

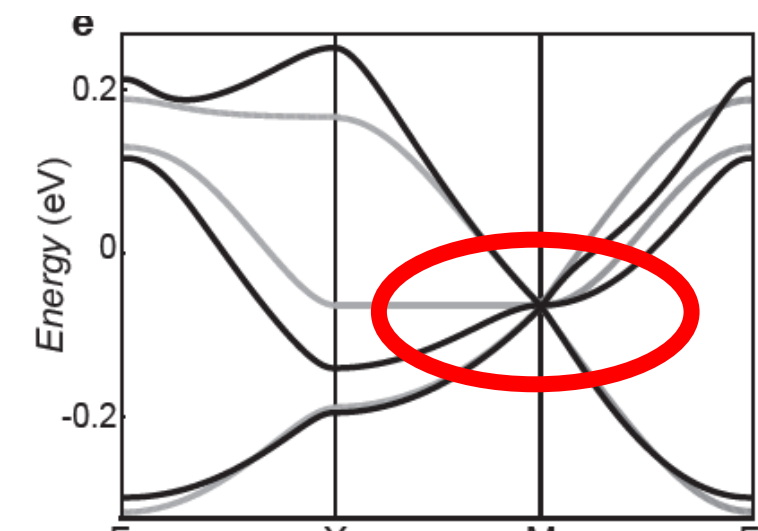
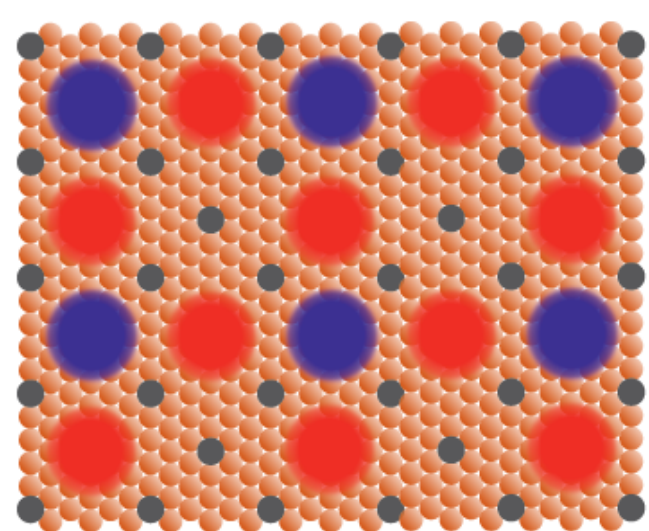
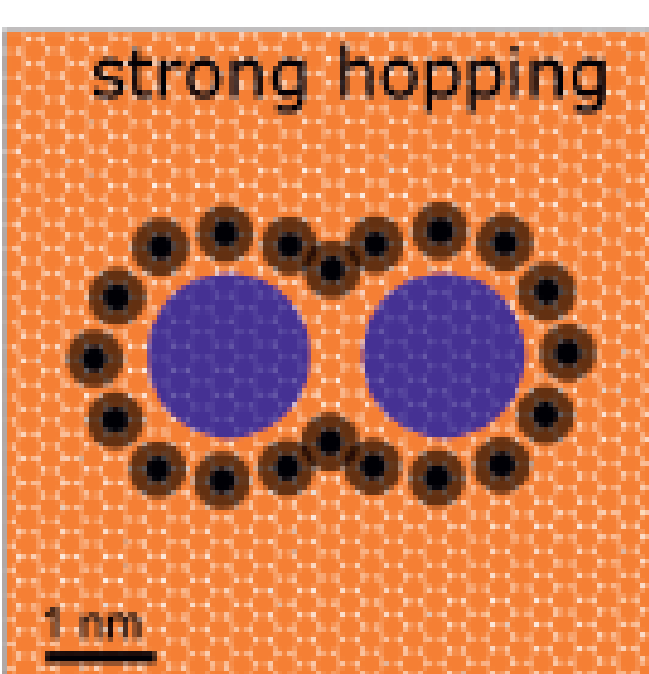
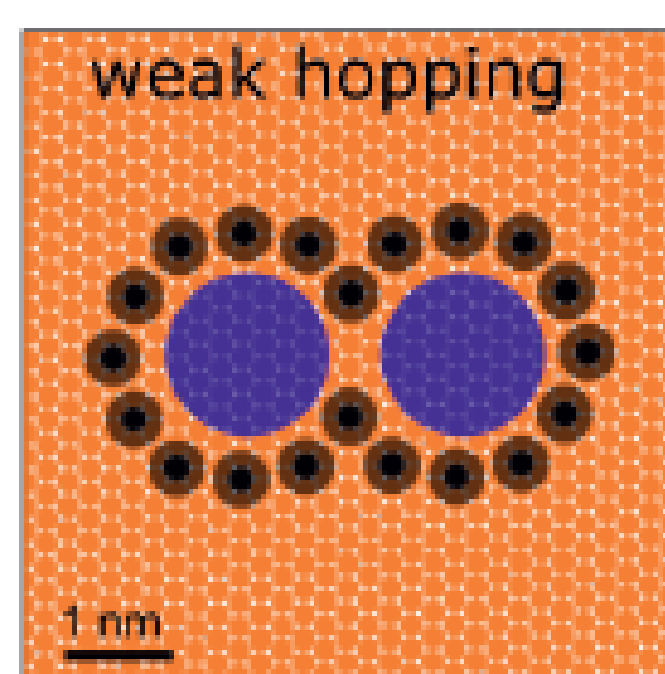
\*ma.jimenez.herrera@gmail.com

