Designing the Kitaev model in new metal-organic frameworks:
towards topological quautum computation

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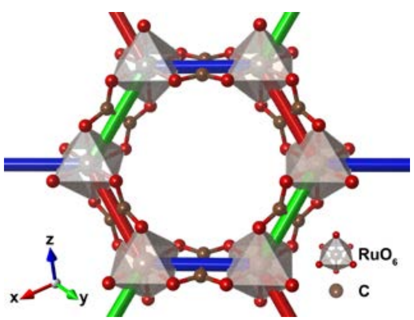
arXiv:1605.04471



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Outline

- Motivation from quantum information
- Introduction to the Kitaev model and metal-organic frameworks
- Proposal for new metal-organic frameworks
- Order estimation => almost Kitaev model
- Summary

Majorana anyons and topological quantum computation

- spin-1/2 = single qubit

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \leftrightarrow \alpha|\uparrow\rangle + \beta|\downarrow\rangle$$

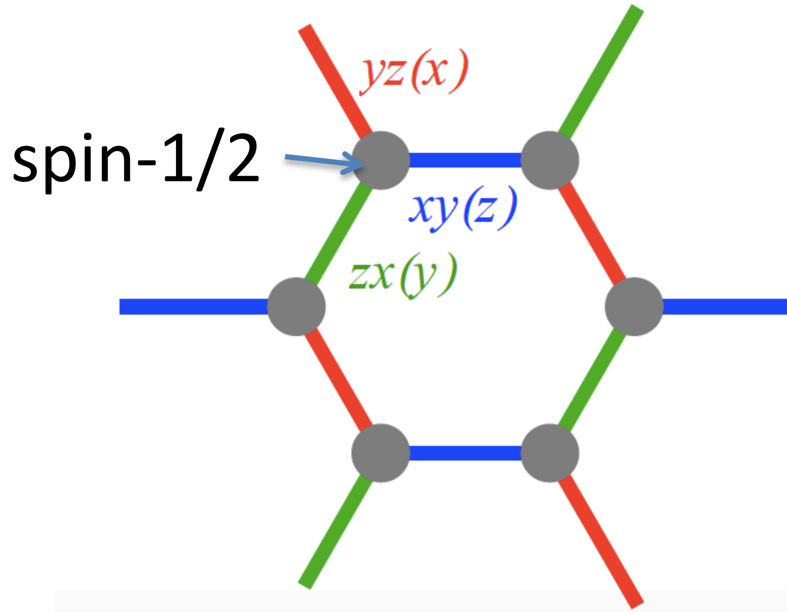
- decoherence due to noise
  => qubit must be stored topologically
- anyon excitations can be entangled, such as by topological braiding
- the Kitaev (honeycomb) model is exactly shown to have such Majorana anyons

For more details, please see Dr. Fujii's lecture note

http://www2.yukawa.kyoto-u.ac.jp/~entangle2016/program.htm

the Kitaev model

- "toy" model for spin liquid
  = no magnetic order
- exactly-solvable with
  Majorana anyon excitation
- more anisotropic than
  the ordinary Heisenberg model
  => difficult to realize experimentally

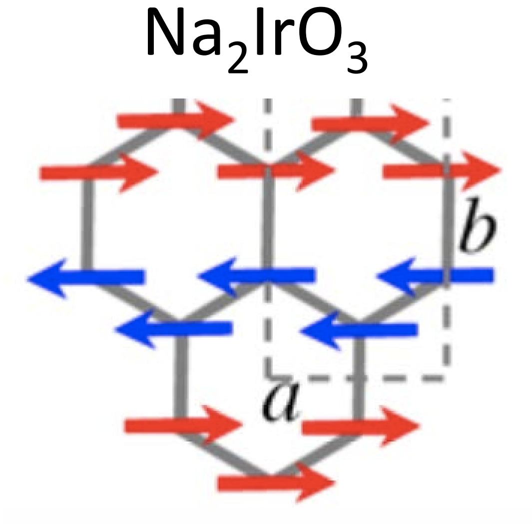


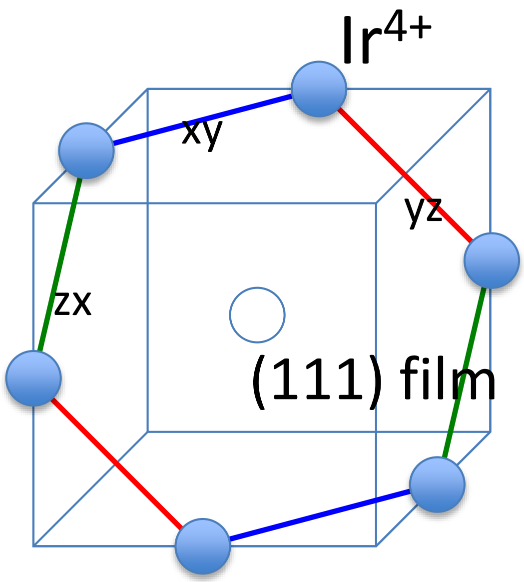
$$H = K_x \sum_{\langle ij \rangle \in yz(x)} S_i^x S_j^x + K_y \sum_{\langle ij \rangle \in zx(y)} S_i^y S_j^y + K_z \sum_{\langle ij \rangle \in xy(z)} S_i^z S_j^z .$$

