Emergent 1D physics in a 3D molecular crystal, $Mo_3S_7(dmit)_3$

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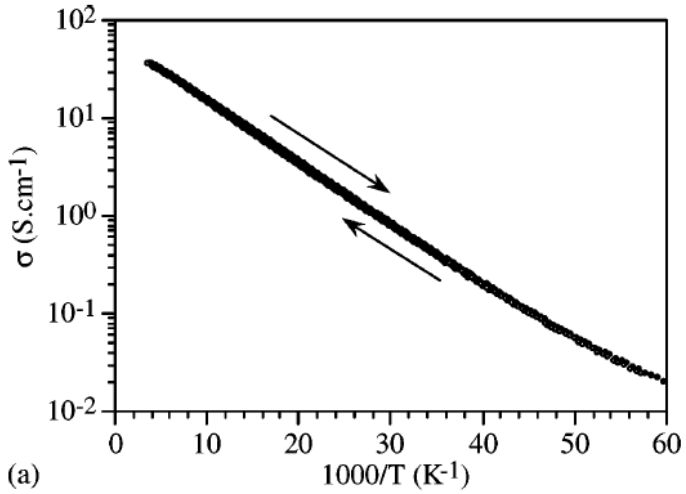
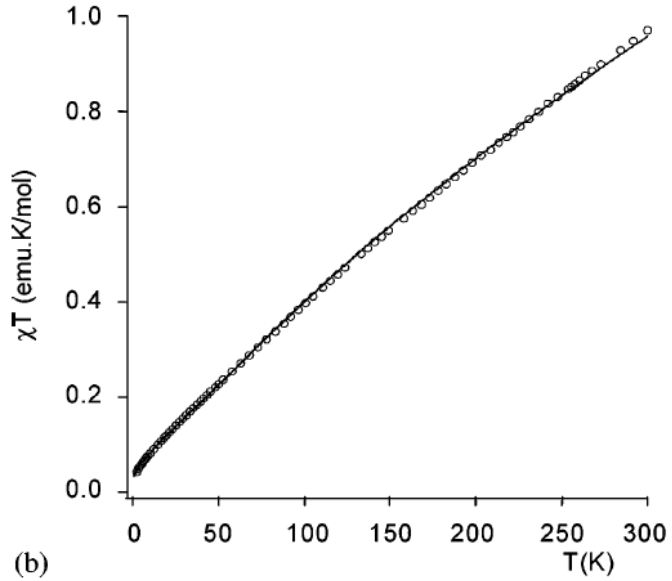
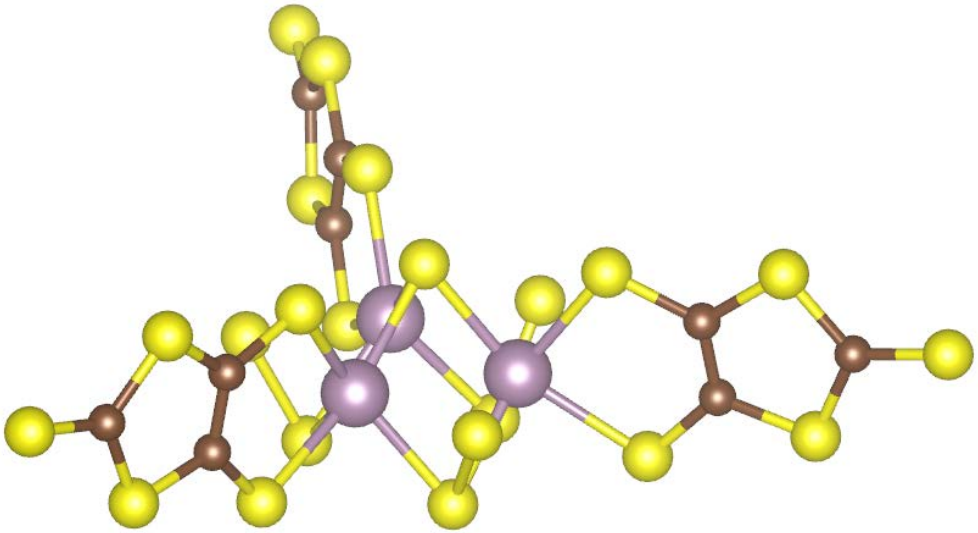
$Mo_3S_7(dmit)_3$





Activated conductivity,

$\Delta \sim 16$ meV

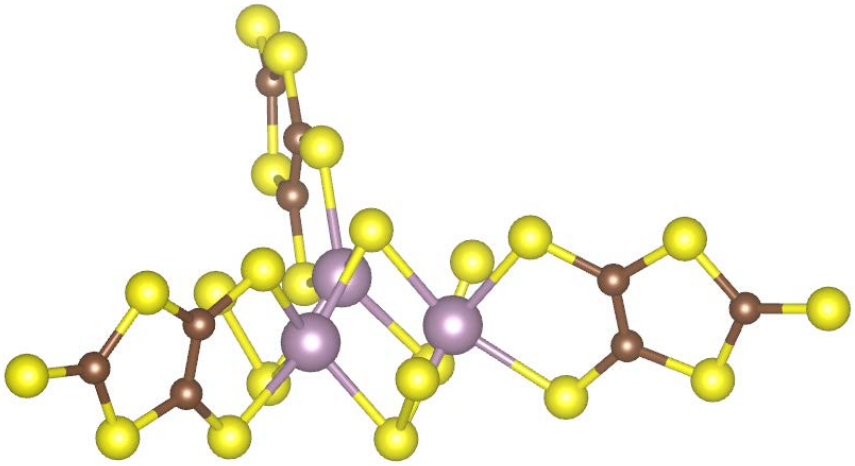


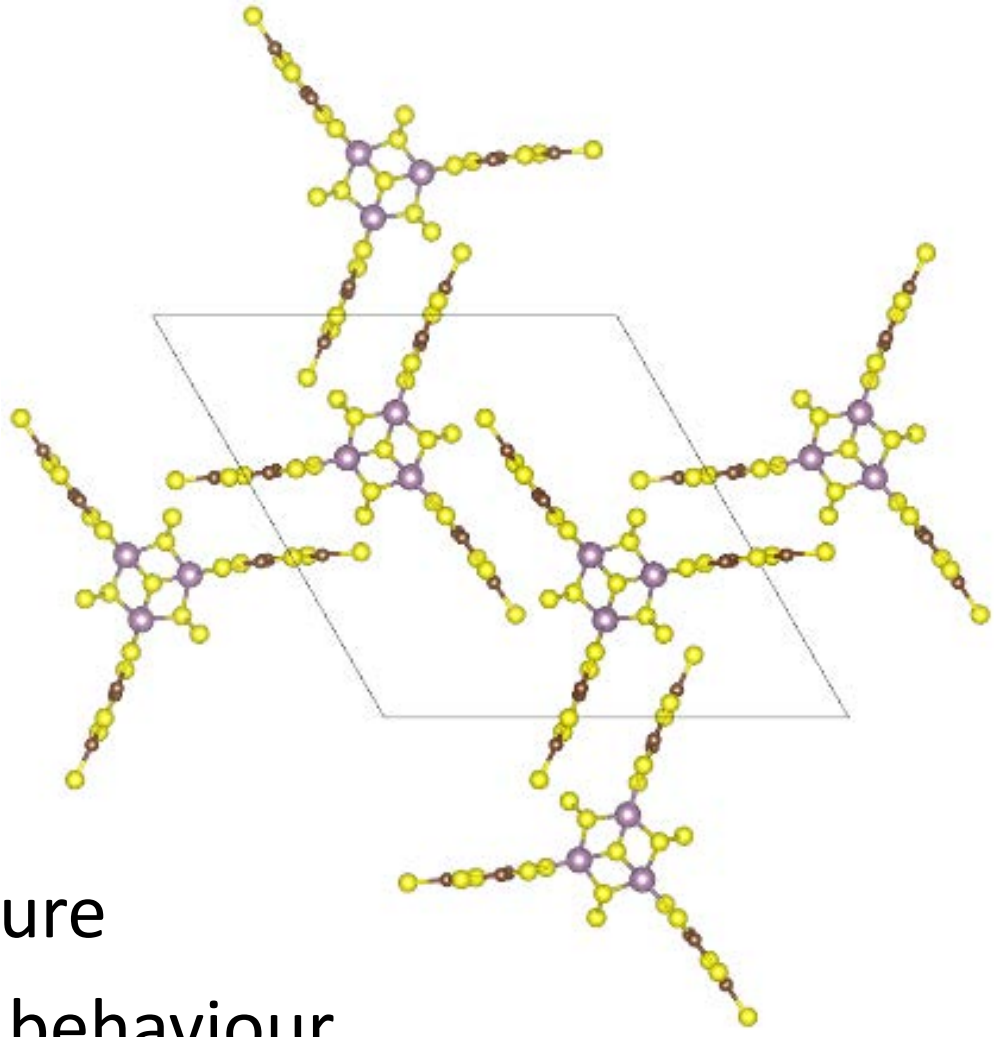
Unpaired spins, & no sign of magnetic order, $J/T \approx 50$.