## Muffin tin method: designing antilattices



Place CO molecules on top of Cu(111),  
Solve Schrödinger by plane wave expansion

$$\left(\frac{1}{2}(\mathbf{k}-\mathbf{G})^2-\mathcal{E}_n\right)c_{\mathbf{k}-\mathbf{G}}^n+\sum_{\mathbf{G}'}V_{\mathbf{G}'-\mathbf{G}}c_{\mathbf{k}-\mathbf{G}'}^n=0$$



M.R. Slot *et al*, Physical Review X **9**, 011009 (2019)  
M.R. Slot *et al*, Nature Physics **13**, 672 (2017)

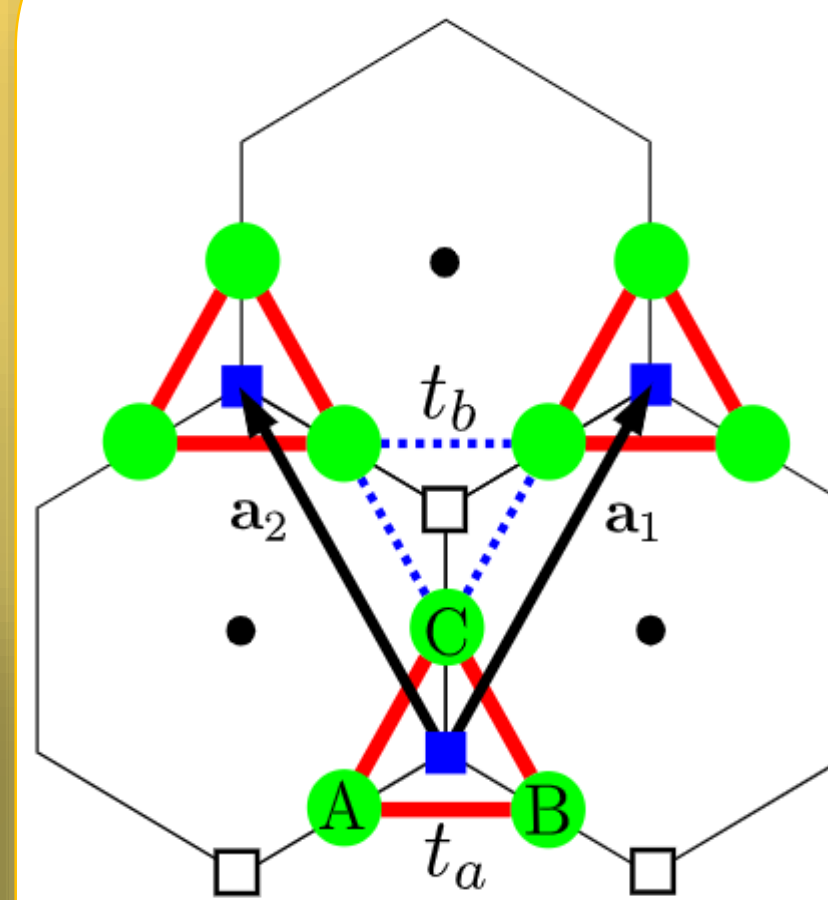
Pros:

- Electronic quantum simulator.
- Simple mathematical solution.

