Role of layer packing for the electronic properties of the organic superconductor 
(BEDT-TTF)$_2$Ag(CF$_3$)$_4$(TCE)

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The charge transfer compound (BEDT-TTF)$_2$Ag(CF$_3$)$_4$(TCE) crystallizes in three polymorphs with different alternating layers: While a phase with a ω packing motif has a low superconducting transition temperature of $T_c = 2.6$ K, two phases with higher $T_c$ of 9.5 K and 11 K are multi-layered structures consisting of α’ and ω layers. We investigate these three systems within density functional theory and find that the α’ layer shows different degrees of charge order for the two ω-α’ systems and directly influences the electronic behavior of the conducting κ layer. We discuss the origin of the distinct behavior of the three polymorphs and propose a minimal Hubbard-like Hamiltonian for the description of these systems based on projective molecular Wannier functions.

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I. INTRODUCTION

Since a few decades organic charge transfer salts (CT) built of donor and acceptor molecular complexes have attracted a lot of attention due to the variety of ground states in their phase diagrams. Application of external or chemical pressure can lead to antiferromagnetic insulating, charge ordered, spin density wave, spin liquid or unconventional superconducting ground states. Tendencies in the dimensionality of the electronic transport are often determined by the choice of conducting molecules: Compounds containing TMTTF (tetramethyltetrathiafulvalene) molecules for example are typically one-dimensional, whereas several phases of BEDT-TTF (bisethylenedithio-tetrathiafulvalene) based salts show two-dimensional behavior. However, the arrangement of the (donor) molecules in these complexes is decisive. Among the BEDT-TTF family of CT salts, many different packings classified as α, α’, β, β’, β”, δ, κ and θ have been experimentally realized and a wide range of different physical properties was found. Depending on the preparation conditions, different polymorphs of one structure can be synthesized; for example (BEDT-TTF)$_2$I$_3$ crystallizes in α, β, θ and κ forms. Polymorphs provide an opportunity to explore the influence of the packing motif on the electronic properties. Effects originating from differences in the anion layer composition can be excluded in this case since this layer remains unaltered in the polymorph family.

Here we consider the polymorph charge transfer salt family (BEDT-TTF)$_2$Ag(CF$_3$)$_4$(TCE) (see Fig. 1 first synthesized by Schlüter and collaborators. TCE stands for 1,1,2-trichloroethane and in the following we will make use of the common abbreviation ET for BEDT-TTF. These systems show a metallic behavior at low temperatures and a $T_c$ of 2.6 K to a superconducting state was measured for the single-layered compound (Fig. 1 (a)) where the ET molecules form dimers arranged in a so-called κ pattern. The term κ phase was coined for this structure, with the index L referring to the low $T_c$. Structural refinement of the other two multi-phase polymorphs (Figs. 1 (b), (c) and Fig. 2) showed the presence of charge-ordered layers in α’ packing between the κ-type layers; α’ phases have also been characterized as Mott-Hubbard insulators. Even though as insulating layers they do not contribute directly to superconductivity, their existence seems to enhance the superconducting transition temperature in (BEDT-TTF)$_2$Ag(CF$_3$)$_4$(TCE). While the dual-layered κ-α’ phase exhibits superconductivity at a critical temperature of 9.5 K which is approximately 3.5 times higher than the $T_c$ of the κ- phases, the four-layered κ-α’$_2$ phase shows superconductivity at 11 K and therefore belongs to the organic superconductors with the highest measured critical temperatures.

In this work we perform density functional theory (DFT) calculations for the three polymorphs. We especially focus on the effects of the α’ layers on the electronic properties of the κ layers in the dual and four-layered systems and perform a comparative analysis of the three systems in terms of $ab$ initio-derived tight-binding Hamiltonians using the projective Wannier method. While all three systems show apparently similar κ-bands, the charge ordering in the α’ layer in κ-α’$_1$ and κ-α’$_2$ influences significantly the magnitude of the hoppings in the conducting κ layer. Analysis of the degree of frustration within a minimal triangular lattice model hints to the different superconducting $T_c$ in these systems.

