Charge density wave and superconductivity in transition metal dichalcogenides

Sudipta Koley, Narayan Mohanta, and Arghya Taraphder

1 Department of Physics, North Eastern Hill University, Shillong, Meghalaya 793022, India
2 Department of Physics, Indian Institute of Technology Kharagpur, W.B. 721302, Kharagpur, India
3 Department of Physics and Centre for Theoretical Studies, Indian Institute of Technology Kharagpur, W.B. 721302, Kharagpur, India

Received 25 October 2019 / Received in final form 28 February 2020
Published online 4 May 2020
© EDP Sciences / Società Italiana di Fisica / Springer-Verlag GmbH Germany, part of Springer Nature, 2020

Abstract. Competing orders in condensed matter give rise to the emergence of fascinating, new phenomena. Here, we investigate the competition between superconductivity and charge density wave in the context of layered-metallic compounds, transition metal dichalcogenides, in which the superconducting state is usually suppressed by the charge density wave. We show, using real-space self-consistent Bogoliubov-de Gennes calculations and momentum-space calculations involving density-functional theory and dynamical mean-field theory, that there is a surprising reappearance of superconductivity in the presence of non-magnetic disorder fluctuations, as observed in recent experiments.

1 Introduction

The issue of disorder and Coulomb interaction, competing with each other, is an old one. In the absence of interaction, disorder is known to localize electronic states. The problem appears in systems where superconductivity (SC) competes with long-range orders like charge density wave (CDW) [1–3] and spin density wave (SDW) [4]. There is a large body of literature on the competition between SC and SDW in presence of disorder [5], while much less is discussed on SC and CDW competing with each other.

In the weak coupling case, these orders compete for the same Fermi surface and when disorder suppresses one, the other grows at its expense. Note that for s-wave SC, non-magnetic disorder (unless very strong) has little effect, while it pushes the CDW instability down. From a traditional view point, superconductivity and CDW are considered as weak coupling Fermi surface instabilities mediated by phonons [7]. There have been reports of both cooperation [6] and competition [1,8] between the two, though on the face of it, they compete for the same electrons. The original idea of a CDW due to Fermi-surface nesting (Peierls instability) has rarely been borne out in real systems where nesting is scarce. Moreover, even if it exists, nesting appears at the wrong wave vectors and away from the Fermi surface quite often [8,9]. Therefore, such single-particle mean-field pictures, invoking large segments of the Fermi surface nested with each other, need to be abandoned in favor of an alternative, strong coupling view. The strong coupling approach is further supported by the finding of $2\Delta/k_B T_{sc} > 5$ (where $\Delta$ is the superconducting pairing gap at zero temperature and $T_{sc}$ is the superconducting transition temperature) in many transition metal dichalcogenides (TMDs) [10] (about 7 for 1T-TiSe$_2$ and 10 for 2H-TaSe$_2$).

The TMDs have typically shown bad metallic resistivity above $T_{CDW}$, the CDW ordering temperature, becoming quadratic and more metallic below it. There is often little or no anomaly across the transition. The linear resistivity at high temperature is persistent till fairly high temperatures [11,12]. In spite of such overwhelming indications to the contrary, and the near-absence of required Fermi-surface nesting, much of the theoretical work on TMDs took recourse to mean-field considerations. Mottness has not been considered important for TMDs, except for 1T-TaS$_2$ [13] long back and for 2H-TaSe$_2$ [12,14] and 1T-TiSe$_2$ [16] lately. Large spectral weight transfer and absence of phonon signatures at typical energies in ARPES data, along with momentum-independent self-energy [17] are strong pointers to physics beyond (mean-field) single-particle processes.
Superconductivity in most of the TMDs also possesses interesting questions. It usually appears when the CDW is suppressed by disorder, intercalation or pressure [18]. One such approach has recently been taken by Li et al. [19] where, in 2H-TaSe$_2$, Se is replaced by sulphur (S) gradually, all the way to 2H-TaS$_2$. They report an emergence of robust superconducting order in single crystal TaSe$_{2−x}$S$_x$ (0 < x < 2) alloy. The SC transition temperature ($T_{SC}$) of the alloy is more than that of the two end-members TaSe$_2$ and TaS$_2$. The conductivity near the middle of the alloy series is also found to be higher than that of either 2H-TaSe$_2$ and 2H-TaS$_2$. This observation clearly suggests that superconductivity in this system is in competition with CDW.