Cons:

- Not very large clusters of molecules.
- Symmetry of the substrate may affect the symmetry of the lattice.

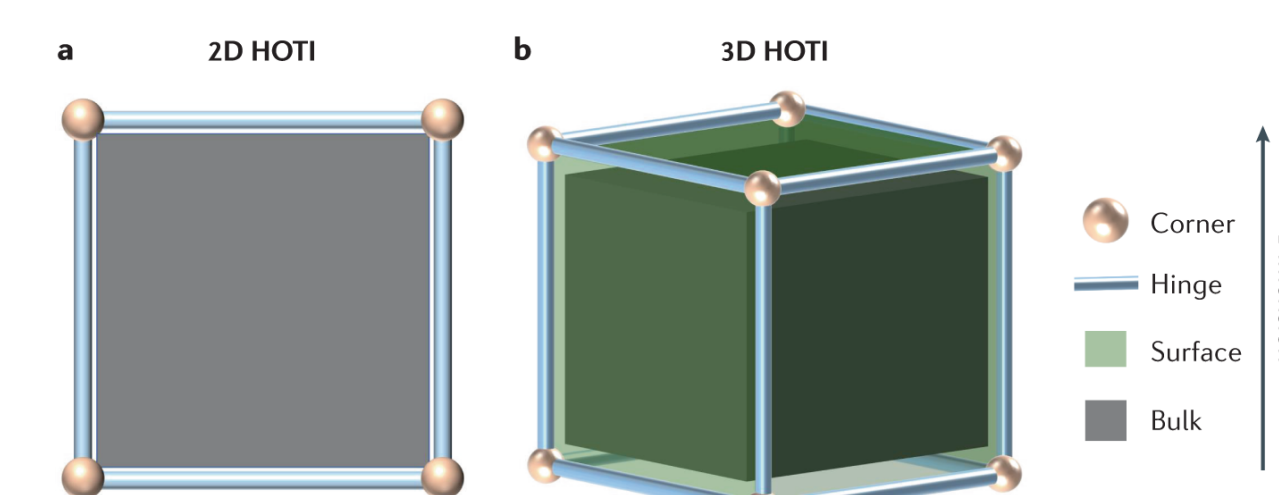
## Breathing kagome lattice



Kagome lattice with different intra- and inter-cell hopping amplitudes.

The breathing process reduces the symmetry from p6mm to p3m1. Displays two phases, one with corner modes (non-trivial) and another without them (trivial).

Such corner modes have suggested that non-trivial breathing kagome is **HOTI**, when **it is not**.

