanning tunneling microscopy,” Phys. Rev. B 38, 10734 (1988).
[5] P. W. Anderson, “Resonating valence bonds: a new kind of insulator?” Mater. Res. Bull. 8, 153 (1973).
[6] Martin Klanišek, Andrej Zorko, Rok Žitko, Jernej Mravlje, Zvonko Jagličić, Pabitra Kumar Biswas, Peter Prelovšek, Dragan Mihailovic, and Denis Arčon, “A new high-temperature quantum spin liquid with polaron spins,” Nat. Phys. 13, 1130 (2017).
[7] K. T. Law and P. A. Lee, “1T-TaS$_2$ as a quantum spin liquid,” Proc. Natl. Acad. Sci. USA 114, 6996 (2017).
[8] M. Kratochvilo, A. D. Hillier, A. R. Wildes, L. Wang, S.-W. Cheong, and J. G. Park, “The low-temperature highly correlated quantum phase in the charge-density-wave in 1T-TaS$_2$,” Npj Quantum Mater. 2, 42 (2017).
[9] A. Ribak, I. Silber, C. Baines, K. Chashka, Z. Salman, Y. Dagan, and A. Kanigel, “Gapless excitations in the ground state of 1T-TaS$_2$,” Phys. Rev. B 96, 195131 (2017).
[10] Y. J. Yu, Y. Xu, L. P. He, M. Kratochvilo, Y. Y. Huang, J. M. Ni, L. Wang, S.-W. Cheong, Je-Geun Park, and S. Y. Li, “Heat transport study of the spin liquid candidate 1T-TaS$_2$,” Phys. Rev. B 96, 081111(R) (2017).
[11] Y. Liu, R. Ang, W. J. Lu, W. H. Song, L. J. Li, and Y. P. Sun, “Superconductivity induced by Se-doping in layered charge-density-wave system 1T-TaS$_{2−x}$Se$_x$,” Appl. Phys. Lett. 102, 192602 (2013).
[12] L. J. Li, W.J. Lu, X.D. Zhu, L.S. Ling, Z. Qu, and Y. P. Sun, “Fe-doping–induced superconductivity in the charge-density-wave system 1T-TaS$_2$,” European Physics Letters 97, 67005 (2012).
[13] B. Sipos, A. F. Kusmartseva, A. Akrap, H. Berger, L. Forró, and E. Tútis, “From Mott state to superconductivity in 1T-TaS$_2$,” Nat. Mater. 7, 960 (2008).
[14] L. Stojchevska, I. Vaskivskyi, T. Mertelj, P. Kušar, Prelovšek, Jernej Mravlje, and Dragan Mihailovic.
crystals,” Sci. Adv. 1, e1500606 (2015).
[16] I. Vaskivskyi, I. A. Mikhailovic, S. Brazovskii, J. Gospodarić, T. Mertelj, D. Svetin, P. Sutar, and D. Mikhailovic, “Fast electronic resistance switching involving hidden charge density wave states,” Nat. Commun. 7, 11442 (2015).
[17] L. Ma, C. Ye, Y. Yu, X. F. Lu, X. Niu, S. Kim, D. Feng, D. Tománek, Y.-W. Son, X. H. Chen, and Y. Zhang, “A metallic mosaic phase and the origin of Mott-insulating state in 1T-TaS₂,” Nat. Commun. 7, 10956 (2016).
[18] D. Cho et al., “Nanoscale manipulation of the Mott insulating state coupled to charge order in 1T-TaS₂,” Nat. Commun. 7, 10453 (2016).
[19] D. Svetin, I. Vaskivskyi, Brazovskii S, and D. Mikhailovic, “Three-dimensional resistivity and switching between correlated electronic states in 1T-TaS₂,” Sci. Reports 7, 46048 (2017).
[20] Yaroslav A. Gerasimenko, Igor Vaskivskyi, and Dragan Mikhailovic, “Dual vortex charge order in a metastable state created by an ultrafast topological transition in 1T-TaS₂,” arXiv:1704.08149 (2017).
[21] Yaroslav Gerasimenko, Igor Vaskivskyi, Jan Ravnik, Jaka Vodeb, Viktor V. Kabanov, and Dragan Mikhailovic, “Ultrafast jamming of electrons into an amorphous entangled state,” arXiv:1803.00255 (2018).