II. CRYSTAL STRUCTURE

κ phase.- The single-layered phase crystallizes in the orthorhombic Pnma space group and its unit cell contains two donor layers which are separated by an insulating layer consisting of the anion [Ag(CF$_3$)$_4$]$^-$ and the solvent TCE. However, the anion layer is disordered. In order to simplify the density functional theory calculations we choose one of the two symmetry-allowed orien-
FIG. 1: Crystal structures of the three polymorphs of (BEDT-TTF)$_2$Ag(CF$_3$)$_4$(TCE).

FIG. 2: Crystal structure of $\kappa$-1$'$-(BEDT-TTF)$_2$Ag(CF$_3$)$_4$(TCE) together with cuts illustrating the two alternating ET patterns. In (b) and (c), colored outlines mark symmetry inequivalent ET molecules.

FIG. 3: Schematic of BEDT-TTF molecule arrangement in the considered materials. (a) $\kappa$-type packing in the low $T_c$ (BEDT-TTF)$_2$Ag(CF$_3$)$_4$(TCE) compound. (b) $\kappa$-type packing in the two high $T_c$ compounds. $\alpha'$-type packing in the two-layer compound. (c) $\alpha'$-type packing in the four-layer compound. Symmetry inequivalent molecules are marked by numbers and colored differently. R (L) indicate tilting of the molecules to the right (left) in the $\alpha'$ layers.

layer.

$\kappa$-$\alpha'_1$ phase.- The triclinic crystal structure $P\overline{1}$ of the dual-layered compound is shown in Fig. 1(b). Compared to the single-layered phase, the layer in the center of the unit cell is here replaced by an $\alpha'$ packed layer. This packing motif is characterized by molecules that are lined up on a rectangular lattice (see Fig. 2 and Fig. 3(c)). The rows of molecules along $b$ alternate between a right and a left tilt with respect to the $a$ axis. This leads to the characteristic cross pattern when viewed along $a$ (Fig. 2 and Fig. 3(c)). In contrast to other $\alpha'$ packed structures, no dimerization and therefore also no shift along the long unit cell axis has been observed. The low symmetry of the space group means that the two ET molecules in a dimer are still related by inversion symmetry but there are two symmetry inequivalent dimers and in the $\alpha'$ layer, there are even four inequivalent ET molecules (see Fig. 2 and Figs. 3(b) and (c)).

$\kappa$-$\alpha'_2$ phase.- The polymorph with the highest superconducting critical temperature has the largest unit cell (Fig. 1(c)). Due to the monoclinic $P_{21}/n$ symmetry (space group No. 14), every second $\kappa$($\alpha'$) layer is shifted by half the lattice vector $a$. Note that DFT codes usually allow only one setting of space group No. 14; we therefore perform the calculations in a $P2_1/c$ setting. As in the case of $\kappa$-$\alpha'_1$, the monoclinic space group leads to two symmetry inequivalent (ET)$_2$ dimers in the $\kappa$ layer; the two ET molecules in a dimer are related by inversion symmetry (see Fig. 2(b)). The symmetry also leads to a checkerboard pattern of symmetry related ET molecules in the $\alpha'$ layer as displayed in Fig. 3(d).
III. ELECTRONIC STRUCTURE

We determine the electronic structure of (BEDT-TTF)$_2$Ag(CF$_3$)$_4$(TCE) using the all electron full potential local orbital basis as implemented in the FPLO code\cite{21} and the generalized gradient approximation functional\cite{22}. A $6 \times 6 \times 6 \ k$ mesh was employed to converge the energy and charge density.

κ phase.- The band structure and density of states (DOS) of the κ phase is presented in Fig. 4. There are eight bands in the energy window $[-0.6 \text{ eV}, 0.4 \text{ eV}]$ deriving exclusively from the highest occupied molecular orbitals (HOMOs) of the eight ET molecules in the unit cell. As there is only a very small dispersion in the stacking direction (Γ-Z path) the bands originating from the two layers in the unit cell are almost degenerate. The dimerization of the ET molecule pairs is reflected in the bonding ($[-0.3 \text{ eV}, 0.4 \text{ eV}]$) antibonding ($[-0.6 \text{ eV}, -0.3 \text{ eV}]$) character of the bands.

Integrating the partial densities of states for symmetry inequivalent molecules in the range $[-0.6, 0] \text{ eV}$ results in a charge transfer of one hole per (ET)$_2$ dimer to the anion layer.

