Band structure and reciprocal space topology of 2D materials

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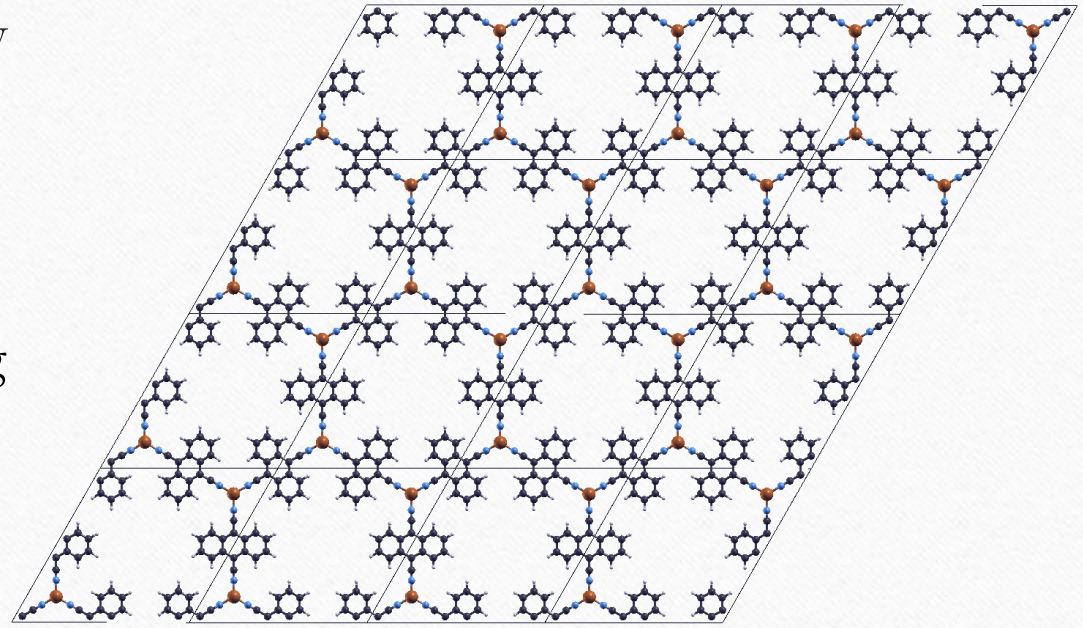
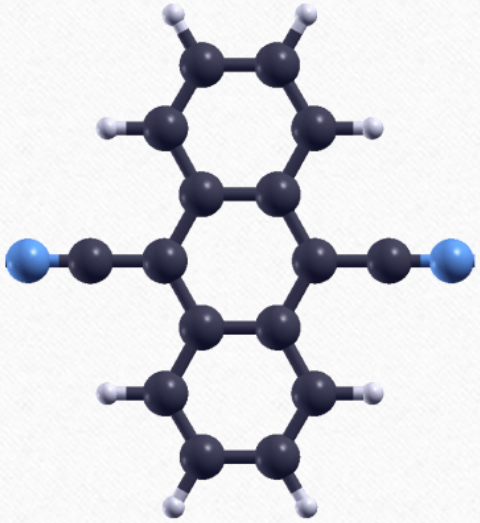
Metal-organic frameworks (MOFs)

- Array of organic molecules linked by metal atoms
  - 4th row: Mn, Fe, Co, Cu
  - 5th and 6th row: Pd, Pt, Ag, Au…
- Porous MOFs might have interesting electronic properties, but often that's not the most stable structure
  - Close packing of the molecules and metals = boring insulators :/



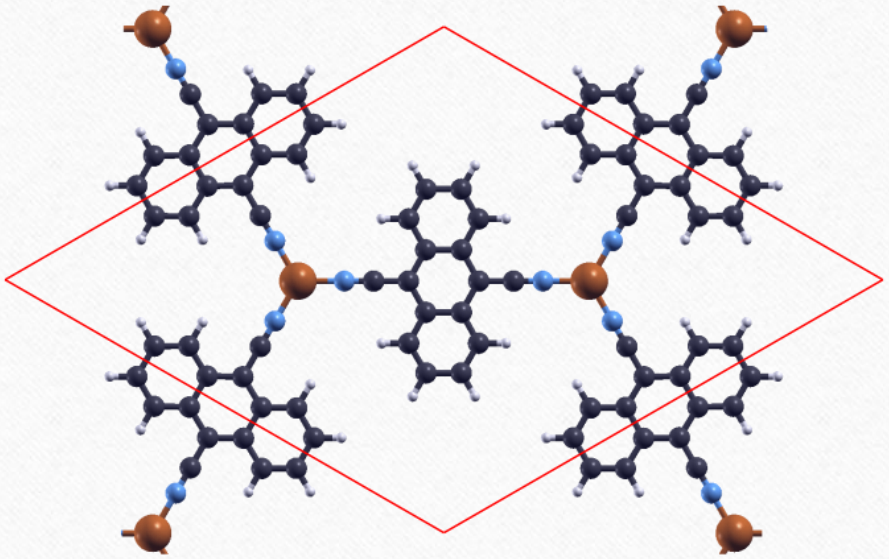
Metal-organic frameworks (MOFs)