In order to understand this competition, we take up the problem of co-existing CDW and SC and add non-magnetic disorder to it. Two kinds of disorder are studied: random disorder (uniform probability in real space with fixed strength) and clusters of disordered regions of fixed strengths. Using a self-consistent Bogoliubov-de-Gennes (BdG) formulation, we observe the evolution of SC and order parameter $\Delta_{CDW}$ as a function of increasing disorder. Such work has been used in the context of disordered superconductivity during the heyday of high $T_c$ superconductivity [21,22].

In addition, we also approach the alloy problem from a strong-coupling point of view at specific dopings. A density functional theory, followed by multi-orbital dynamical mean field theory (DFT+MO-DMFT) calculations for TaSe$_{2−x}$S$_x$ (at x = 0 and 1) are performed to understand the nature of the competition between CDW and SC. The disorder-induced competition is introduced via doping of sulfur which affects the band structure slightly, while acting as a substitutional disorder. The strong-coupling approach views the CDW as a condensate out of a pre-formed excitonic liquid [14,16] of bad metals. The unconventional CDW found in the parent dichalcogenide is a Bose-condensate of pre-formed excitons from high temperature. As there is no magnetism found in TMD, the alloy is a bad metal without magnetic fluctuations. Therefore direct comparisons can be drawn with non-magnetic disorder that degrades CDW and facilitates SC at low temperatures. The paper is arranged as follows: we discuss the methods employed in the following section. We then discuss the results and draw our conclusions at the end.

2 Methods

To investigate the interplay between charge density wave and superconductivity in the presence of real-space potential fluctuations, we use a self-consistent BdG formalism in which the s-wave superconducting pairing gap ($\Delta_{SC}$) and charge density wave order parameter ($\Delta_{CDW}$) are computed for a given disorder configuration.

2.1 Self-consistent BdG formalism

In this method, we consider a square lattice of size $N = 41 \times 41$, with open boundary conditions, and the order parameters, $\Delta_{SC}$ and $\Delta_{CDW}$, are computed self-consistently, until convergence is achieved at each lattice site.

We consider the following BdG Hamiltonian for disorder-affected superconductor on a square lattice

$$\mathcal{H}_{BdG} = -t \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + H.c.) - \sum_{i,\sigma} (\mu - V_i c_{i\sigma}^\dagger c_{i\sigma}) + \sum_i (\Delta_{SC}^{i\dagger} c_{i\uparrow}^\dagger c_{i\downarrow} + H.c.)$$

(1)

where $t$ is the nearest-neighbor electron hopping energy, $V_i$ is the local non-magnetic disorder in the chemical potential $\mu$. Two types of configuration of the onsite disorder $V_i$ have been considered in this study: (i) clustered regions of the disorder as shown in Figure 1d and (ii) randomly distributed disorder as shown in Figures 1g and 1f. The onsite disorder $V_i$ is varied within a range $-V_d \leq V_i \leq V_d$, where $V_d$ is the strength of the disorder. $\mathcal{H}_{BdG}$ is diagonalized via a Bogoliubov-Valatin transformation $c_{i\sigma} = \sum_{\sigma'} u_{i\sigma\sigma'} c_{n\sigma'} + v_{i\sigma\sigma'} c_{n\sigma'}^\dagger$, which gives the following equation for the local superconducting order parameter $\Delta_{SC}^{i} = -U_{SC} \langle c_{i\sigma}^\dagger c_{i\sigma} \rangle$, where $U_{SC}$ is the strength of the pairwise electron-electron attractive interaction, in terms of the Bogoliubov quasiparticle and quasihole amplitudes $u_{i\sigma}$ and $v_{i\sigma}$

$$\Delta_{SC}^{i} = -U_{SC} \sum_n [u_{n\uparrow} v_{n\downarrow}^* (1 - f(E_n)) + u_{n\downarrow} v_{n\uparrow}^*]$$