$$\chi T = C + \chi_0 T$$

Llusar et al., JACS **126** 12076 (2004)

$Mo_3S_7(dmit)_3$



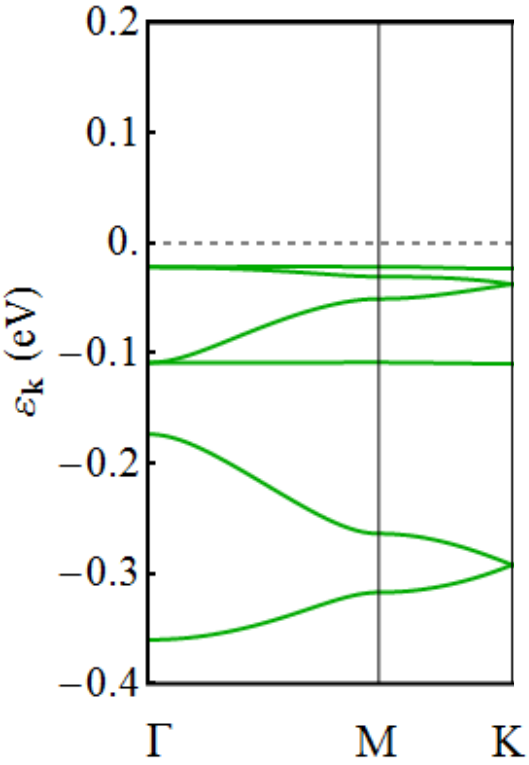


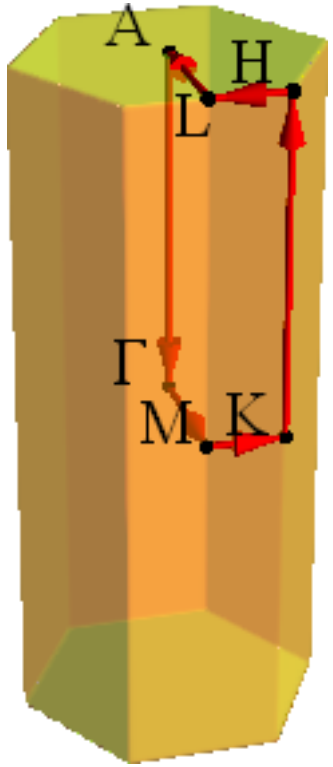
- Spin-liquid candidate (magnetic susceptibility)
- Interesting crystal structure
- Suggestions of quasi-1D behaviour