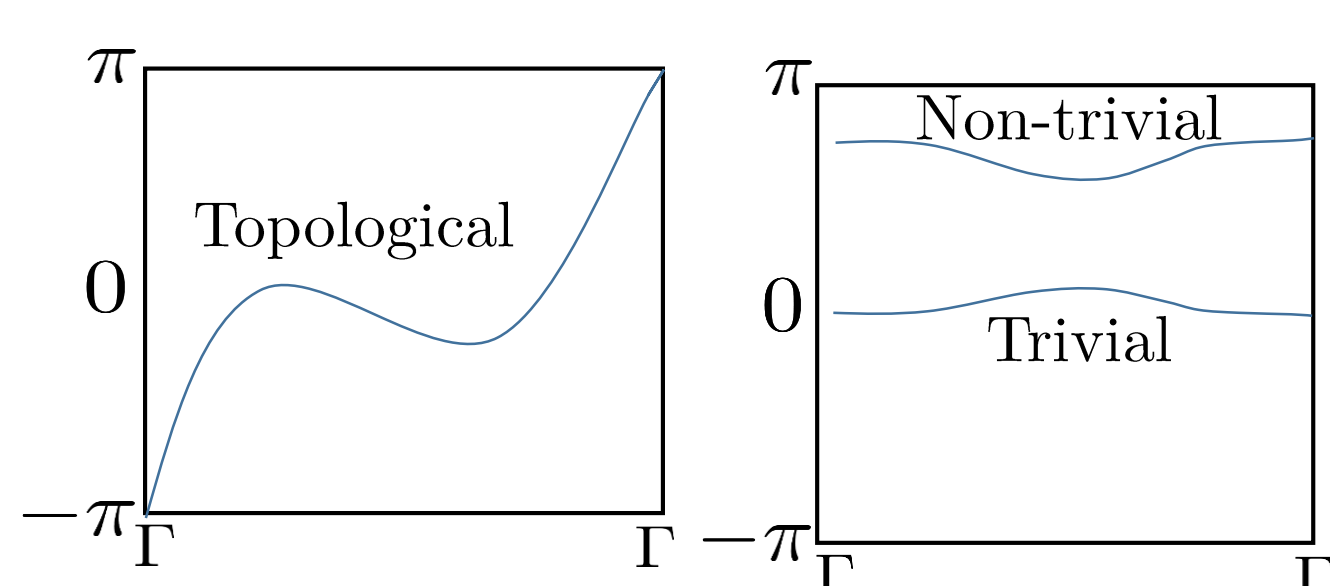


## Wilson loops and Wannier center

$$W_\ell^n = \mathcal{P} \exp \left\{ -i \int_\ell d\ell \cdot \mathbf{A}_n \right\}$$

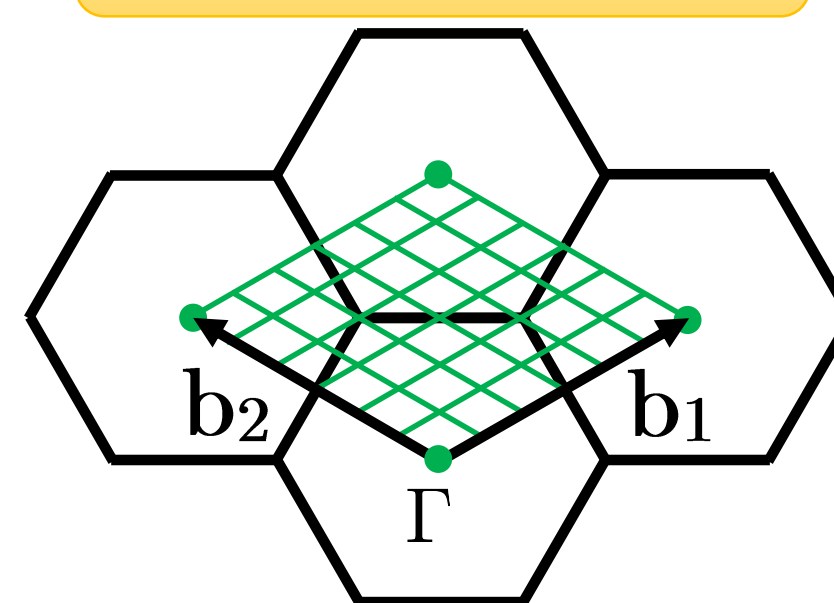
Discretization

$$\begin{aligned} W_{\mathbf{k}+\mathbf{b}_1 \leftarrow \mathbf{k}}^n &= W_{\mathbf{b}_1}^n(k_2) = \\ &= \langle u_n(\mathbf{k} + \mathbf{b}_1) | \prod_{j=1}^{N-1} \mathcal{P}(\mathbf{k}^j) | u_n(\mathbf{k}) \rangle \end{aligned}$$



Non-topological phases  $\mathbf{r}_{WC} = \frac{\vartheta^1}{2\pi} \mathbf{a}_1 + \frac{\vartheta^2}{2\pi} \mathbf{a}_2$