(2)

where $f(E_n) = 1/(1 + e^{E_n/kT})$ is the Fermi function at temperature $T$ and at the $n$th energy eigenvalue $E_n$. The quasiparticle and quasihole amplitudes $u_{i\sigma}$ and $v_{i\sigma}$ are determined by solving the following BdG equations

$$\mathcal{H}_{BdG} \phi_n^i = \epsilon_n \phi_n^i$$

(3)

written in the basis $\phi_n = [u_{n\uparrow}, u_{n\downarrow}, v_{n\uparrow}^*, v_{n\downarrow}^*]$. The above equations (Eqs. (2) and (3)) are solved self-consistently on a finite, two dimensional square lattice with open boundary conditions and the superconducting order parameter is determined using $\Delta_{SC} = \frac{1}{N} \sum_i \Delta_{SC}^{i}$, averaged over several realizations of disorder configuration.

The CDW order is modeled via a real-space modulation of the onsite potential, expressed by the following Hamiltonian, which is added to equation (1) for the self-consistent solution,

$$H_{CDW} = -U_{CDW} \sum_i (\cos(Q_x x + \alpha) + \cos(Q_y y + \beta)) c_{i\uparrow}^\dagger c_{i\downarrow} + \text{h.c.}$$

(4)

where $U_{CDW}$ defines the strength of the CDW order, $Q_x, Q_y$ are the CDW wave vectors, $\alpha$ and $\beta$, when non-zero, give incommensurate CDW. The local CDW order parameter is calculated using $\Delta_{CDW}^i = (1/U_{CDW})(2n - \xi_i)$, where $n = (1/N) \sum_i (\xi_{i\sigma} c_{i\sigma})$ is the total average.
carrier density at a given set of parameters and $\xi_i$ is the local carrier density due to CDW. The mean CDW order parameter is obtained, as in the previous case of SC order parameter, by averaging over all lattice sites $\Delta_{CDW} = (1/N) \sum_i \Delta_{CDW}$. In the present study, we consider CDW order to be dominant over the SC order in the homogeneous situation ($V_d = 0$) and choose $U_{SC} = 2t$ and $U_{CDW} = 4t$ throughout the manuscript, with no qualitative change in the result for other choices, as long as $U_{CDW} > U_{SC}$. Also, we express all energies for the results present here, obtained from the BdG analysis, in units of the hopping energy scale $t$ as wet set $t = 1$.

2.2 Combined DFT+DMFT approach

2H-TaSe$_2$ has a layered hexagonal structure (space group P63/mmc). The crystal structure contains layers of transition metals and chalcogens, arranged along the z direction; these layers are separated by van der Waals gap. First principles calculations were performed using WIEN2k [24] full-potential linearized augmented plane wave (FP-LAPW) ab initio package within the DFT formalism to get the band structure, density of states (DOS) and related quantities. A $10 \times 10 \times 10$ k-mesh (with the cutoff parameter, $R_{k_{\text{max}}} = 7.5$) is used here.
and a generalized gradient approximation Perdew-Burke-
Ernzerhof (GGA-PBE) exchange correlation potential
is chosen. The muffin-tin radius, R_{mt} is chosen to be
2.5 a.u. for Ta, 2.39 for Se, and 2.21 for S (used for
doping). The cell parameters are derived from an ear-
lier experiment [19]. Finally the self-consistent field (scf)
calculations are evaluated with an accuracy of 0.0001 eV
and the energy-minimized crystal structure is obtained
for the parent and doped dichalcogenide. From the con-
verged structure we determined the band structure and
DOS. To carry out transport calculations, a fully charge-
self-consistent dynamical mean field theory (DMFT) is
used. In a strongly-correlated system, like a TMD, DFT,
combined with DMFT, has been successful in explaining
a host of experimental results. The multi-orbital iterated
perturbation theory (MO-IPT), a computationally fast
and effective impurity solver, has been used here. Though
not exact, it works nicely in real systems for both high and
low temperature regimes. Here we have used multi-orbital
Hubbard model with reasonable intra and inter-orbital
Coulomb interactions. The total Hamiltonian is expressed
as,
\[ H = \sum_{k,a,b} t_{k,a,b} c_{k,a}^\dagger c_{k,b} + U \sum_{i,a} n_{i,a\uparrow} n_{i,a\downarrow} + U' \sum_{i,a,b} n_{i,a} n_{i,b} \]
(5)
where \( a, b \) denote the DFT conduction (Ta-d) band and
valence (Se-p and S-p) bands) with dispersions \( t_{aa}, t_{bb} \)
(calculated from WIEN2K program). \( t_{ab} \) is the interorbital
hopping and \( U \) and \( U' \) are the intra- and inter-orbital
Coulomb repulsions. Initially \( t_{ab} \) is taken as 0.4 eV for
2H-TaSe\(_2\) which is effectively modified inside DMFT self
consistency equation according to the modified band
structure and doping. \( U \) and \( U' \) are chosen as 1.0 eV and
0.5 eV after checking for the possible values to show the
CDW induced changes in resistivity.