2D Electronic Structure

Flat bands - totally localised states

Dirac points

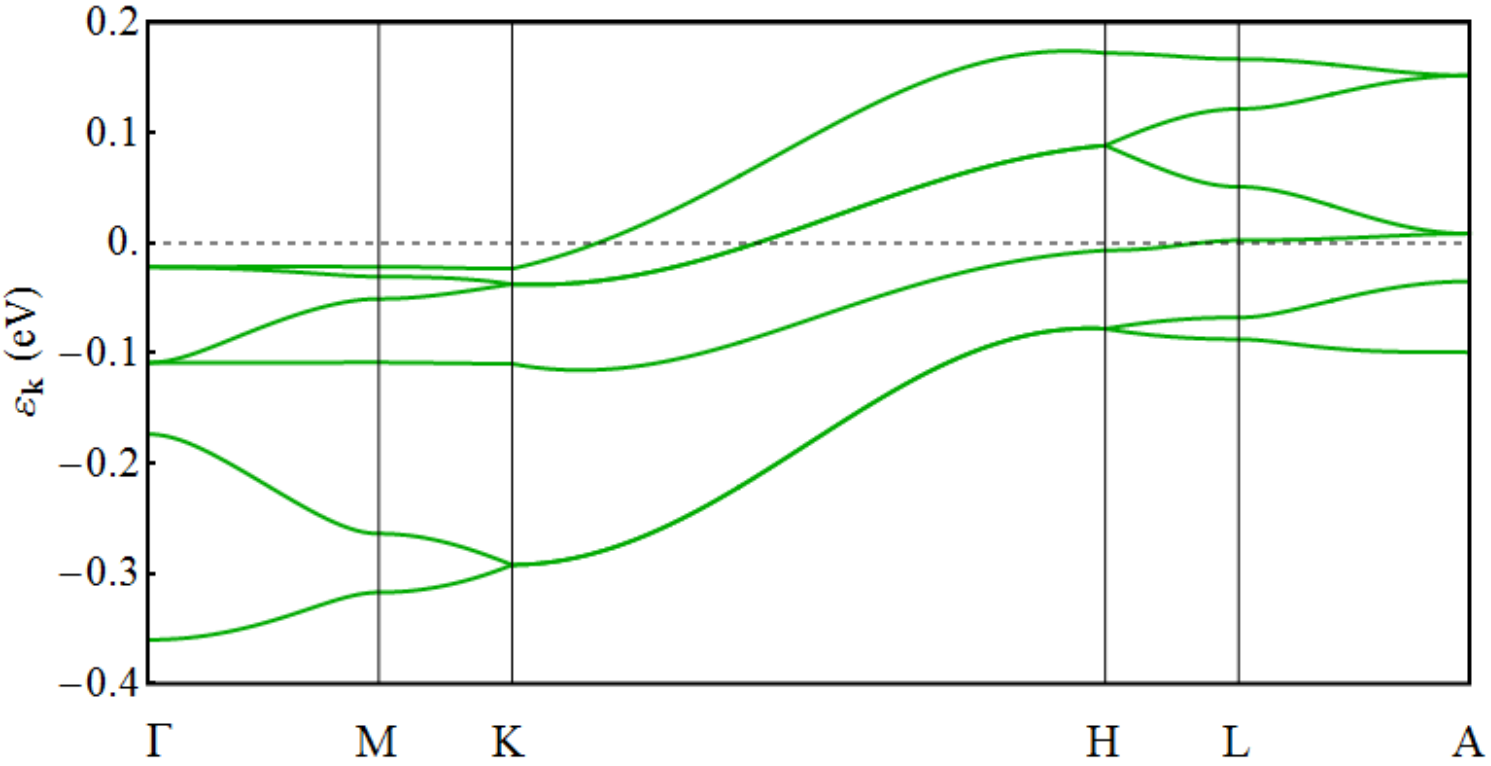


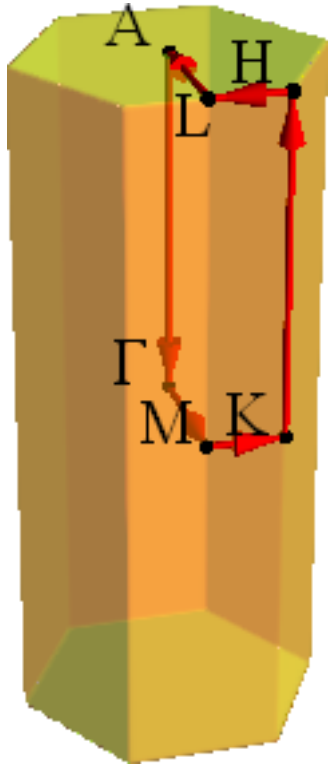


3D Electronic Structure

Flat bands → quasi-1D bands

Dirac lines

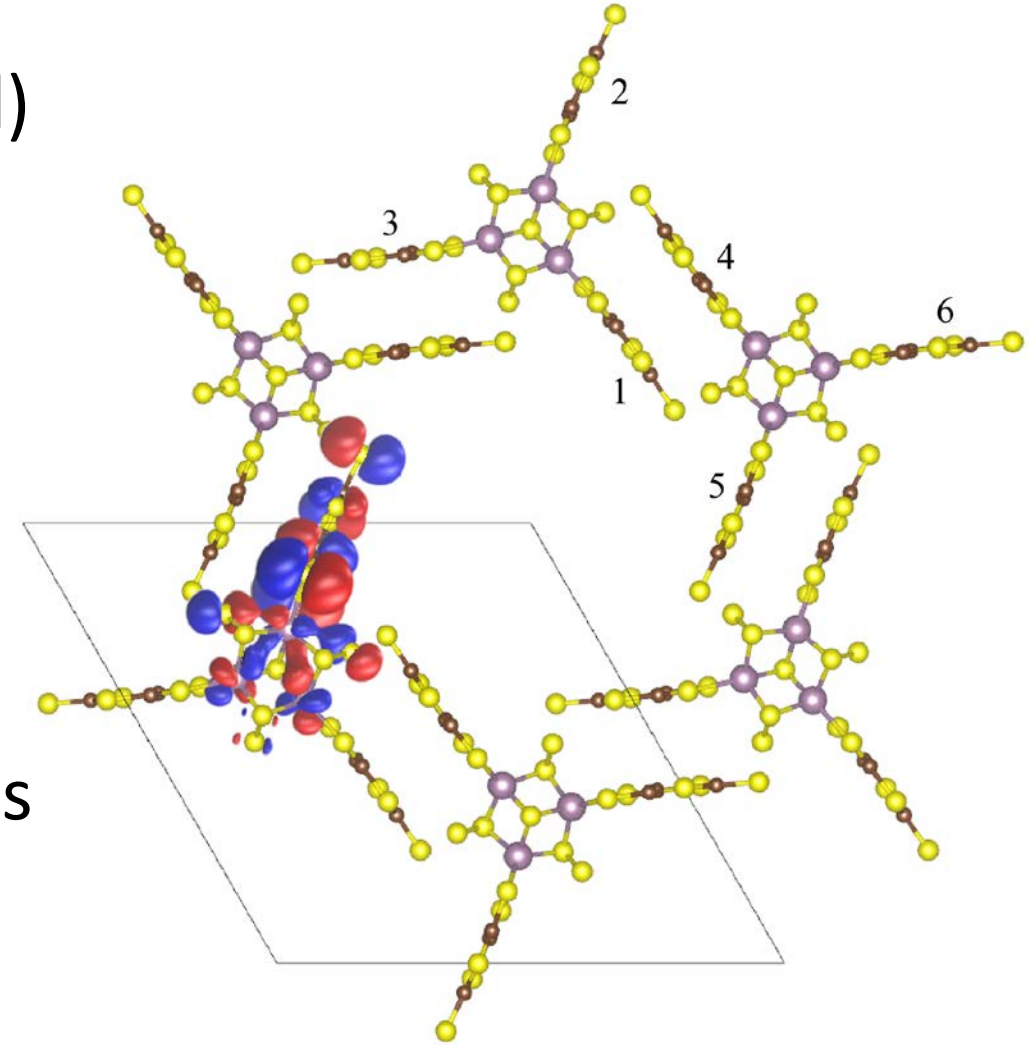




Wannier Orbitals

- 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.