## Discretization



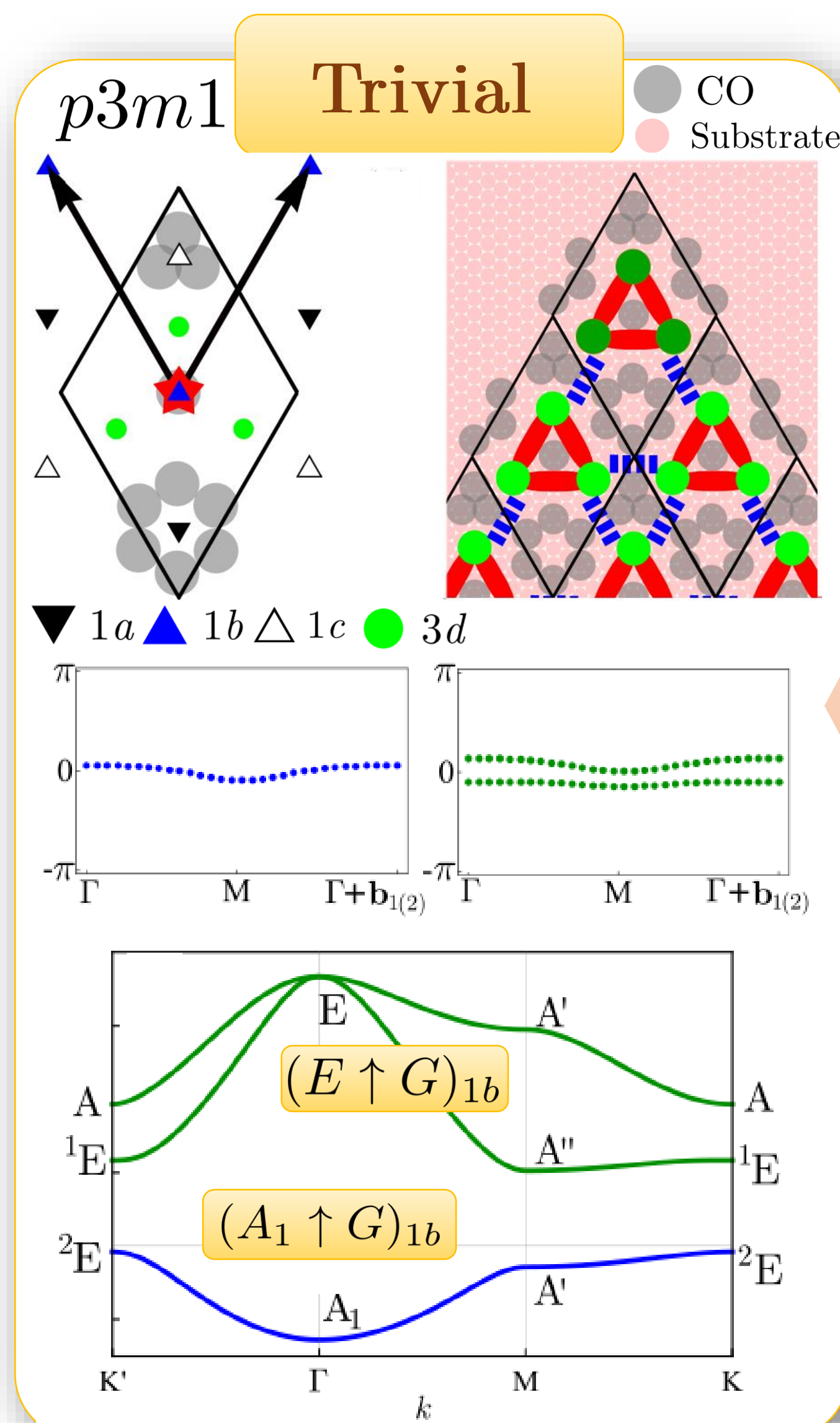
# Topological quantum chemistry

Space group + Irrep assignment + Wannier center