3 Results

3.1 Results from self-consistent BdG calculations

We present our results from the BdG calculation on
an extended Hubbard model first. In our model, we have
considered a 2D s-wave superconductor with CDW
order and non-magnetic disorder. With the parameters
(unit of energy \( t = 1 \)) mentioned above we averaged all
the observables for 200 independent realizations of two
different types of disorder: (i) a random choice of disor-
der sites without any bias and (ii) a clustered disorder
configuration.

For better understanding we provided here spatial dis-
tribution of CDW order and superconducting gap with
different disorder strengths in both random and clustered
disorder configurations in Figure 1. The spatial profiles
of disorder ((a), (d), (g), (j)), \( \Delta_{SC} \) ((b), (e), (h), (k)) and
\( \Delta_{CDW} \) ((c), (f), (i), (l)) are shown in Figure 1. Though
the disorder is completely uncorrelated from site to site, emer-
gence of superconducting islands increases with increasing
disorder. These superconducting islands are separated
from one another by very small CDW regions and the
size of the islands is the measure of coherence length and
can be tuned with disorder strength and superconducting
pair potential. For initial assumption we considered here
incommensurate CDW and start from an initial guess of
CDW and superconducting order. We find that:

- Random potential fluctuations which are not spa-
tially coherent cannot lead to the reappearance of
superconductivity.

- There is a connection between the coherence length of
superconductivity and the wavelength of CDW
vectors.

- We have considered disorder on a microscopic scale
and the combination of the pairing interaction,
disorder concentration and amplitude of the impur-
ities. This combination leads to superconducting
islands separated by insulating region. Our results
on the disorder strength dependence of supercon-
ducting and CDW order for the two types of
disorder are shown in Figure 2. For both ran-
domly distributed and clustered disorder, CDW
order parameter decreases slowly while the SC
order parameter increases, indicating that the emergence
of superconducting order takes place in a highly-
disordered situation. For both kinds of disorder
enhancement of superconductivity may be related
to disorder induced changes in stoicheometry and
lattice bond lengths. In our model, a disorder term
essentially describes a random fluctuation in the
chemical potential. In reality, however, such poten-
tial fluctuations could appear from any change in the
stoicheimetry and/or bond lengths.

However a clustering of impurities is the most
probable scenario for a macroscopic superconducting
order to appear. For impurities distributed randomly
over the two-dimensional space, the reappearance
of robust superconducting order will require large
concentration of impurities (more than 20 percent).

- The spectral gap (Fig. 3) in one-particle density of
states persists through all the ranges of disorder
in spite of growing number of sites. Not only does the
spectral gap persist in the disordered state, it
increases with increasing disorder.