A. Kitaev, Ann. Phys. 321, 2 (2006)

possible condensed matter realization

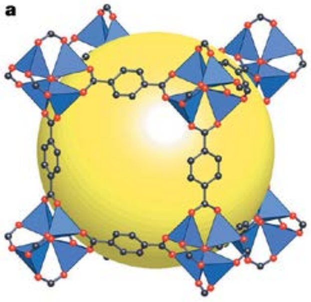
- iridium oxides (iridates) / $RuCl_3$
  - proposed by Jackeli and Khaliullin (2009)
  - not perfect Kitaev model, i.e. does not show a long-range entangled ground state





MOF (Metal-Organic Framework)

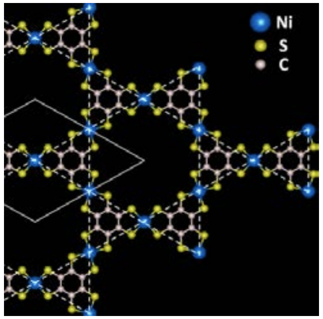
- MOF: metal-organic framework : a kind of coordination polymer consisting of metal ions and organic ligands

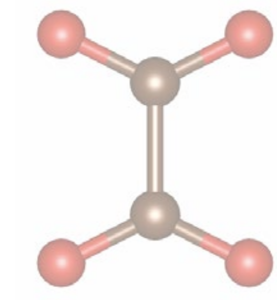


- 2D MOF: honeycomb / kagome

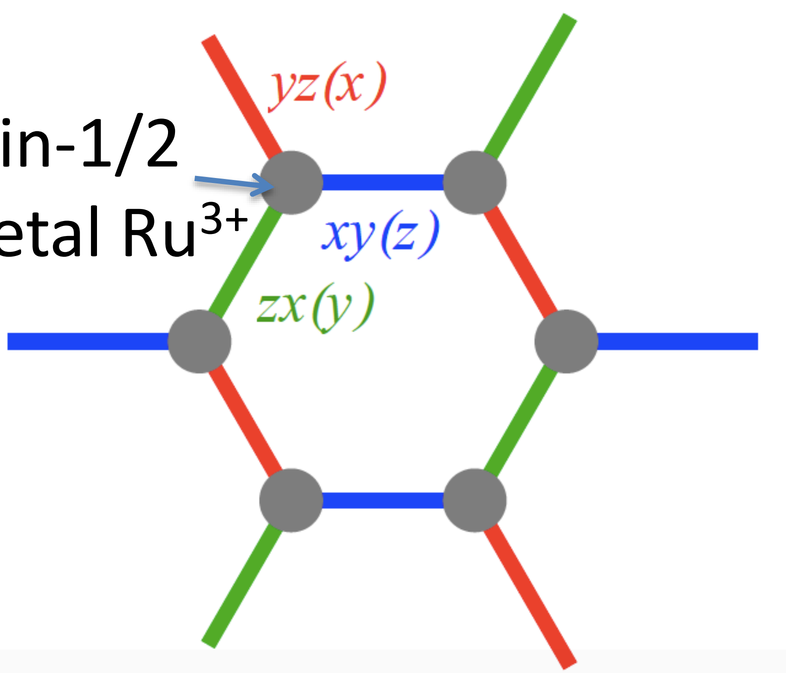
Yaghi *et al.,* Nature **423**, 705 (2003)