[22] Y. I. Joe, X. M. Chen, P. Ghaemi, K. D. Finkelstein, G. A. de La Peña, Y. Gan, J. C. T. Lee, S. Yuan, J. Geck, G. J. MacDougall, T. C. Chiang, S. L. Cooper, E. Fradkin, and P. Abbamonte, “Emergence of charge density wave domain walls above the superconducting dome in 1T- TiSe₂,” Nat. Phys. 10, 421 (2014).
[23] Shichao Yan, Davide Iaia, Emilia Morosan, Eduardo Fradkin, Peter Abbamonte, and Vidya Madhavan, “Influence of domain walls in the incommensurate charge density wave state of Cu intercalated 1T-TiSe₂,” Phys. Rev. Lett. 118, 106405 (2017).
[24] S. Qiao, X. Li, N. Wang, W. Ruan, C. Ye, P. Cai, Z. Hao, H. Yao, X. Chen, J. Wu, Y. Wang, and Z. Liu, “Orbital-driven Mottness collapse in 1T-TaS₂−aSe₂ transition metal dichalcogenide,” Phys. Rev. X 7, 041054 (2017).
[25] Doohye Cho, Gyeongcheol Gye, Jinwon Lee, Sung-Hoon Lee, Lilai Wang, Sang-Wook Cheong, and Han Woong Yeom, “Correlated electronic states at domain walls of a Mott-charge-density-wave insulator 1T-TaS₂,” Nat. Comm. 8, 392 (2017).
[26] K. Rossnagel, “On the origin of charge-density waves in select layered transition-metal dichalcogenides,” J. Phys.: Condens. Matter 23, 213001 (2011).
[27] P. Darancet, A. J. Millis, and C. A. Marianetti, “Three-dimensional metallic and two-dimensional insulating behavior in octahedral tantalum dichalcogenides,” Phys. Rev. B 90, 045134 (2014).
[28] Ju-Jin Kim, W. Yamaguchi, T. Hasegawa, and K. Kitazawa, “Observation of Mott localization gap using low temperature scanning tunneling spectroscopy in commensuare 1T-TaS₂,” Phys. Rev. Lett. 73, 2103 (1994).
[29] L. Perfetti, P. A. Loukakos, M. Lisowski, U. Bovensiepen, H. Berger, S. Biermann, P. S. Cornaglia, A. Georges, and M. Wolf, “Time evolution of the electronic structure of 1T-TaS₂ through the insulator-metal transition,” Phys. Rev. Lett. 97, 067402 (2006).
[30] L. Perfetti, P. A. Loukakos, M. Lisowski, U. Bovensiepen, M. Wolf, H. Berger, S. Biermann, and A. Georges, “Femtosecond dynamics of electronic states in the Mott insulator 1T-TaS₂ by time resolved photoelectron spectroscopy,” New J. Phys. 10, 053019 (2008).
[31] M. Ligges, I. A. Avigo, D. Golež, H. U. R. Strand, L. Stojchevska, M. Malliøre, K. Rossnagel, M. Eckstein, P. Werner, and U. Bovensiepen, “Ultrafast doublon dynamics in photo-excited 1T-TaS₂,” arXiv:1702.05300 (2017).
[32] P. Karpov and S. Brazovskii, “Modeling of networks and globules of charged domain walls observed in pump and pulse induced states,” Scientific Reports 8, 4043 (2018).
[33] Masatoshi Imada, Atsushi Fujimori, and Yoshinori Tokura, “Metal-insulator transitions,” Rev. Mod. Phys. 70, 1039 (1998).
[34] F. Gebhardt, The Mott metal-insulator transition (Springer, Berlin, 1997).
[35] K. Aryapour, W. E. Pickett, and R. T. Scalettar, “Dynamical mean-field study of the Mott transition in the half-filled Hubbard model on a triangular lattice,” Phys. Rev. B 74, 085117 (2006).
[36] L. Perfetti, T. A. Gloor, F. Mila, H. Berger, and M. Greioni, “Unexpected periodicity in the quasi-two-dimensional Mott insulator 1T-TaS₂ revealed by angle-resolved photoemission,” Phys. Rev. B 71, 153101 (2005).