In the present setting (shown in Fig. 1) the CDW wave-
length is small to start with: in Figure 1b for example, the
CDW is like a checkerboard pattern. What we find is that
if we take longer CDW wavelength, SC is not suppressed
much (or by negligible amount) by CDW in the absence of
disorder. This is also understandable as the density modu-
lation due to CDW occurs over a large length scale which
does not affect SC. On the other hand, if CDW has a
small wave vector (i.e., rapidly changing carrier density)
SC is strongly affected. The macroscopic superconduct-
ing coherence sets in over a coherence length which the
short-wavelength CDW militates against. There is, there-
fore, a connection between the CDW wave vector and SC
coherence length. Disorder sets in its own length scale in
the problem by localizing charges, disturbing the existing
charge-density profile, facilitating SC order to emerge.
Fig. 2. Variation of $\Delta_{CDW}$ and $\Delta_{SC}$ with disorder strength in (a) clustered disorder configuration and (b) random disorder configuration. In clustered disorder $\Delta_{CDW}$ decreases with disorder strength and it follows the same trend in random disorder. With both disorder at a concentration strength $V_d = 7$ both superconductivity and CDW coexists and superconducting order parameter increases with increasing $V_d$.

Fig. 3. Spatial profile of the carrier density modulation $\xi_i$, revealing the CDW pattern at different Q vectors (a) $(Q_x, Q_y) = (1,1)$, (b) $(Q_x, Q_y) = (0.75,0.75)$, (c) $(Q_x, Q_y) = (0.5,0.5)$ and (d) $(Q_x, Q_y) = (0.25,0.25)$.

We varied the Q values as described in Figure 4. The charge density modulation can have larger period and the checkerboard pattern (shown in plot (a) in figure below), obtained at $(Q_x, Q_y) = (1,1)$, is the case that we focus in our description. We find that the suppression of the superconductivity by the CDW order decreases with increasing CDW period (or decreasing the values of $Q_x$ and $Q_y$). With a smaller CDW period (e.g., in plot (a)), the carrier density fluctuation is stronger and the lattice sites lose long-range superconducting coherence. So a large superconducting coherence length will help the global superconductivity for its resilience against the CDW order.

In the TMD compounds, for example TaS$_2$ or TaSe$_2$, the Ta ions form a triangular lattice. However, the problem that we discuss in this work i.e. the competition between the order parameters of superconductivity and charge density wave in the presence of the non-magnetic disorder is a general one and it does not depend explicitly on the underlying lattice geometry. The main observation, i.e. the reentrance of superconductivity in the presence of non-magnetic potential fluctuation, that we extract from our analysis of square lattice is expected to be present in a triangular lattice also.

3.2 DFT+DMFT results

As discussed above, the normal state of TMDs are dominated by incoherent scattering of electrons condensing in to a more coherent CDW state at $T < T_{CDW}$. To study the competition between superconductivity and CDW order, we have used DFT+DMFT calculation on the transition metal dichalcogenide 2H-TaSe$_2$, where Se is substituted gradually by S, as reported by Li et al. [19]. A random concentration of substitution by this method entails huge computational efforts. We work therefore at only two composition (equal Se and S, $x = 1$ and $x = 0$). As we show, the chemical substitution does indeed lead to a competition between CDW and SC and our theory captures the essential results of Li, et al. Band structures for 2H-TaSe$_2$ and 2H-TaSe$_2$-$x$S$_x$ have been computed within the WIEN2K. The crystal structure of the unit cell is shown in Figure 4a. The band structures for both the structures are calculated from WIEN2K. Band diagram (Figs. 4b and 4c) of 2H-TaSe$_2$ shows strong Ta-d$_z^2$ character hybridized with Se-p in the two metallic bands crossing the Fermi level due to the two layers of TaSe$_2$ coupled by van der Waals interaction.

The two bands should be degenerate at the K point but a small difference appears due to the overestimation of potential in WIEN2K. However, this was seen earlier also [25], and our band structure is in close agreement with it.
the Fermi level with slight modification. The Fermi surface (Figs. 5f and 5g) also reveals the same features. The parent structure shows a Fermi surface with hexagonal symmetry and six hole pockets which remain almost same in the doped structure. The evolution of unit cell parameters with doping is consistent with experimental data [19]. Since the basic structures of 2H-TaSe$_2$ and 2H-TaSe$_{2-x}$S$_x$ are same, the small changes in parent band structure due to doping can be considered as crystallographic disorder. We will now show how it helps in destroying CDW and stabilizing superconductivity.