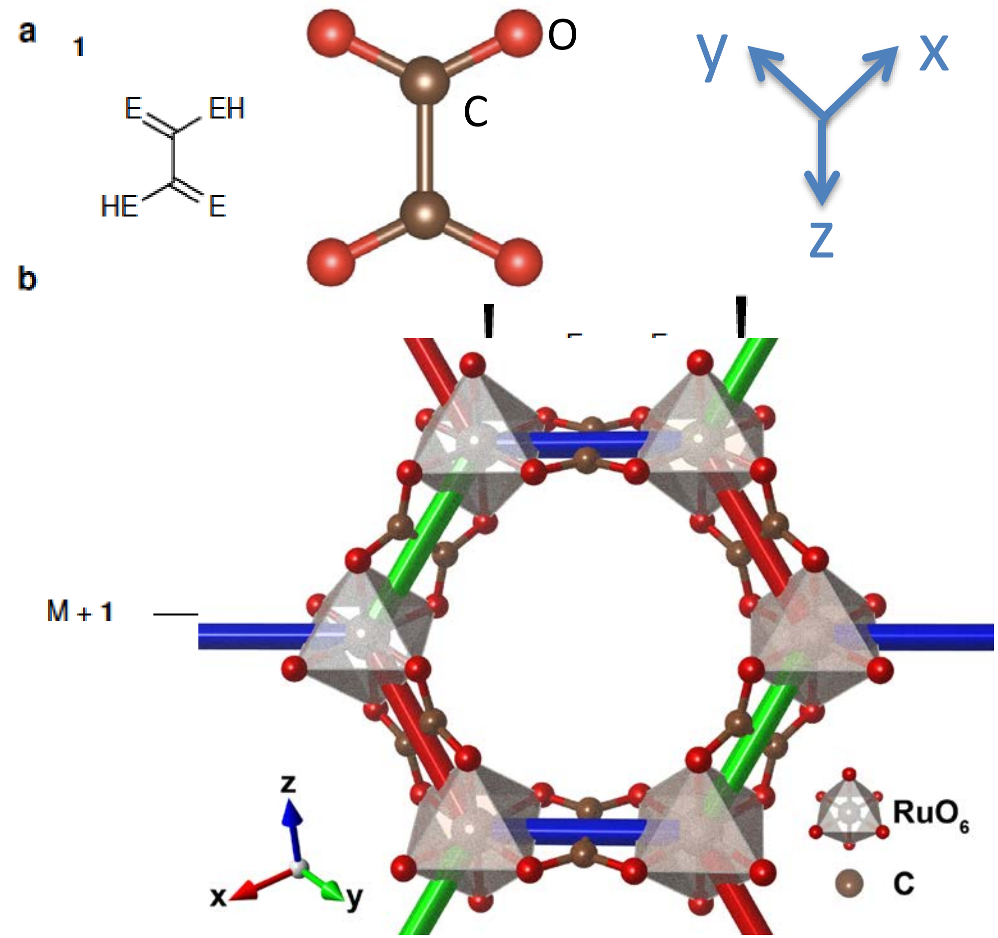
- kagome lattice by Kambe, *et al.*, JACS **135**, 2462 (2013).
  Sheberla, *et al.*, JACS **136**, 8859 (2014).
  - proposal for organic topological insulators
    Wang, *et al.*, Nano Lett. **13**, 2842 (2013).
    M.G.Y., *et al.*, arXiv:1510.00164



