Emergent 1D physics in a 3D molecular crystal, Mo$_3$S$_7$ (dmit)$_3$

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$\text{Mo}_3\text{S}_7(\text{dmit})_3$  

Activated conductivity,  
$\Delta \sim 16 \text{ meV}$

Unpaired spins, & no sign of magnetic order, $J/T \approx 50$.  

$\chi_T = C + \chi_0 T$

Llussar et al., JACS 126 12076 (2004)
Mo$_3$S$_7$(dmit)$_3$

- Spin-liquid candidate (magnetic susceptibility)
- Interesting crystal structure
- Suggestions of quasi-1D behaviour
2D Electronic Structure

Flat bands - totally localised states

Dirac points
3D Electronic Structure

Flat bands $\rightarrow$ quasi-1D bands

Dirac lines
Wannier Orbitals

- a (physically meaningful) basis of **localised orbitals** → Wannier orbitals
- Localised to dmit
- 6 per unit cell

A small Hilbert space of physically meaningful basis states.

Jacko, arXiv:1508.07735
Model from Wannier Orbitals

*ab initio* model construction – Compute a single, meaningful set of tight-binding parameters

→ *ab initio* tight binding model

Jacko, arXiv:1508.07735

Kagomene

What are the key features of the model?

Kagomene

2D \textit{ab initio} model – Kagomene

Kagomene

2D \textit{ab initio} model – Kagomene

Kagomene Lattice

$t_k \rightarrow \infty$

DFT

$t_g = \frac{3}{2} t_k$

$t_g \rightarrow \infty$

Molecular limit

Dimer limit

Flat Band States

Interference from adjacent sites on the triangle → no amplitude can leave the triangle
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Interference from adjacent sites on the triangle \(\rightarrow\) no amplitude can leave each triangle

Topological states: degeneracy depends on boundary conditions
Kagomite

3D *ab initio* model – Kagomite

Stacked layers of the Kagomene lattice:

Kagomite

All of these hopping integrals are similar magnitude.

The **topology** of the lattice leads to 1D behaviour.

Monomers in Hubbard Model

Solve monomer Hubbard model exactly at 2/3 filling

Monomers in Hubbard Model

Solve monomer Hubbard model exactly at 2/3 filling $\rightarrow$ Low energy spin-1 degree of freedom

Solve monomer Hubbard model exactly at 2/3 filling.

Perturbatively couple dimers: two possibilities → two exchange couplings.

$\tau_z \approx \tau_g$

Dimers in Hubbard Model

Solve monomer Hubbard model exactly at 2/3 filling.

Perturbatively couple dimers: two possibilities → two exchange couplings.

\[ J_z > J_g \]

The perturbative model is predominantly 1D.

Emergent 1D behaviour from 3D lattice: topological and many-body effects.

Mo$_3$S$_7$(dmit)$_3$ and related compounds need more experimental investigation!

*ab initio* models: Jacko, *arXiv*:1508.07735


Ben Powell’s talk