κ-α'$_1$ phase.- In Fig. 5 we show the band structure and layer-resolved density of states of the dual-layered compound. The anion layer has no weight at the Fermi level. The elliptical shapes are due to the bands arising from the ET molecules of the κ-layer, while the wiggly lines are the almost one-dimensional features resulting from the α'-layer.

In Fig. 6 we show the band structure and layer-resolved density of states of the κ-α'$_2$ phase. The DFT band structure is shown with black lines, while the Wannier bands are displayed with blue (κ) and red (α') symbols.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig4.png}
\caption{DFT band structure and density of states of the κ phase. The blue bands are determined by the projective Wannier function method and originate from the ET HOMO orbitals.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig5.png}
\caption{Band structure and density of states (DOS) of the κ-α'$_1$ phase. The Wannier bands (blue symbols for κ orbitals and red symbols for α' orbitals) are in excellent agreement with the DFT bands.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig6.png}
\caption{Calculated Fermi surface of the dual layered compound: The elliptical shapes are due to the bands arising from the ET molecules of the κ-layer, while the wiggly lines are the almost one-dimensional features resulting from the α'-layer.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig7.png}
\caption{Band structure and density of states of the κ-α'$_2$ phase. The DFT band structure is shown with black lines, while the Wannier bands are displayed with blue (κ) and red (α') symbols.}
\end{figure}
level and therefore does not contribute to the electronic transport. The bands originating from the $\kappa$ layer are similar in shape to the bands of the $\alpha'$ phase (Fig. 1) while the $\alpha'$ bands are narrower and less dispersive than the $\kappa$ bands. The corresponding Fermi surface of the $\kappa$-$\alpha'_1$ phase is shown in Fig. 5. Here, the elliptical shape corresponds to the $\kappa$ layer and is typical for this packing motif.\cite{22} In contrast, the $\alpha'$ Fermi surface (wiggly lines in Fig. 5) is quasi-one-dimensional and has no dispersion in the $k_z$ direction.

Recent de-Haas-van-Alphen experiments for the dual-layered compound observed only elliptic orbitals originating from the $\kappa$ band\cite{13} and no $\alpha'$ bands were detected. However, one should mention that on the one hand the $\alpha'$ packed systems have been reported in the past as Mott-Hubbard insulators\cite{13,10} and, on the other hand, DFT underestimates correlation effects and cannot reproduce the insulating behavior of a Mott system. A better treatment of correlations beyond DFT in organic material\cite{13} (presently beyond the scope of this study) could lead to an opening of a gap at the Fermi level in the $\alpha'$ bands and to a Fermi surface with only $\kappa$ bands. Note, however, that direct hybridization between $\alpha'$ and $\kappa$ layers is almost negligible (maximum $\alpha'$ to $\kappa$ hopping parameters in $\kappa$-$\alpha'_1$ and $\kappa$-$\alpha'_2$ are 0.2–0.3 meV) so that it is clearly justified to focus our investigation on the properties of the $\kappa$ layers even in $\kappa$-$\alpha'_1$ and $\kappa$-$\alpha'_2$ as these layers will be responsible for the observed superconductivity.

The charge transfer in this system has more features than in the pure $\kappa$ phase compound due to the low symmetry and the presence of the $\alpha'$ layer. We find that the right tilted ET molecules in the $\alpha'$ plane contribute a charge of the order of $1/3$ electron (0.343 for ET molecule 3 as denoted in Fig. 3(c) and 0.316 for molecule 4). The other two left tilted molecules show a larger charge transfer of the order of $2/3$ of an electron (0.658 for molecule 1 and 0.705 for molecule 2). For clarity, we depict in Fig. 8 this charge ordering. A similar charge disproportionation has already been observed in other $\alpha'$ charge transfer salts (i.e., in $\alpha'$-ET$_2$Ag(CN)$_2$ \cite{20}, where the homogeneous charge transfer of the ET molecules at high temperature is redistributed to a $1/3$ vs. $2/3$ order upon cooling.