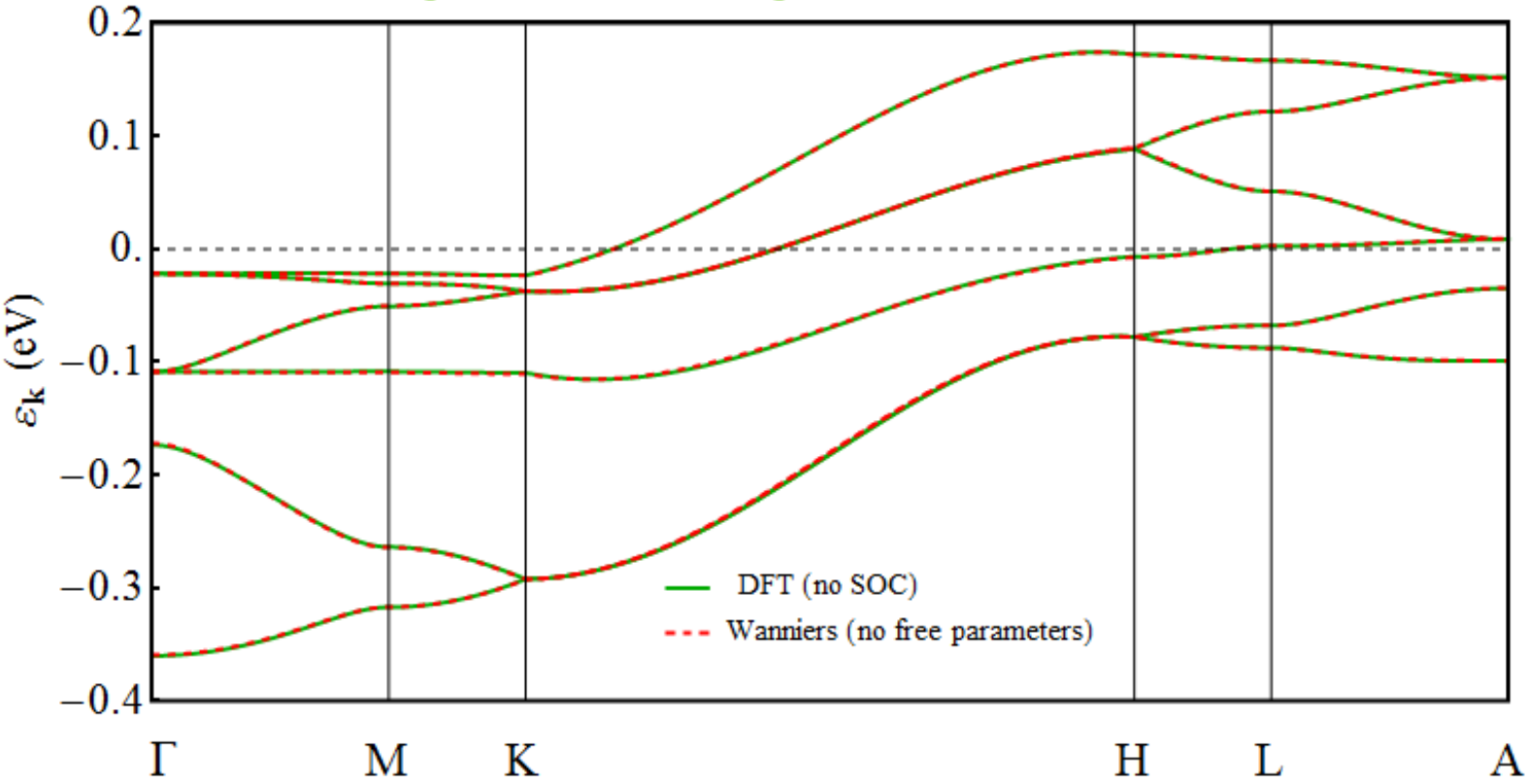
Jacko, **arXiv:**1508.07735

Jacko *et al*, **Phys. Rev. B 91**, 125140 (2015)

Model from Wannier Orbitals

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

→ ***ab initio* tight binding model**

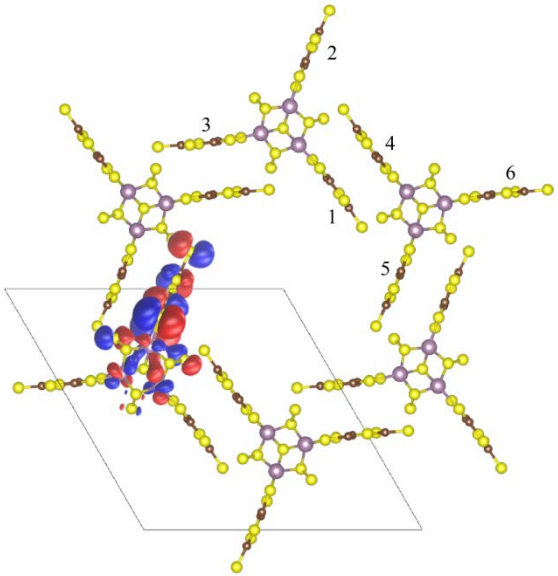


Jacko, **arXiv:**1508.07735

Jacko *et al*, **Phys. Rev. B 91**, 125140 (2015)

Kagomene

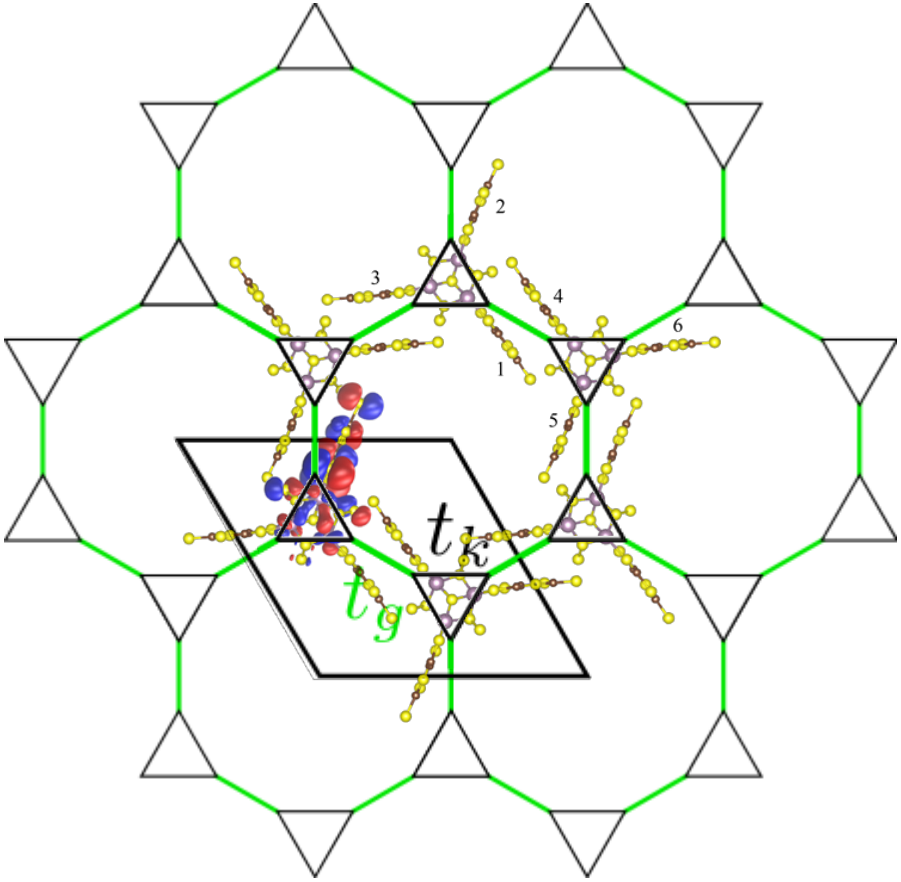
What are the key features of the model?



Jacko *et al*, **Phys. Rev. B 91**, 125140 (2015)

Kagomene

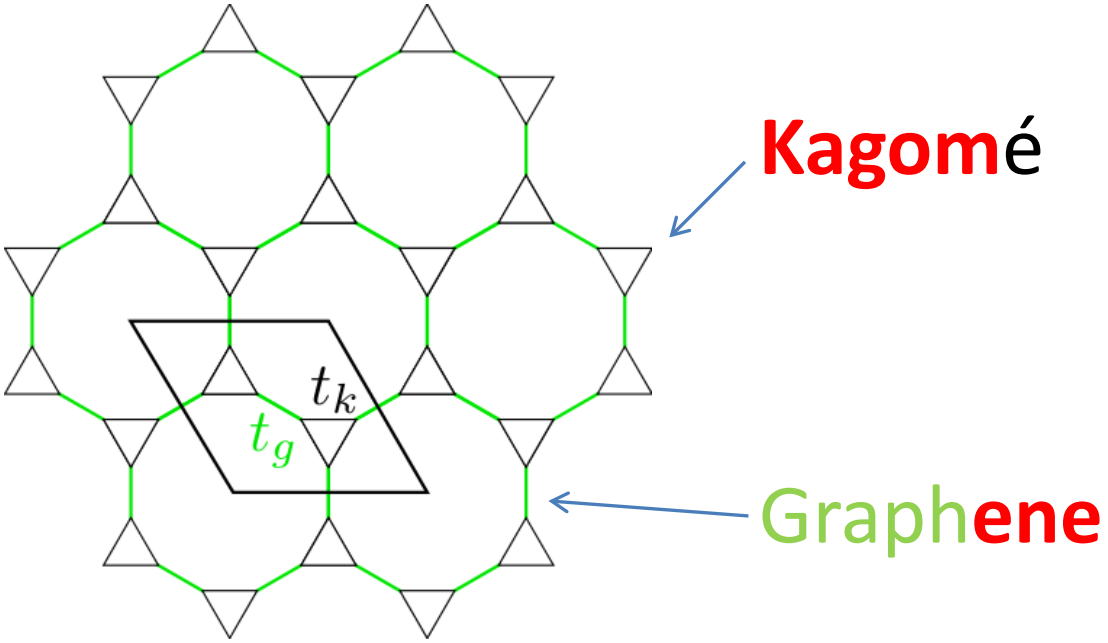
2D *ab initio* model – Kagomene



Jacko *et al*, **Phys. Rev. B 91**, 125140 (2015)