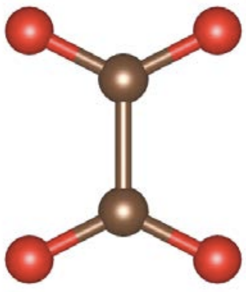
proposed MOFs with 

- M = Ru, Os, E = O, S, NH

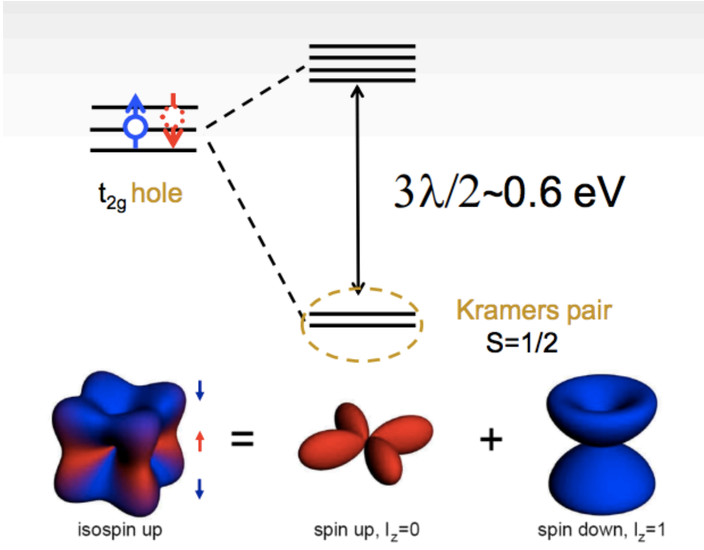




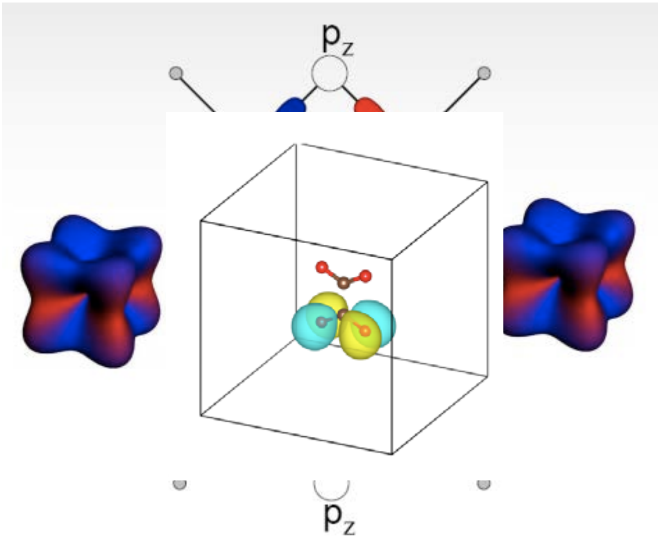
Jackeli-Khaliullin mechanism in



- ordinary spin model = Heisenberg term
- strong spin-orbit coupling in Ir^{4+} or Ru^{3+}



- Superexchange int. becomes Kitaev-type!