The parent compound 2H-TaSe$_2$ has two CDW transitions (120 K and 90 K) down to low temperatures and the reported superconductivity is below 1 K (∼0.14 K). It is well known that DMFT is an excellent approximation to compute transport coefficients (directly from DMFT Green’s function) since irreducible vertex corrections vanish for one-band model and are small for multiband situations. Examination of CDW state through resistivity in this dichalcogenide shows a change in slope of resistivity around 120 K in 2H-TaSe$_2$ (Fig. 6a) which is the onset of incommensurate CDW. The resistivity decreases monotonically thereafter without any feature (Fig. 6a inset). The onset of commensurate CDW order at 90 K does not reflect in the resistivity as the condensation of pre-formed excitons already began at a higher temperature [14]. We then calculate the resistivity from DMFT (Fig. 6a, red lines) for 2H-TaSe$_2$ and found that there is no signature of a CDW for $x = 1$ compound. Below 5 K, the resistivity suddenly drops shapely to a very small value indicating the onset of an SC transition at 5 K as $x = 1$ alloy.

In the excitonic CDW scenario [14], the carrier scattering above $T_{CDW}$ is due predominantly to incoherent pre-formed excitonic fluctuations in TMD systems. The CDW transition is argued as a coherence-restoring transition of these pre-formed excitons. In order to discuss a CDW or SC state from a single-site DMFT, we follow the excitonic route [14] discussed earlier. An effective model for the incoherent metal is written down and a mean-field analysis for the CDW instability is performed thereon (vide Refs. [14,16]). The partial restoration of coherence in the low temperature phase is achieved through excitonic condensation. The superconductivity follows in a similar manner when the instability is in the particle-particle channel. The resistivity above the instabilities, tellingly, reflects this excitonic fluctuation with a linear behaviour at high temperature (exponent $n = 1$) until CDW or SC order sets in.

Disorder brings in a new length scale in the problem and degrades CDW order by localizing charges and suppressing excitonic fluctuations. However, superconductivity is not affected by disorder, unless it is too strong. This is primarily the reason why SC shows up at the expense of CDW as disorder increases. This also implies that the resistivity actually goes down with disorder initially (till disorder-induced charge localization comes into effect) in the CDW state, seen in our DMFT calculations.

Next we present the superconducting order parameter $\Delta_{SC} \propto \langle c_{\alpha\uparrow} c_{\alpha\downarrow} \rangle$ (shown in Fig. 6b) at $x = 1$, calculated self-consistently from DMFT, to directly check the SC transition seen in resistivity at 5 K. The order parameter follows $(1 - T/T_c)^{1/2}$ behaviour and vanishes near 4.5 K (where the resistivity also drops). Thus both qualitative and quantitative agreement of our theoretical results with earlier experiments strongly support the argument that disorder or doping degrades CDW and facilitates superconducting order. Vanishing of CDW with doping also leads to an increase in carrier density with doping. So the substitutional disorder stabilizes SC at a higher temperatures than the putative $T_c$. We presented a detailed study of the effect of disorder on the CDW transition, and it appears that in certain parameter regimes, disorder may facilitate an SC state at the expense of charge density order.

Tuning from CDW to SC phase can be accomplished by intercalation, doping and pressure and has been explored largely through experiments. The above findings have important indications for SC arising in disordered state. We have introduced disorder in the TMD by isoelectronic substitution. Substituting Se by S increases superconducting $T_c$ and at $x = 1$ there is no sign of CDW and resistivity varies linear in $T$ due to disorder induced scattering. A finite doping increases carrier density at the Fermi level and disorder redistributes electrons and holes in the system, analogous to disordered chemical potential which in turn weakens CDW order. In excitonic CDW, as found earlier in parent system [14] when excitonic fluctuations are maximized CDW is destroyed. In disordered square lattice we also found that CDW order is destroyed with increasing disorder strength or fluctuation in both clustered and random disorder. These constitute the critical collective fluctuations which lead to multiband SC with
Fig. 5. (a) Crystal structure of 2H-TaSe$_2$, band structure of (b) 2H-TaSe$_2$ and (c) 2H-TaSeS along Γ − M − k − Γ direction. Density of states and Fermi surface of (d) and (f) 2H-TaSe$_2$ and (e) and (g) 2H-TaSeS. Slight modification in the band structure can be observed due to doping which can be taken as an effect of disorder due to doping.