In the $\kappa$ layer, the symmetry of the crystal leads to two symmetry inequivalent (ET)$_2$ dimers with distances between the ET molecules in a dimer of $d_A = 3.77$ Å and $d_B = 3.74$ Å. However, the charge transfer from these dimers to the anion layer is the same within the computational accuracy (0.493 electrons for ET molecule A (see Fig. 3(b)) and 0.494 for molecule B).

$\kappa$-$\alpha'_2$ phase.- Fig. 7 shows the band structure and density of states of the four-layered compound. As the unit cell consists of four donor layers, there are sixteen bands corresponding to the HOMOs of the ET molecules. However, as the dispersion along the stacking direction is extremely small, the bands originating from the two identically packed layers in the unit cell are nearly pairwise degenerate and the band structure is very similar to that of the $\kappa$-$\alpha'_1$ compound. Nevertheless, the subtle quantitative differences between the electronic structure of the two systems, in particular in the $\alpha'$ bands, have important consequences on the behavior of the materials as it is reflected, for instance, in the charge transfer. The $P 2_1/c$ symmetry in $\kappa$-$\alpha'_2$ poses stronger restrictions on the charge transfer in the $\alpha'$ layer compared to the $P 1$ $\kappa$-$\alpha'_1$ system. The symmetry equivalent ET molecules form a checkerboard pattern on the rectangular lattice as shown in Fig. 3(d). The ET molecules on one of the $\alpha'$ sublattices donate 0.367 electrons, while the other molecules transfer approximately 0.611 electrons. Thus, the average charge transfer from the $\alpha'$ layers to the anion layer is slightly less than half an electron per ET molecule.

As in the $\kappa$-$\alpha'_1$ system, there are two symmetry inequivalent (ET)$_2$ dimers in the $\kappa$ layer. The distances of the molecules within the dimers differ slightly, at $d_A = 3.76$ Å and $d_B = 3.73$ Å. There is a small charge disproportionation between the dimers, with ET molecules of dimer A transferring 0.520 electrons to the anion, while those of dimer B transfer 0.500 electrons (compare Fig. 3(b)). Thus, the $\kappa$ layer compensates for the slightly too low charge transfer of the $\alpha'$ layer.

An important difference between the $\kappa$-$\alpha'_1$ and $\kappa$-$\alpha'_2$ phases is that the constraint imposed by the higher symmetry in $\kappa$-$\alpha'_2$ translates into a more symmetric charge order in the $\alpha'$ layer in $\kappa$-$\alpha'_2$ than in $\kappa$-$\alpha'_1$ and the corresponding $\alpha'$-$\kappa$ stacking in $\kappa$-$\alpha'_2$ shows the (ET)$_2$ dimers of the $\kappa$ layers always aligned on top of the stronger charged ET molecule in the $\alpha'$ layer, contrary to what happens
in $\kappa$-$\alpha_1'$ (Fig. 8). This has important consequences on
the Hamiltonian description of these systems as we show
below.

**IV. TIGHT-BINDING HAMILTONIAN**

We use the projective Wannier function method as im-
plemented in FPLO in order to obtain the tight-binding
parameters for the conducting $\kappa$ layers in (BEDT-
TTF)$_2$Ag(CF$_3$)$_4$(TCE) from Wannier function overlaps.
Considering the centers of the ET molecules as sites, the
tight-binding (TB) Hamiltonian can be written as:

$$H = \sum_{\langle ij \rangle, \sigma} t_{ij} (c_{i\sigma}c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + \sum_{[ij]} t'(c_{i\sigma}c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma})$$

(1)

where $c_{i\sigma}^\dagger$ creates (destroys) an electron on site $i$.

When the dimerization of the ET molecule pairs is
strong, the separation between bonding and antibonding
bands is large and the analysis of the low-energy tight-
binding Hamiltonian can be reduced to the two partially
occupied antibonding bands. This case corresponds to
a half-filled anisotropic triangular lattice where the sites
denote the centers of the (ET)$_2$ dimers:

$$H = \sum_{\langle ij \rangle, \sigma} t (c_{i\sigma}c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + \sum_{[ij]} t' (c_{i\sigma}c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma})$$

(2)

$t$ and $t'$ correspond to nearest and next nearest neigh-
bors hopping contributions. The hoppings between
dimers [Eq. (2)] can be connected to the hoppings between
molecules [Eq. (1)] using geometrical as well as analytical
considerations:

$$t \approx \frac{|t_2| + |t_4|}{2}, \quad t' \approx \frac{|t_3|}{2} \quad \text{and} \quad U \approx 2|t_1|$$

(3)

Here $t_1$ can be identified as the intradimer hopping pa-
rameter, while $t_2$ and $t_4$ are the hoppings between one
molecule and the two closest molecules on the orthogo-
nal oriented dimer. $t_3$ belongs to the hopping between
the closest ET molecules on neighboring equally oriented
dimers.