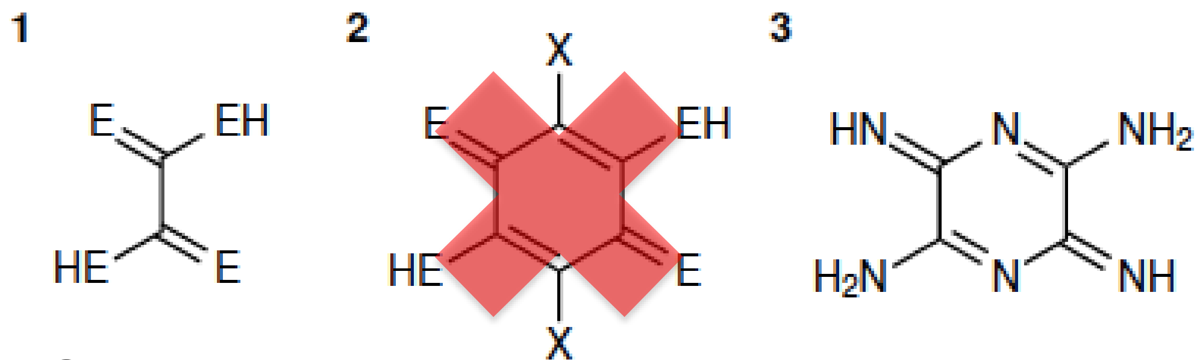


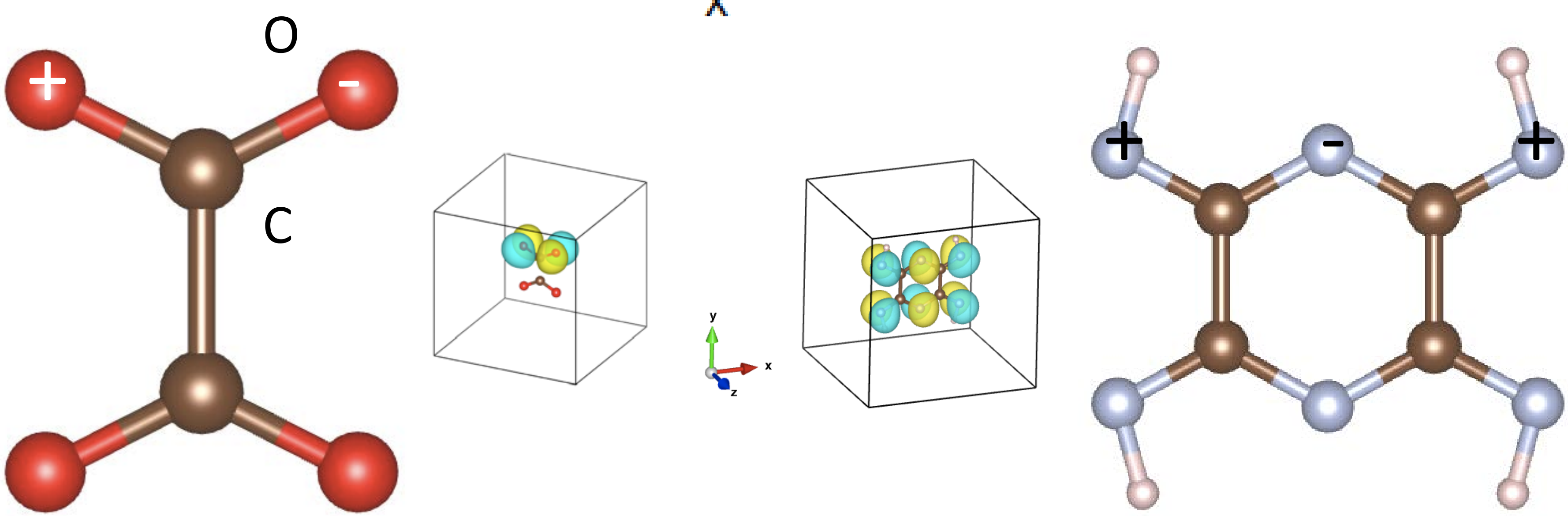
- cf. zigzag edge state of graphene

G. Jackeli and G. Khaliullin, PRL **102**, 017205 (2009).
http://online.kitp.ucsb.edu/online/fragnets_c12/jackeli/pdf/Jackeli_Fragnets12Conf_KITP.pdf

1: oxalate / 3: tetraaminopyrazine

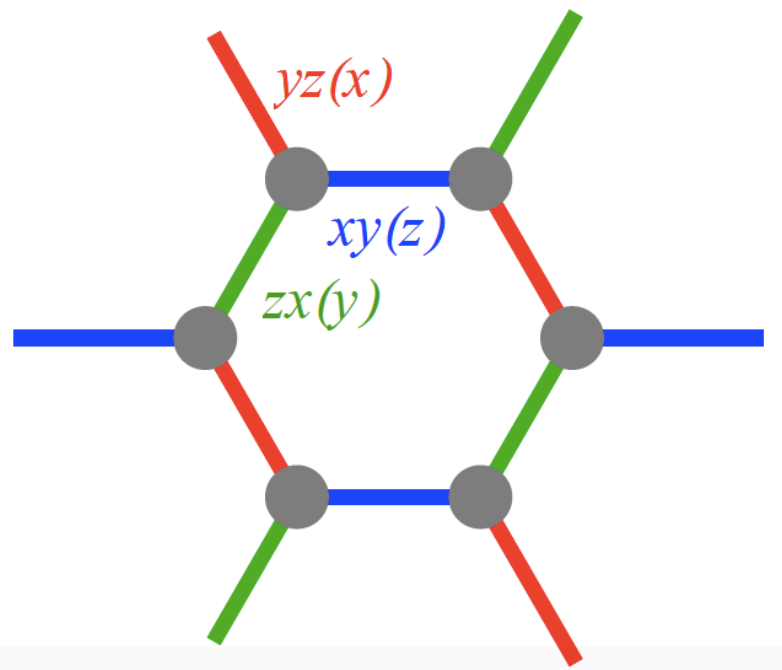
- degenerate edge states (HOMOs) in 1 and 3





the extended Kitaev model
= the JKΓ model

- Heisenberg term J
- Kitaev term K
- symmetric off-diagonal exchange Γ



$$H = \sum_{\langle ij \rangle \in \alpha\beta(\gamma)} [J \boldsymbol{S}_i \cdot \boldsymbol{S}_j + \boxed{K S_i^\gamma S_j^\gamma} + \Gamma (S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha)], \quad (1)$$

Kitaev term

Order Estimation

$$J = \frac{16(\mathbb{A} - \mathbb{B})}{9} t_1^2,$$

$$K = \frac{8\mathbb{B}}{3}(t_1^2 - 3t_2^2),$$

$$\Gamma = \frac{16\mathbb{B}}{3} t_1 t_2,$$

$\mathbb{A} \sim 0.6 \text{ eV}^{-1}$ and $\mathbb{B} \sim 0.05 \text{ eV}^{-1}$.

$t_1 = t_{\pi\pi} t_{d\pi}^2 / (V_\pi^2 - t_{\pi\pi}^2)$ and $t_2 = V_\pi t_{d\pi}^2 / (V_\pi^2 - t_{\pi\pi}^2)$.

experimental value

$$E_{\text{LUMO}} = V_{\pi^*} - t_{\pi^*\pi^*} \sim 2.6 \text{ eV},$$

$t_{\pi\pi} = 0.153$ eV and $t_{\pi^*\pi^*} = 1.631$ eV from the DFT calculations,