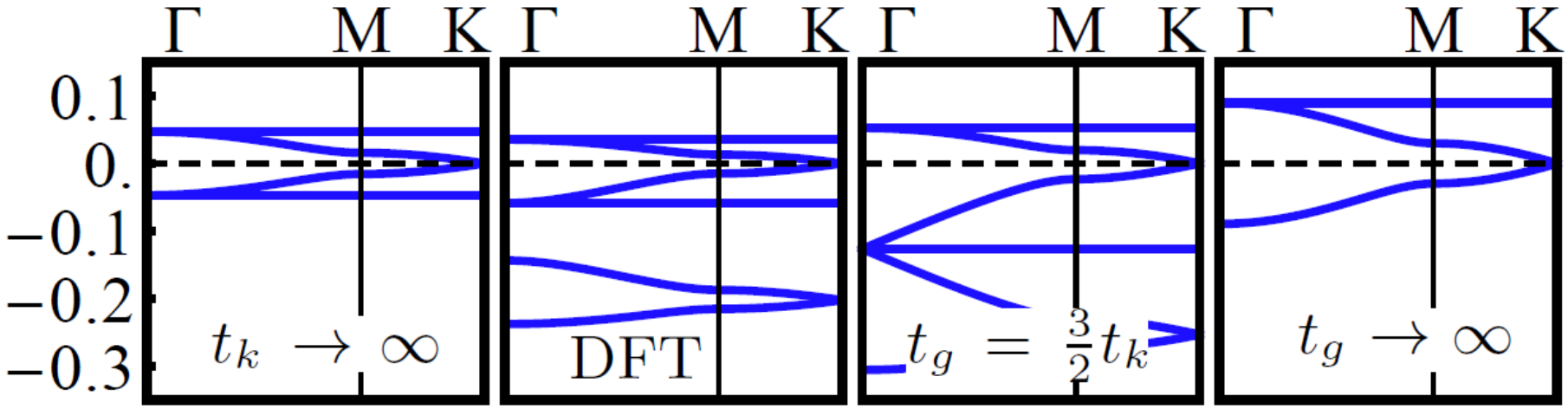
Kagomene

2D *ab initio* model – Kagomene



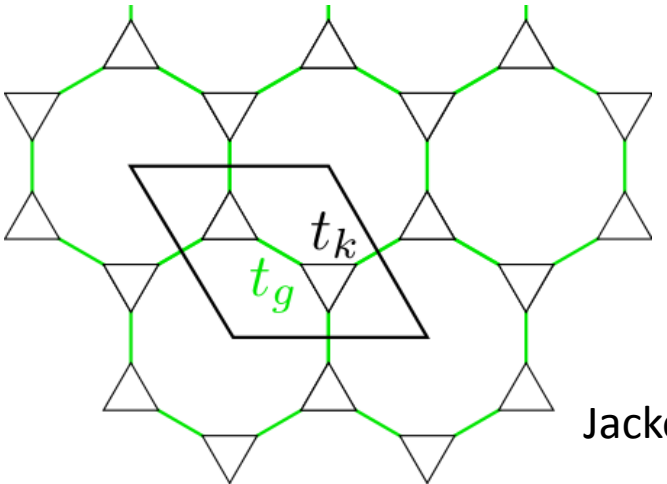
Jacko *et al*, **Phys. Rev. B 91**, 125140 (2015)

Kagomene Lattice



Molecular limit

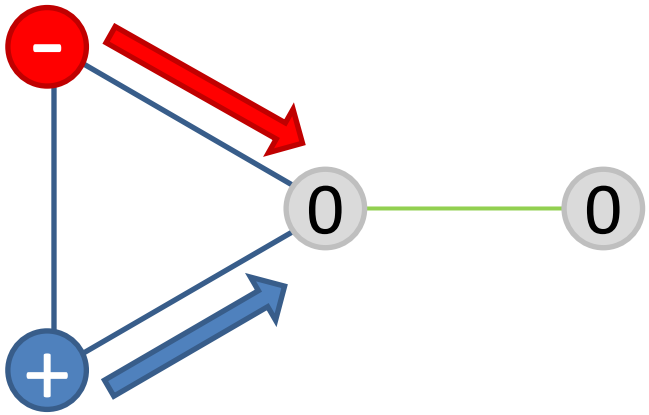
Dimer limit



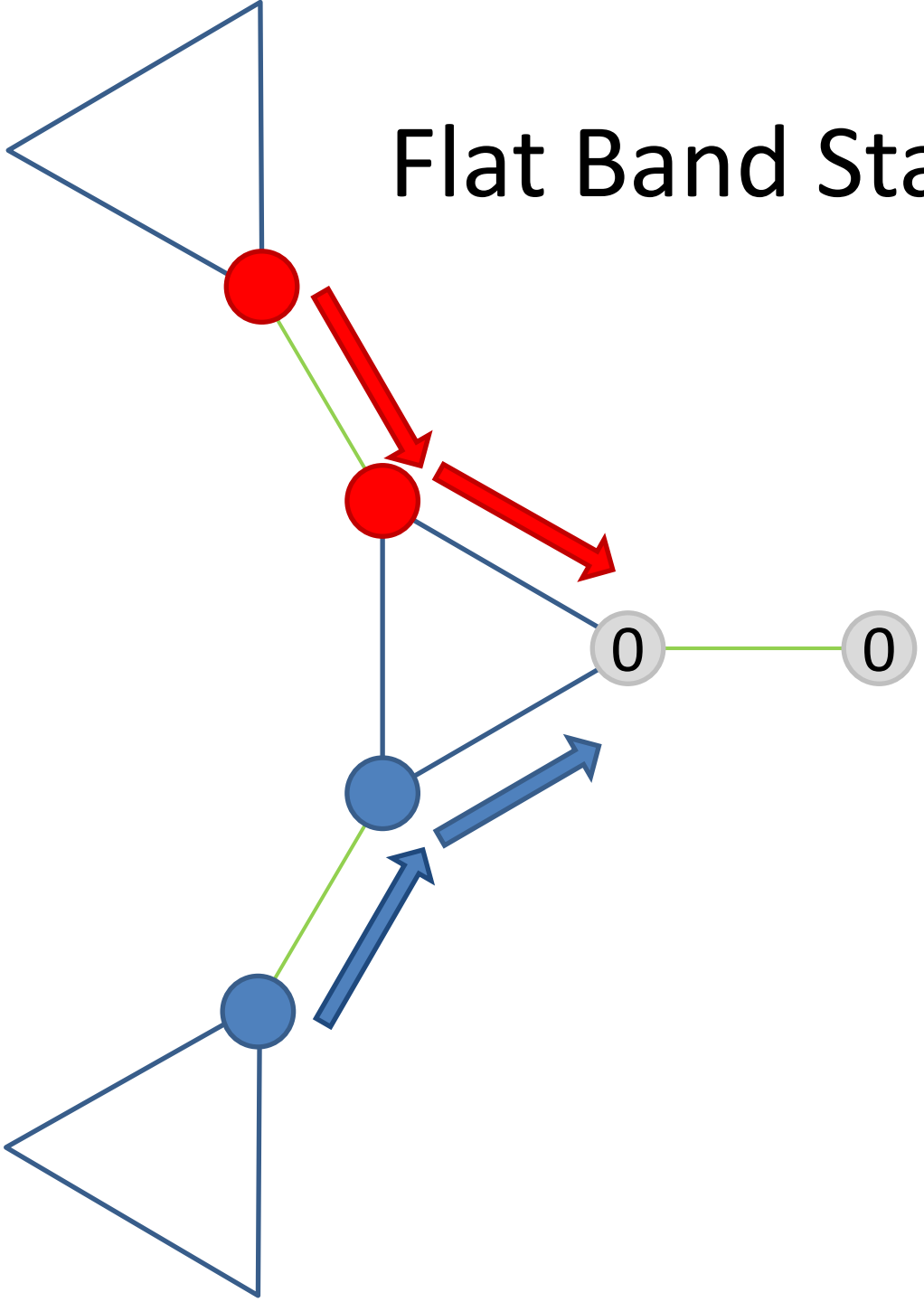
Jacko *et al*, **Phys. Rev. B 91**, 125140 (2015)