In Table I we list the hopping parameters between ET
molecules (Eq. (1) and Fig. 9 (a)) in the $\kappa$ layer of the three
polymorphs (BEDT-TTF)$_2$Ag(CF$_3$)$_4$(TCE). Due to the
presence of two inequivalent (ET)$_2$ dimers in $\kappa$-$\alpha_1'$ and
$\kappa$-$\alpha_2'$, these phases have twice as many TB parameters
compared to the $\kappa$ phase. For the $\kappa$-only system $A=B$. In
Table II, the tight-binding parameters for the dimer
model (Eq. (2) and Fig. 9 (b)) are listed.

A detailed analysis on the hopping parameters for $\kappa$-$\alpha_1'$
in Table I shows that the tight-binding parameters differ-
entiate between the two inequivalent (ET)$_2$ dimers and
reflect the stripy charge transfer found for the $\alpha'$ layer
and illustrated in Fig. 5. The more tightly bound dimers
(A) are above the stronger charged $\alpha'$ ET molecules with
a 2/3 hole, the less tightly bound dimers (B) are above
the weakly charged $\alpha'$ ET molecules with a 1/3 hole.

In $\kappa$-$\alpha_2'$, the strength of the dimerization as defined by
the size of the intradimer hoppings $t_1^\alpha$ and $t_1^\gamma$ is smaller
than in the other two polymorphs. Here, contrary to
the $\kappa$-$\alpha_1'$ case, the TB parameters don’t show the stripy
pattern from $\kappa$-$\alpha_1'$ since both the A and B (ET)$_2$ dimers
are aligned on top of a charge-rich ET molecule in the $\alpha'$
layer.

In all three polymorphs, the dimer model esti-
mate (Eq. 2) doesn’t give such a good represen-
tation of the band structure as, for instance, in
$\kappa$-(ET)$_2$Cu$_2$(CN)$_3$. This may partly be due
to the weak degree of dimerization in (BEDT-
TTF)$_2$Ag(CF$_3$)$_4$(TCE), but more importantly it re-
lates the fact that the basis defined by the hoppings between
dimer sites is not rich enough to correctly describe de-
tails of the band structure and Fermi surface. Only by
allowing the larger basis defined by the hopping ampli-
tudes between molecules can all relevant details be cap-
tured. Keeping in mind that the parameters of the dimer
models only indicate the relevant parameter range, we
can compare them to other previously examined $\kappa$ struc-

![Image](https://via.placeholder.com/150)
TABLE I: Tight-binding parameters for the $\kappa$ layers of all three phases. Distances between ET molecule centers are listed for identification of hopping paths.

| system       | $t_1$ (meV) | $t_2^A$ | $t_2^B$ | $t_2^A$ | $t_2^B$ | $t_4^A$ | $t_4^B$ | $t_4^A$ | $t_4^B$ |
|--------------|-------------|----------|----------|----------|----------|----------|----------|----------|----------|
| $\kappa$     | 168         | 102      | 33.4     | 60.8     |          |          |          |          |          |
| $d_i$ (Å)    | 3.73        | 5.59     | 6.73     | 6.83     |          |          |          |          |          |
| $\kappa-\alpha'_1$ | 170  | 161      | -98.8    | -98.8    | 64.1     | 67.6     | -38.1    | -32.4    |
| $d_i$ (Å)    | 3.74        | 5.60     | 5.65     | 6.64     | 6.66     | 6.84     | 6.85     |
| $\kappa-\alpha'_2$ | 166  | 163      | -98.0    | -98.8    | 70.5     | 62.9     | -35.2    | -37.4    |
| $d_i$ (Å)    | 3.73        | 5.59     | 5.64     | 6.61     | 6.67     | 6.83     | 6.83     |

FIG. 10: (a) Illustration of the eight nearest neighbor hopping paths in the molecule model for the $\kappa$ layer of the dual-layered phase. (b) Illustration of the tight-binding parameters of the dimer model.