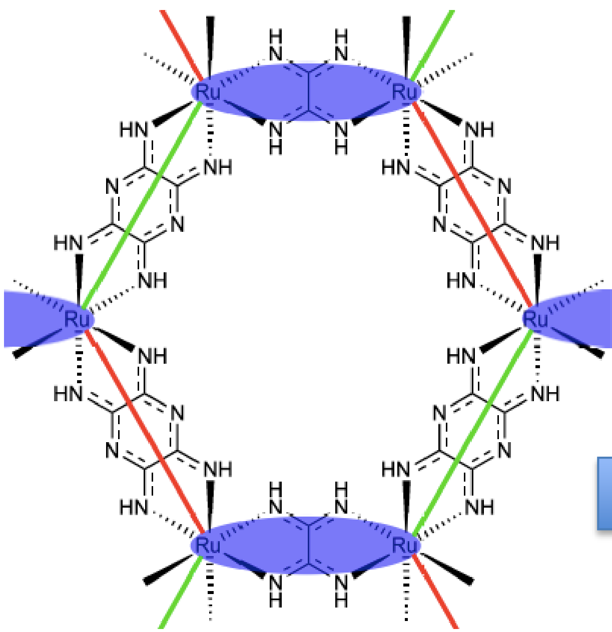
- From the tight binding model and these equations, we made a crude estimation

$$J/|K| = 0.09 \text{ and } |\Gamma|/|K| = 0.03$$

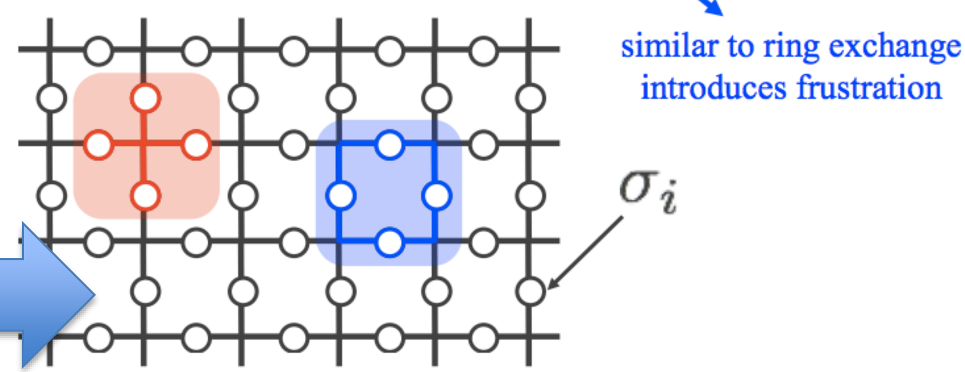
the Kitaev term K strongly dominates!!!

possible gapped toplogical phase

- bond anisotropy or external magnetic field
  -> gapped g. s. w/ Z_2 topological order
  -> topological quantum computation???



$$H_{\mathrm{TC}} = -A\sum_{v} \prod_{j\in \mathrm{vertex}(v)} \sigma_j^z - B\sum_{p} \prod_{j\in \mathrm{plaquette}(p)} \sigma_j^x$$



A. Kitaev, Ann. Phys. **303**, 2 (2003).

http://online.itp.ucsb.edu/online/freedmanfest/shtengel/pdf/Kirill_Shtengel.pdf

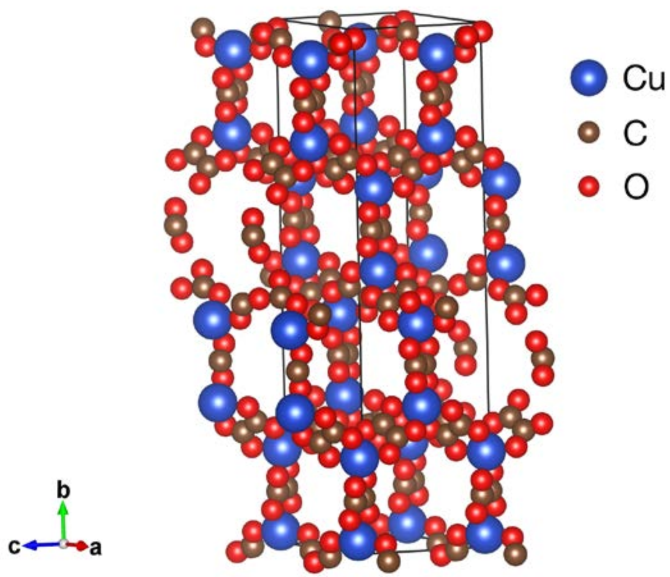
Summary

- We proposed new Ru-based Kitaev MOFs
- possibly Kitaev-dominant with oxalate/tetraaminopyrazine
- a wide variety of organic ligands
  => new way to achieve the toric-code limit
- aiming to the first materials realization of topological order
- possible application to quantum computation