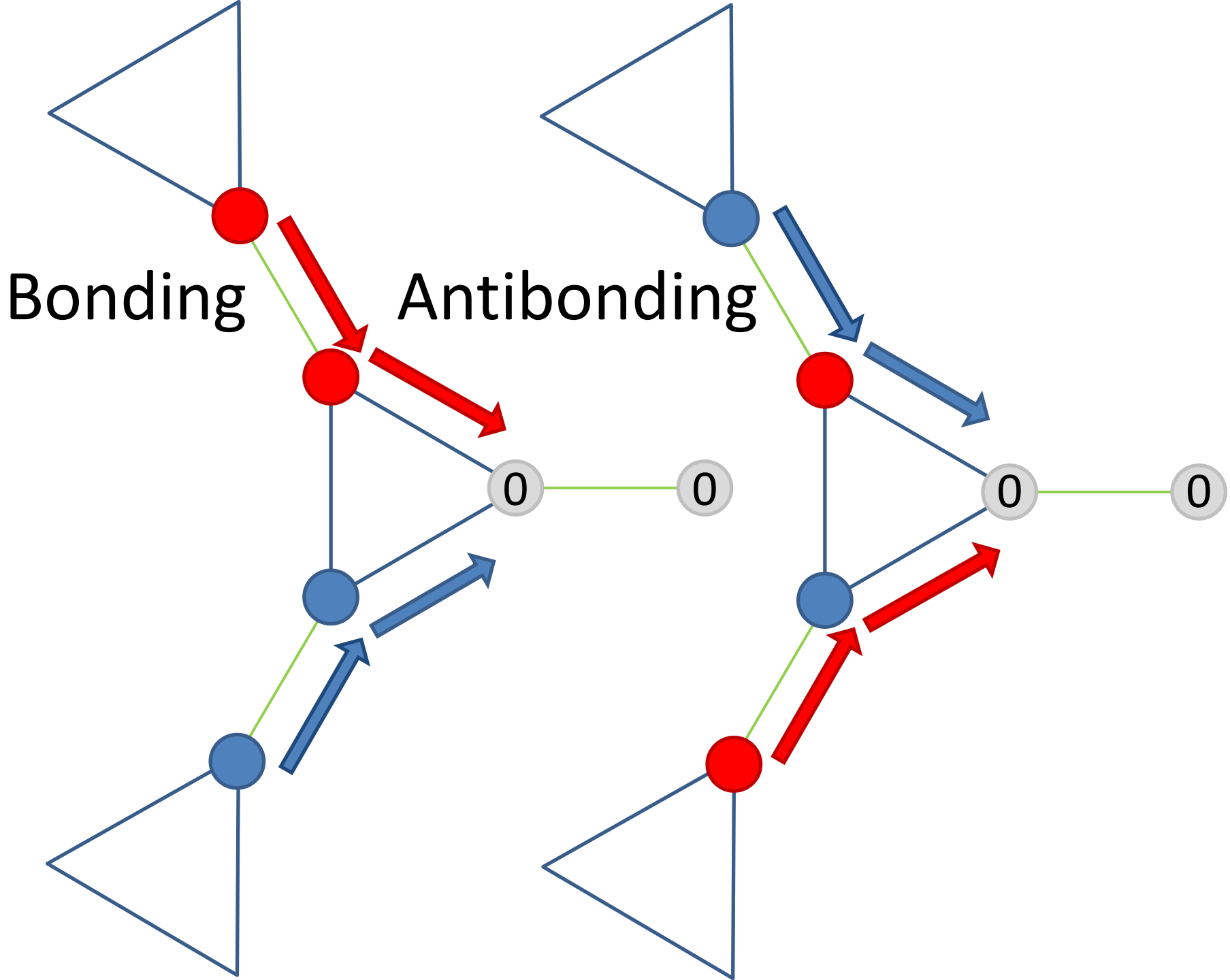
Flat Band States

Interference from adjacent sites on the triangle
→ no amplitude can leave the triangle