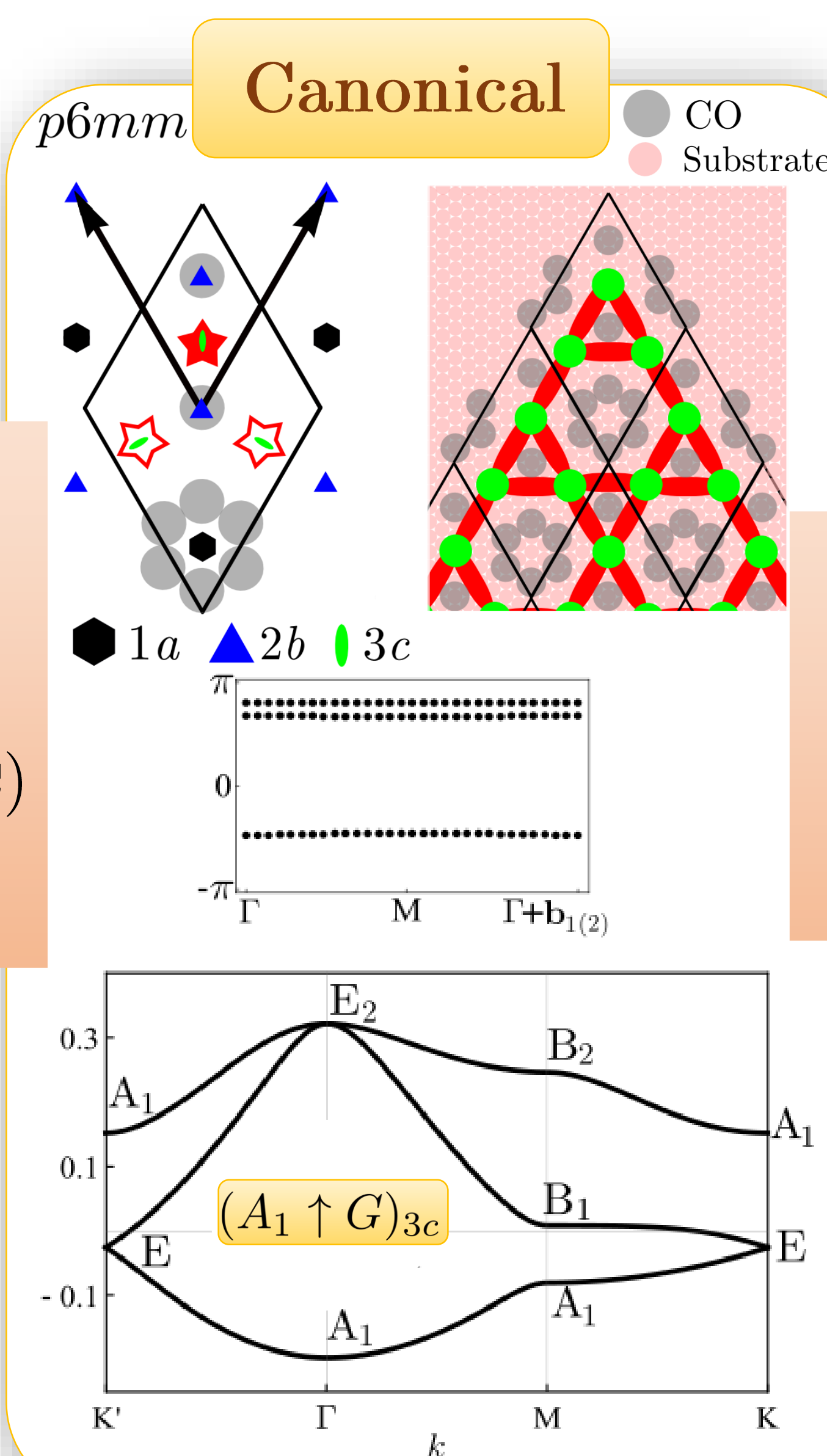
Non-topological band representation +  
Occupied Wyckoff positions