3D structures by self-organization

Hyperhoneycomb (10,3)-b

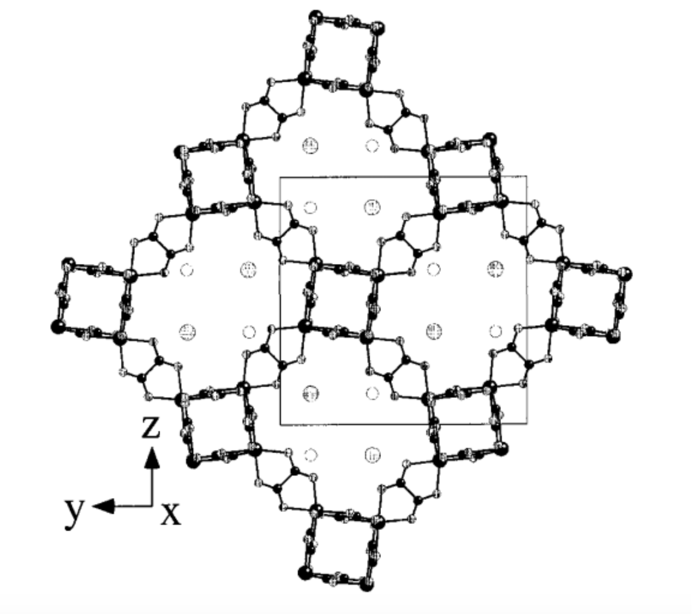
- possible Weyl spin liquid w/ TR symmetry breaking



B. Zhang, Y. Zhang, and D. Zhu, Dalton Trans. 41, 8509 (2012).

Hyperoctagon (10,3)-a New!

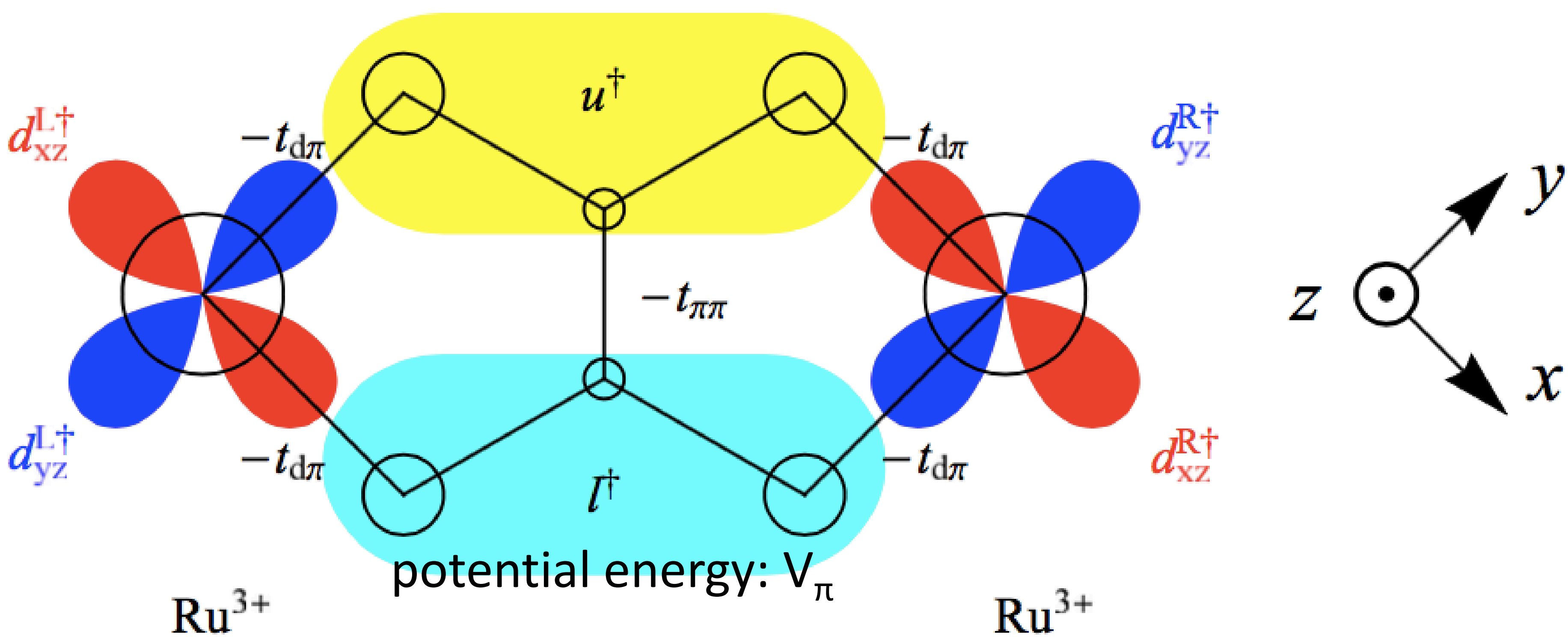
- Majorana Fermi surface -> spin Peierls instability