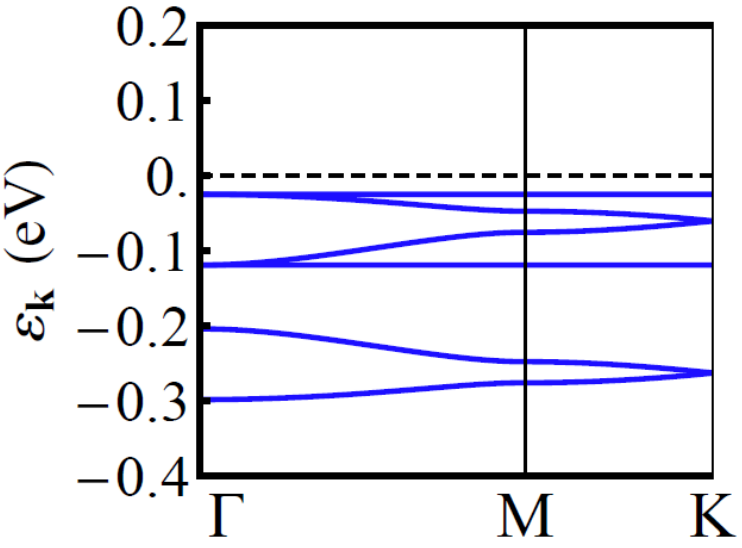
Flat Band States

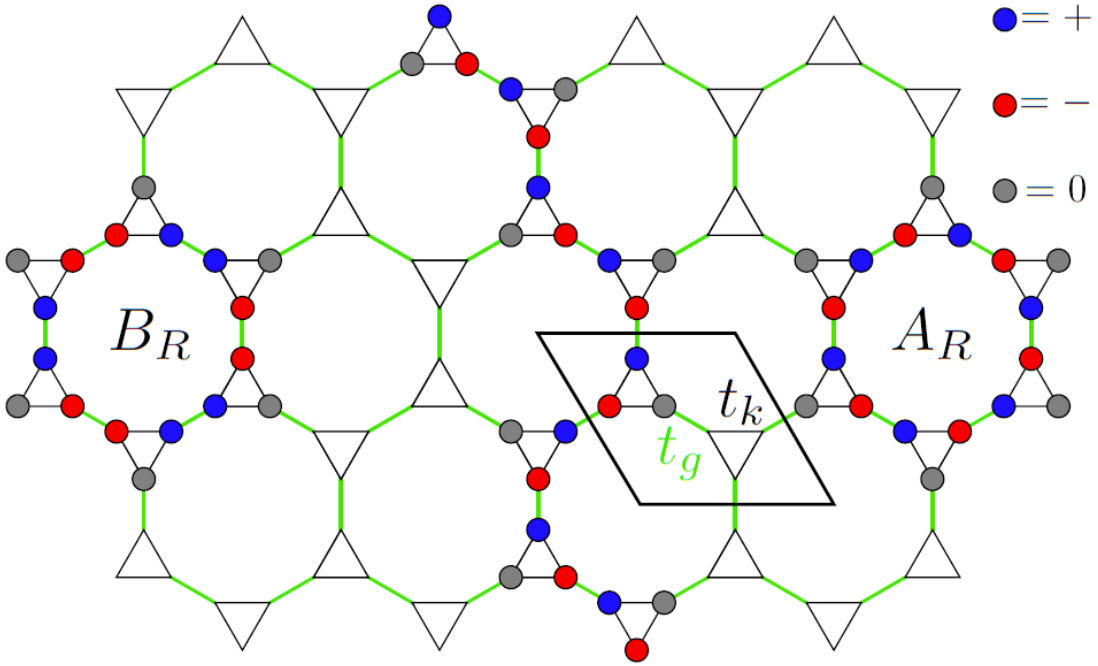



Bonding
Antibonding
0
0
0
0

Flat Band States

Interference from adjacent sites on the triangle
→ no amplitude can leave each triangle





Flat Band States

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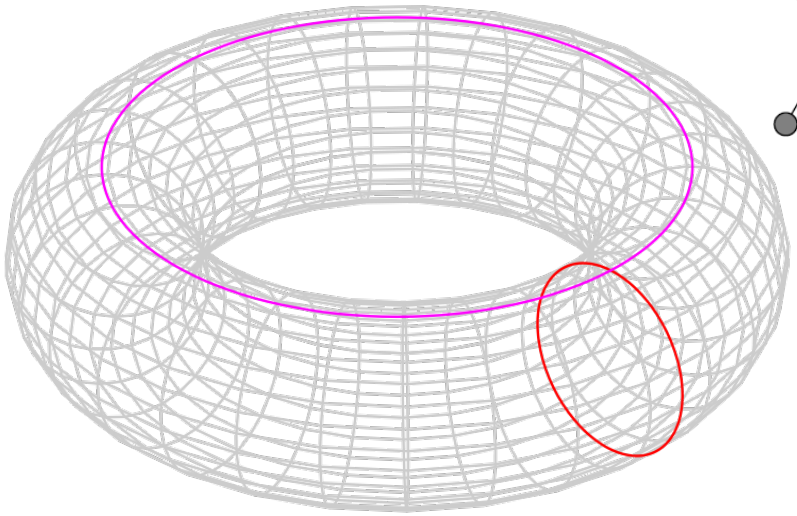
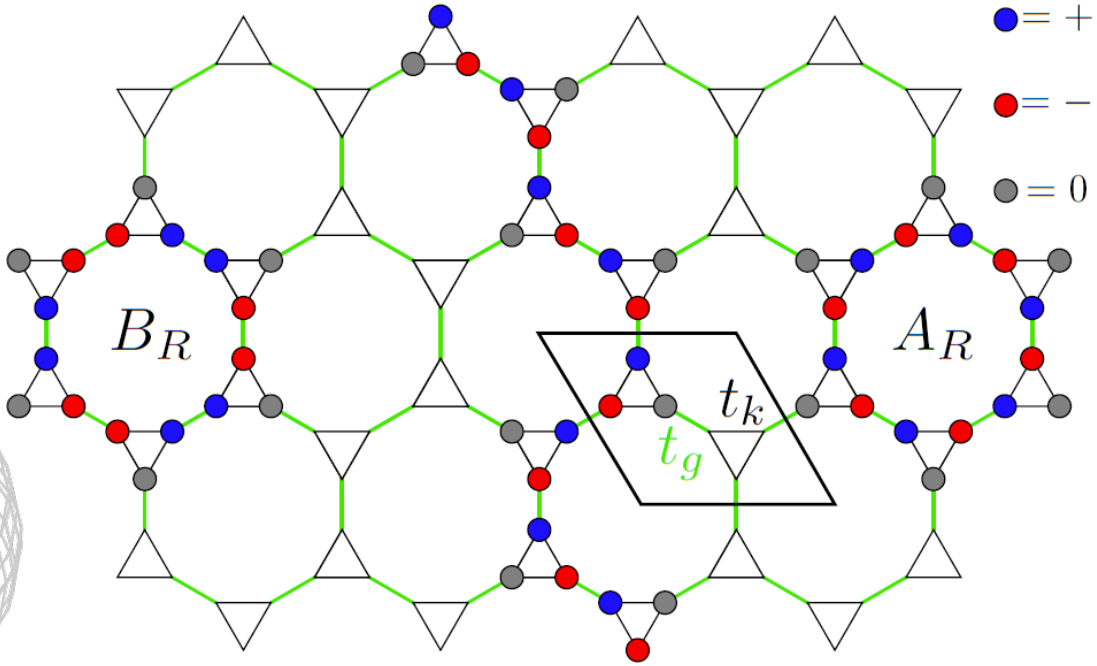
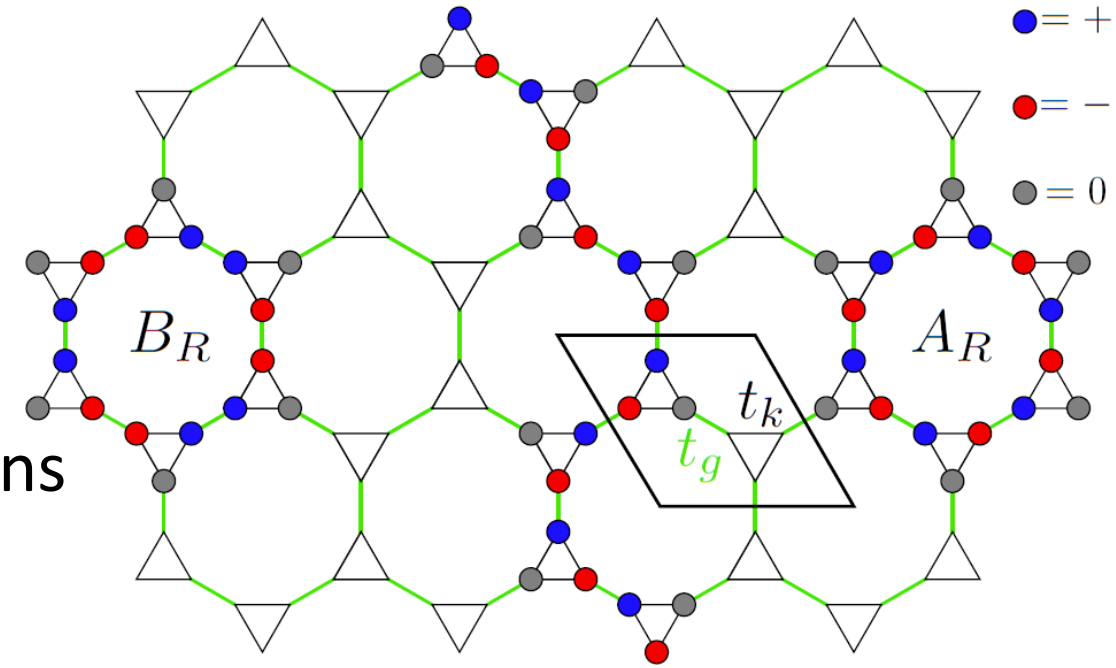