Trivial/non-trivial classification: trivial and obstructed atomic limits

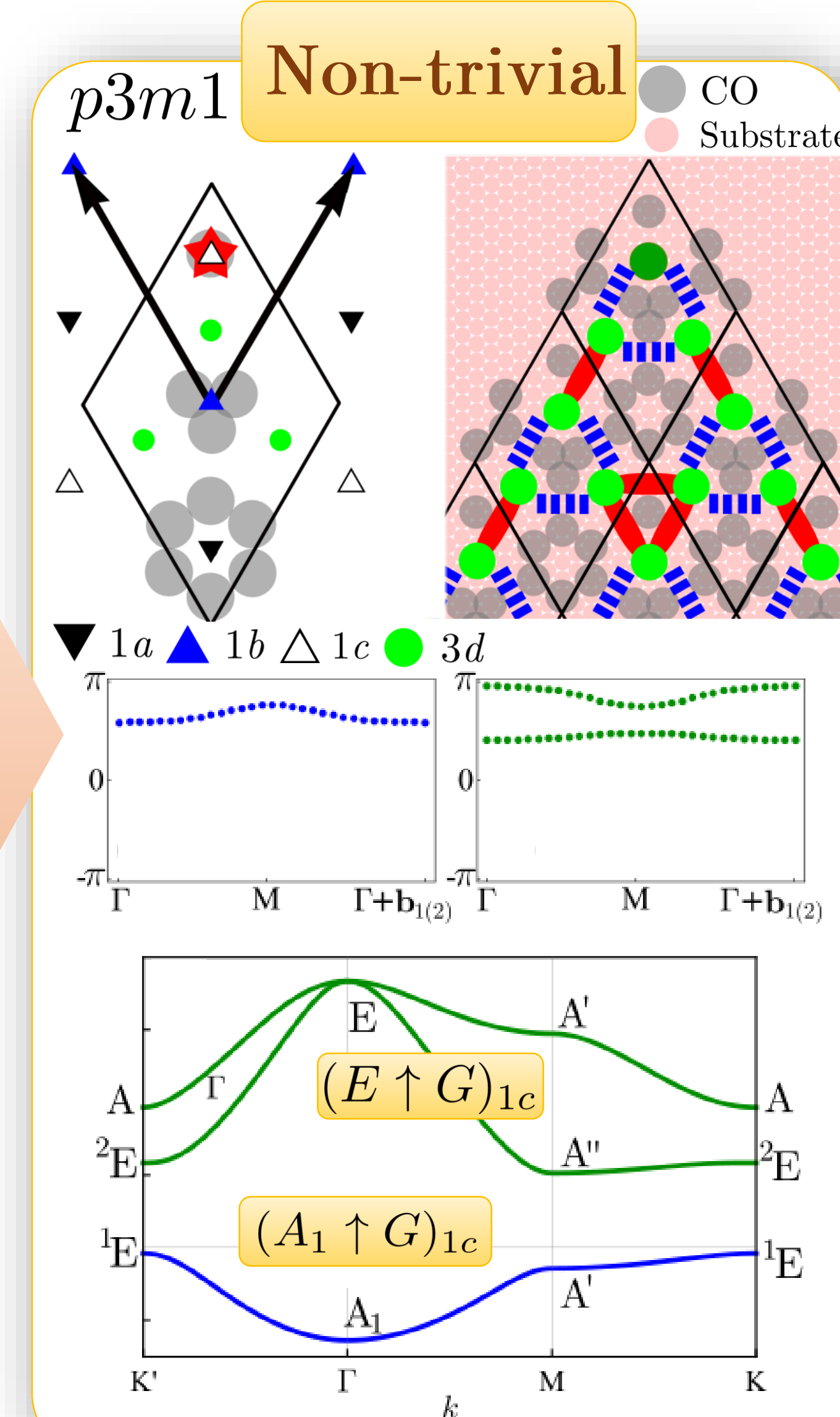
## Breathing kagome lattice + Muffin tin