The frustration, given by the ratio of the next nearest hopping to the nearest hopping $|t'/t|$ (Fig. 10) of the multi-layered phases ($\approx 0.5$) is close to 0.58 obtained for $\kappa$-(ET)$_2$Cu(SCN)$_2$ which is superconducting at a temperature of 10.4 K. The low $T_c$ $\kappa$ phase is less frustrated and the frustration parameter of 0.45 is just slightly higher than the one calculated for the antiferromagnetic insulator $\kappa$-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl.

TABLE II: Table of triangular lattice Hamiltonian parameters $t$, $t'$ and $U$ for the three polymorphs, given in meV.

| system       | $t^A$   | $t^B$   | $t'^A$  | $t'^B$  | $U^A$   | $U^B$   |
|--------------|---------|---------|---------|---------|---------|---------|
| $\kappa$     | 67.9    | 30.4    | 336     |         |         |         |
| $\kappa-\alpha'_1$ | -68.4 | -64.4   | 32.1    | 33.8    | 341     | 322     |
| $\kappa-\alpha'_2$ | -67.0  | -67.7   | 31.5    | 35.2    | 314     | 291     |

V. DISCUSSION AND CONCLUSIONS

Our microscopic analysis of the polymorph family (BEDT-TTF)$_2$Ag(CF$_3$)$_2$(TCE) with density functional theory and projective Wannier function derived tight-binding Hamiltonians showed that, even though the $\alpha'$ layer in these materials is most probably insulating, its electronic structure decisively influences the behavior of the conducting $\kappa$ layer in $\kappa-\alpha'_1$ and $\kappa-\alpha'_2$. In particular, the TB hopping parameters in $\kappa-\alpha'_1$ reflect the stripy-like charge ordered pattern shown by the ET molecules in the $\alpha'$ layer. In $\kappa-\alpha'_2$ there is no such pattern since the (ET)$_2$ dimers in $\kappa-\alpha'_2$ are always aligned on top of the stronger charged ET molecule in the $\alpha'$ layer. This different charge arrangement has its origin on the symmetry constraint imposed by $P2_1/n$ in $\kappa-\alpha'_2$. Our tight-binding model parameters for the molecule-based model (Eq. 1) and Table I provide an adequate and reliable starting point for a many-body description of these systems in terms of a Hubbard-like Hamiltonian where intramolecular and intermolecular Coulomb interaction terms should be added to the tight-binding Hamiltonian.

In contrast, an analysis in terms of the simplified dimer model (Eq. 2 and Table II) shows that the half-filled triangular lattice is not as good a starting point for describing these materials. This is due to the relatively weak dimerization of the (ET)$_2$ dimers and therefore the contribution of the $\kappa$ bonding bands shouldn’t be neglected when describing the electronic properties of these systems. However, the information obtained from the tight-binding hopping parameters in the dimer model is still useful to roughly classify the degree of frustration in (BEDT-TTF)$_2$Ag(CF$_3$)$_2$(TCE) and have first hints for understanding the different superconducting critical temperatures in these systems. Our comparison of the trends of the frustration parameters with earlier studies shows that the $\kappa$-phase system lies in the range of frustration where other $\kappa$ systems are antiferromagnetic insulators, while the multi-layered $\kappa-\alpha'_1$ and $\kappa-\alpha'_2$ show a slightly higher frustration degree as also observed in the superconductor $\kappa$-(ET)$_2$Cu(SCN)$_2$. Nevertheless, a detailed understanding of the different critical temperatures requires a many-body analysis of the molecular Hubbard-like model proposed here which is beyond the scope of the present work.

Summarizing, in this work we demonstrated and quantified the importance of the $\alpha'$ layers in the polymorph family (BEDT-TTF)$_2$Ag(CF$_3$)$_2$(TCE) although probably they are insulating layers and suggested a molecule-based model Hamiltonian to describe these systems. We hope that this work will motivate other groups to investigate these multi-layered materials which hold promise of increasing the superconducting critical temperatures.
in organic charge transfer superconductors.

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