Flat Band States

Interference from adjacent sites on the triangle
→ no amplitude can leave each triangle

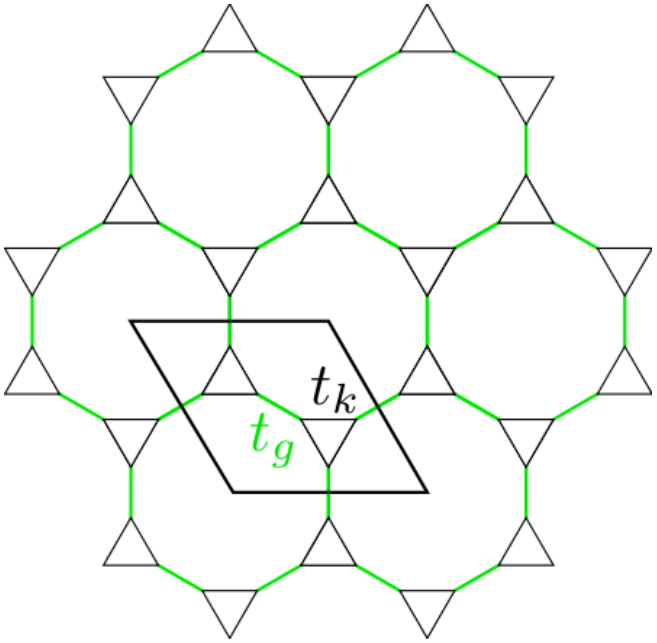
Topological states:
degeneracy depends
on boundary conditions

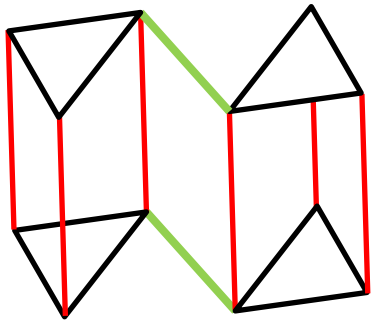


Kagomite

3D *ab initio* model – Kagomite

Stacked layers of the Kagomene lattice:



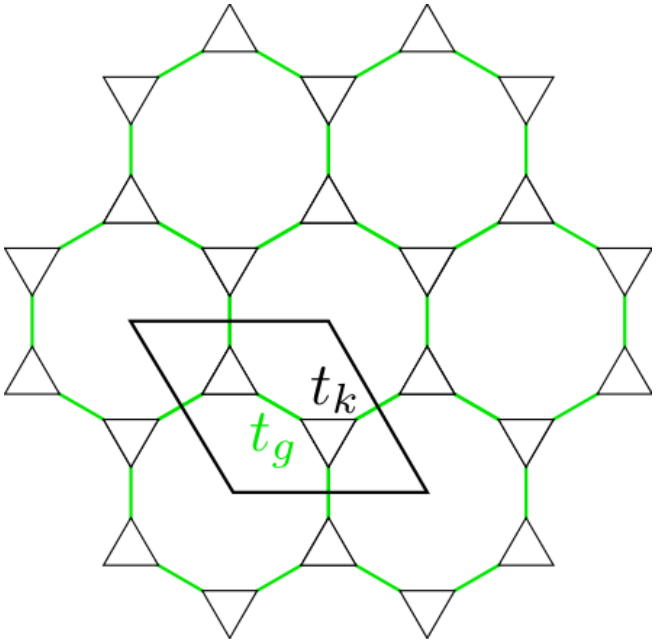


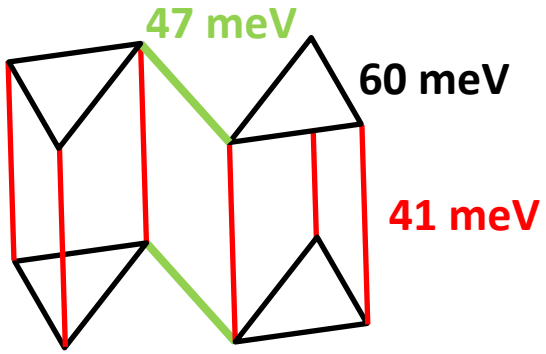
Jacko *et al*, **Phys. Rev. B 91**, 125140 (2015)

Kagomite

All of these hopping integrals are similar magnitude.

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

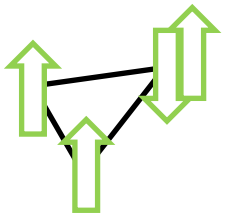




Jacko *et al*, **Phys. Rev. B 91**, 125140 (2015)

Monomers in Hubbard Model

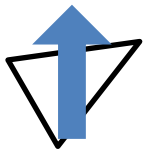
Solve monomer Hubbard model exactly at 2/3 filling



Chander *et al*, **Phys. Rev. B 90**, 035120 (2014)
& **Phys. Rev. Lett. 113**, 267204 (2014)

Monomers in Hubbard Model

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

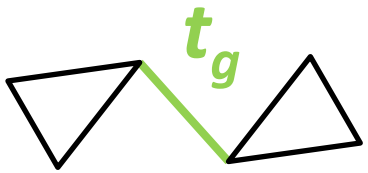


Chander *et al*, **Phys. Rev. B 90**, 035120 (2014)
& **Phys. Rev. Lett. 113**, 267204 (2014)

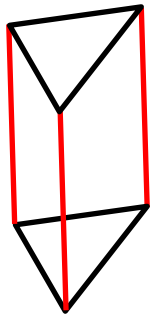
Dimers in Hubbard Model

Solve monomer Hubbard model exactly at 2/3 filling.

Perturbativly couple dimers: two possibilities → two exchange couplings.



$t_z \approx t_g$



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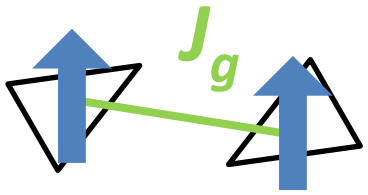

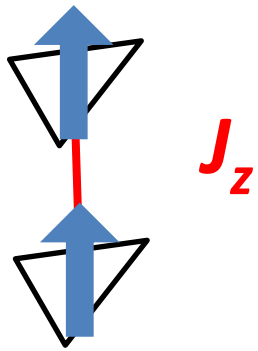

$J_z > J_g$

The perturbative model is **predominantly 1D**.

Jacko *et al*, **Phys. Rev. B 91**, 125140 (2015)

Summary

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

$Mo_3S_7(dmit)_3$ and related compounds need more experimental investigation!

ab initio models:	Jacko, **arXiv**:1508.07735
$Mo_3S_7(dmit)_3$:	Jacko *et al*, **Phys. Rev. B 91**, 125140 (2015)
	Ben Powell's talk