Fig. 6. (a) Main panel shows DMFT resistivity with temperature for $x = 0$ and $x = 1$. Upper inset presents resistivity with parent 2H-TaSe$_2$ around 120 K while lower inset presents resistivity of 2H-TaSeS around 5 K. (b) DMFT superconducting order parameter plot with temperature for 2H-TaSeS: green points represent actual date points while the red line is a fit.
a finite value of superconducting order: this is again in accord with the observation of BdG calculation. In conclusion, here we show that disorder induced fluctuation reduces CDW and maximizes superconductivity both in BdG calculation and also in TMD alloy.

SK acknowledges department of science and technology, Govt of India women scientist scheme (SR/WOS-A/PM-80/2016(G)) for finance.

**Author contribution statement**

AT devised the problem. SK and NM have performed the theoretical calculations. All authors have analysed the results, written and reviewed the manuscript.

**Publisher’s Note** The EPJ Publishers remain neutral with regard to jurisdictional claims in published maps and institutional affiliations.

**References**

1. A. Taraphder, R. Pandit, H.R. Krishnamurthy, T.V. Ramakrishnan, Int. J. Mod. Phys. B 10, 863 (1991)
2. S. Seo et al., Nat. Phys. 10, 120 (2014)
3. K.S. Kim, Phys. Rev. B 75, 075105 (2007)
4. Y. Mizyuki et al. Nat. Commun. 5, 5657 (2014)
5. H. Alloul et al., Rev. Mod. Phys. 81, 45 (2009)
6. T. Kiss et al., Nat. Phys. 3, 720 (2007)
7. G. Gruner, Rev. Mod. Phys. 60, 1129 (1988)
8. S.V. Borisenko et al., Phys. Rev. Lett. 102, 166402 (2009)
9. M.D. Johannes, I.I. Mazin, Phys. Rev. B. 77 165135 (2007)
10. W.L. McMillan, Phys. Rev. 167, 331 (1968)
11. S.V. Dordevic et al., Eur. Phys. J. B 33, 15 (2003)
12. V. Vescoli et al., Phys. Rev. Lett. 81, 453 (1998)
13. P. Fazekas, E. Tosatti, Philos. Mag. B 39, 229 (1979)
14. A. Taraphder, S. Koley, N.S. Vidhyadhiraja, M.S. Laad, Phys. Rev. Lett. 106, 236405 (2011)
15. Dordevich et al., Eur. Phys. J. B 33, 15 (2003)
16. S. Koley et al., Phys. Rev. B 90, 115146 (2014)
17. T. Valla et al., Phys. Rev. Lett. 85, 4759 (2000)
18. A.F. Kusmartseva, B. Sipos, H. Berger, L. Forro, E. Tutis, Phys. Rev. Lett. 103, 236401 (2009)
19. L. Li et al., Nat. Phys. J. Quantum Mater. 2, 11 (2017)
20. N. Mohanta, A. Taraphder, J. Phys.: Condens. Matter 26, 025705 (2014)
21. G. Alvarez, M. Mayr, A. Moreo, E. Dagotto, Phys. Rev. B 71, 014514 (2005)
22. B. Chatterjee, A. Taraphder, Solid State Commun. 148, 582 (2008)
23. S. Koley, Solid State Commun. 251, 23 (2017)
24. P. Blaha, K. Schwarz, G.K.H. Madsen, D. Kvasnicka, J. Luitz, WIEN2k. An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties (Karlheinz Schwarz, Techn. Universitat Wien, Wien, 2001)
25. J. Laverock et al., Phys. Rev. B 88, 035108 (2013)