[37] J. K. Freericks, H. R. Krishnamurthy, Y. Ge, A. Y. Liu, and Th. Pruschke, “Theoretical description of time-resolved pump/probe photoemission in TaS₂: a single-band DFT+DMFT(NRG) study within the quasiequilibrium approximation,” Phys. Status Solidi B 256, 948 (2009).
[38] T. Yoshioka, A. Koga, and N. Kawakami, “Quantum phase transitions in the Hubbard model on a triangular lattice,” Phys. Rev. Lett. 103, 036401 (2009).
[39] Tomonori Shirakawa, Takami Tohyama, Jure Kokalj, Sige-toshi Sota, and Seiji Yunoki, “Ground-state phase diagram of the triangular lattice Hubbard model by the density-matrix renormalization group method,” Phys. Rev. B 96, 205130 (2017).
[40] Antoine Georges, Gabriel Kotliar, Werner Krauth, and Marcelo J. Rozenberg, “Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions,” Rev. Mod. Phys. 68, 13 (1996).
[41] M. Potthoff and W. Nolting, “Surface metal-insulator transition in the Hubbard model,” Phys. Rev. B 59, 2549 (1999).
[42] M. Potthoff and W. Nolting, “Metallic surface of a Mott insulator–Mott insulating surface of a metal,” Phys. Rev. B 60, 7834 (1999).
[43] M. Potthoff and W. Nolting, “Dynamical mean-field study of the Mott transition in thin films,” Eur. Phys. J. B 8, 555 (1999).
[44] J. K. Freericks, “Dynamical mean-field theory for strongly correlated inhomogeneous multilayered nanostructures,” Phys. Rev. B 70, 195342 (2004).
[45] J. Freericks, Transport in Multilayered Nanostructures: The Dynamical Mean-field Theory Approach (Imperial College Press, London, 2006).
[46] S. Okamoto and A. J. Millis, “Spatial inhomogeneity and strong correlation physics: A dynamical mean-field study of a model mott-insulator–band-insulator heterostructure,” Phys. Rev. B 70, 241104(R) (2004).
[47] R. W. Helmes, T. A. Costi, and A. Rosch, “Kondo Proximity Effect: How Does a Metal Penetrate into a Mott Insula-
tor?” Phys. Rev. Lett. 101, 066802 (2008).
[48] M. Jiang, G. G. Batrouni, and R. T. Scalettar, “Density of states and magnetic correlations at a metal-Mott insulator interface,” Phys. Rev. B 86, 195117 (2012).
[49] Juho Lee and Chuck-Hou Yee, “Interfaces in coexisting metals and Mott insulators,” Phys. Rev. B 95, 205126 (2017).
[50] P. Bakalov, D. Nasr Esfahani, L. Covaci, F. M. Peeters, J. Tempere, and J.-P. Locquet, “Electric-field-driven Mott metal-insulator transition in correlated thin films: An inhomogeneous dynamical mean-field theory approach,” Phys. Rev. B 93, 165112 (2016).
[51] Antoine Georges and Werner Krauth, “Numerical solution of the $d = \infty$ Hubbard model: Evidence for a Mott transition,” Phys. Rev. Lett. 69, 1240 (1992).
[52] X. Y. Zhang, M. J. Rozenberg, and G. Kotliar, “Mott transition in the $d=\infty$ Hubbard model at zero temperature,” Phys. Rev. Lett. 70, 1666 (1993).
[53] P. Werner and A. J. Millis, “Doping-driven Mott transition in the one-band Hubbard model,” Phys. Rev. B 75, 085108 (2007).
[54] R. Žitko, D. Hansen, E. Perepelitsky, J. Mravlje, A. Georges, and B. S. Shastry, “Extremely correlated Fermi liquid theory meets dynamical mean-field theory: Analytical insights into the doping-driven Mott transition,” Phys. Rev. B 88, 235132 (2013).
[55] D. E. Logan and M. R. Galpin, “Mott insulators and the doping-induced Mott transition within DMFT: exact results for the one-band Hubbard model,” J. Phys.: Condens. Matter 28, 025601 (2016).
[56] T. Ritschel, J. Trinckauf, K. Koepernik, B. Buchner, M. von Zimmermann, H. Berger, Y. I. Joe, P. Abbamonte, and J. Geck, “Orbital textures and charge density waves in transition metal dichalcogenides,” Nature Phys. 11, 328 (2015).