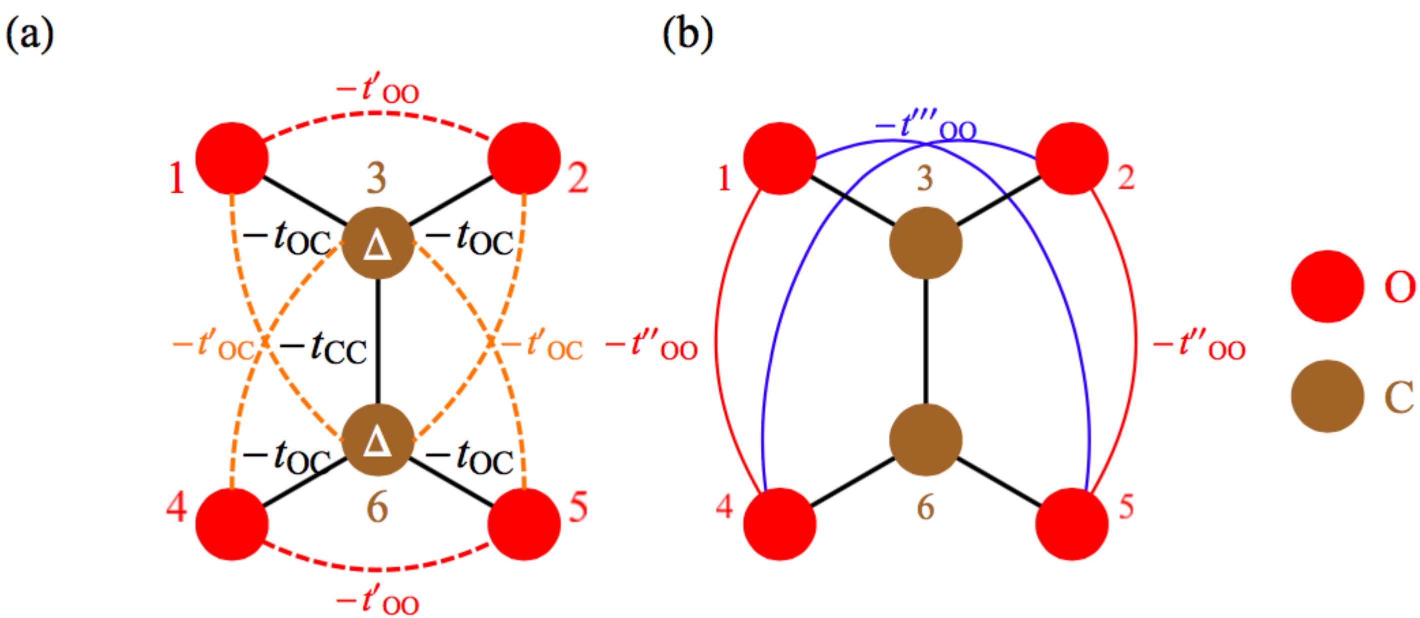
E. Coronado, J. R. Galan-Mascaros, C. J. Gomez-Garcia, and J. M. Martnez-Agudo, Inorg. Chem. 40, 113 (2001)

Derivation of the JKΓ model

- off-diagonal hopping (xz-yz) t_2 produces a Kitaev term
- diagonal (xz-xz/yz-yz) t_1 produces the others



tight-binding explanation



- diagonalize

$$H_{\mathrm{ox}} = \begin{pmatrix} 0 & -t'_{\mathrm{OO}} & -t_{\mathrm{OC}} & -t''_{\mathrm{OO}} & -t'''_{\mathrm{OO}} & -t'_{\mathrm{OC}} \\ -t'_{\mathrm{OO}} & 0 & -t_{\mathrm{OC}} & -t'''_{\mathrm{OO}} & -t''_{\mathrm{OO}} & -t'_{\mathrm{OC}} \\ -t_{\mathrm{OC}} & -t_{\mathrm{OC}} & \Delta & -t'_{\mathrm{OC}} & -t'_{\mathrm{OC}} & -t_{\mathrm{CC}} \\ -t''_{\mathrm{OO}} & -t'''_{\mathrm{OO}} & -t'_{\mathrm{OC}} & 0 & -t'_{\mathrm{OO}} & -t_{\mathrm{OC}} \\ -t'''_{\mathrm{OO}} & -t''_{\mathrm{OO}} & -t'_{\mathrm{OC}} & -t'_{\mathrm{OO}} & 0 & -t_{\mathrm{OC}} \\ -t'_{\mathrm{OC}} & -t'_{\mathrm{OC}} & -t_{\mathrm{CC}} & -t_{\mathrm{OC}} & -t_{\mathrm{OC}} & \Delta \end{pmatrix},$$