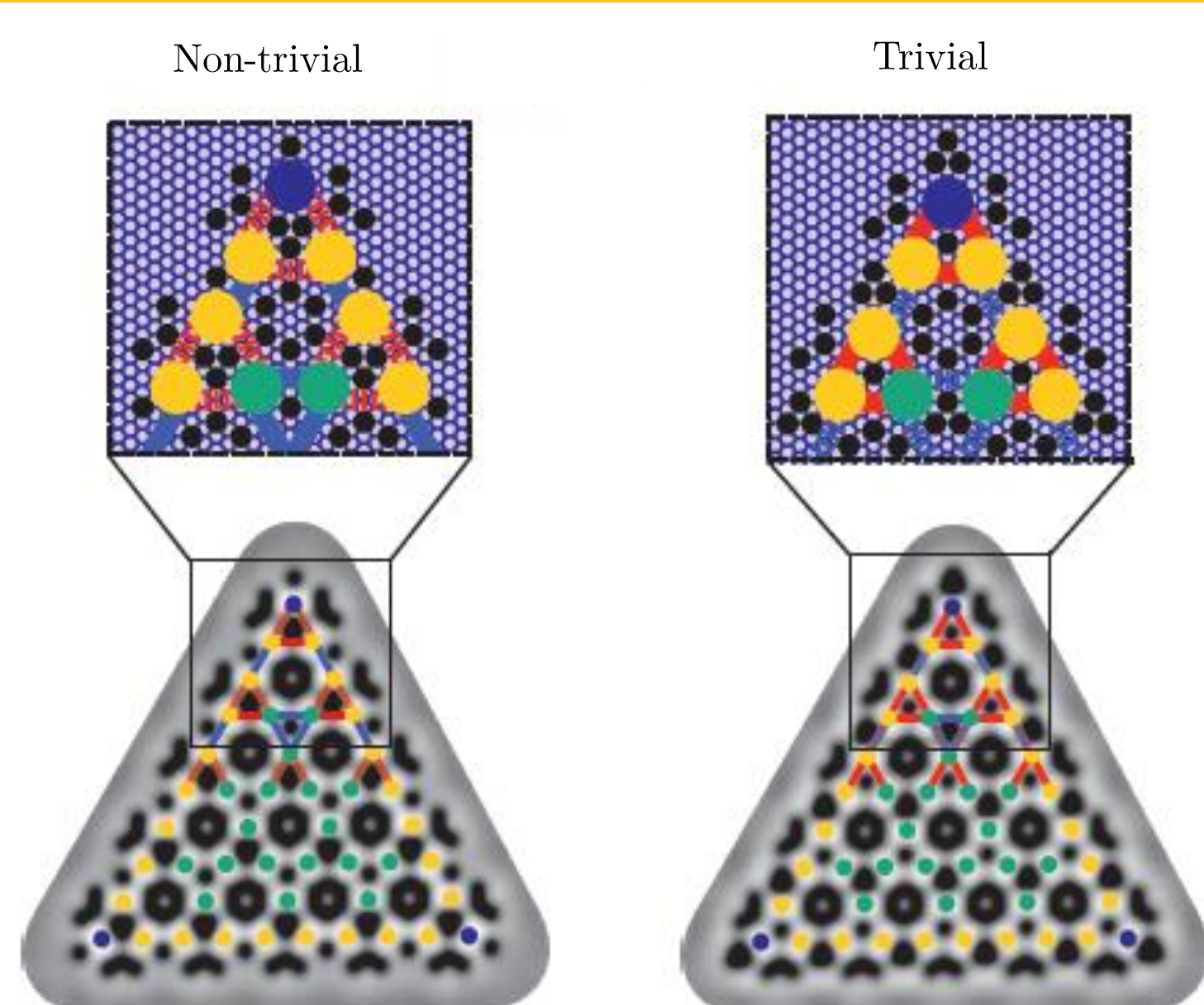
Break  $C_6$  by  
allowing  
intra>inter  
(contracted UC)



Break  $C_6$  by  
allowing  
intra<inter  
(expanded UC)



## Experimental realization



S.N. Kempkes, *et al.* Nature Materials 18, 1292 (2019).

## Conclusions

- The breathing kagome lattice exhibits **two topologically distinct phases**.
- However, these two phases are indeed **non-topological**. They both correspond to (different) **obstructed atomic limits**.
- One of the phases (the non-trivial one) hosts **corner modes**, as well as **edge modes**. Thus, the breathing kagome lattice is **not a HOTI by definition**.
- The corner modes can be perturbed but never removed, so they are robust.
- This robustness depends on three factors: the symmetry of the lattice, the generalized chiral symmetry and in the connectivity of the lattice site.

Check out this work!

 @ma\_jherrera