DCA molecule



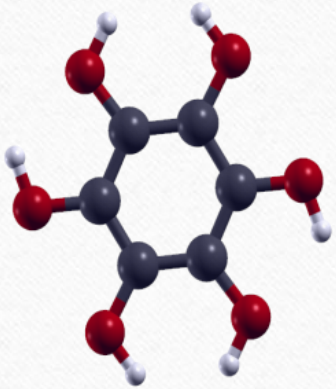
Cu atom

Cu_2DCA_3 2D MOF



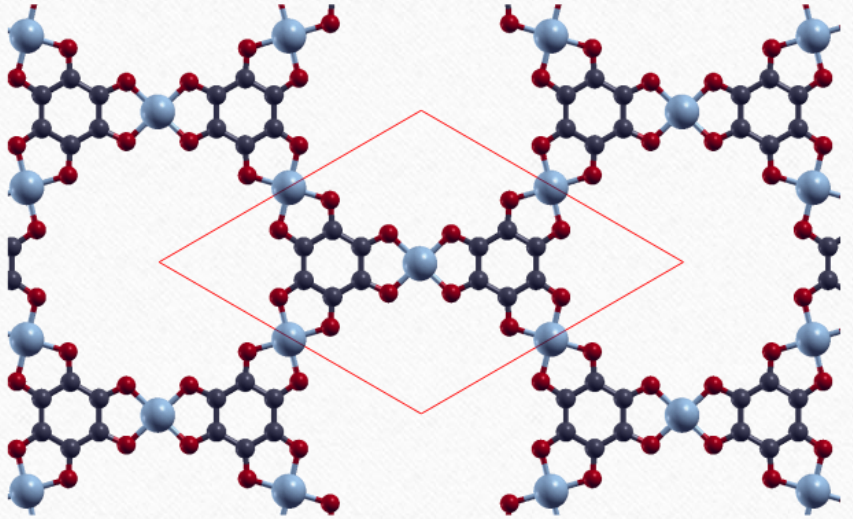
Metal-organic frameworks (MOFs)

HIB molecule

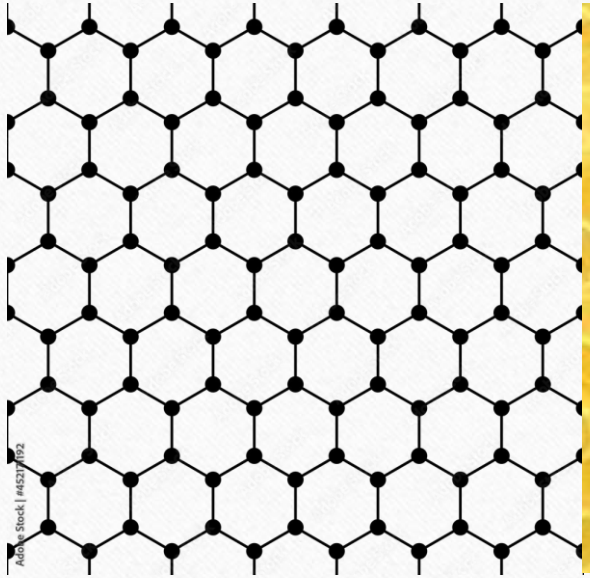


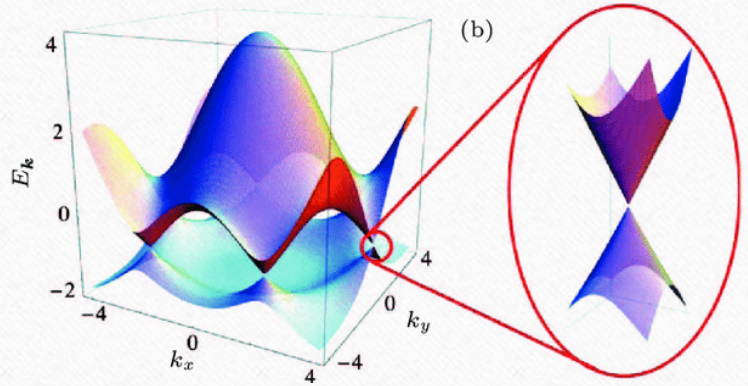
Ni atom

Ni_3HIB_2 2D MOF

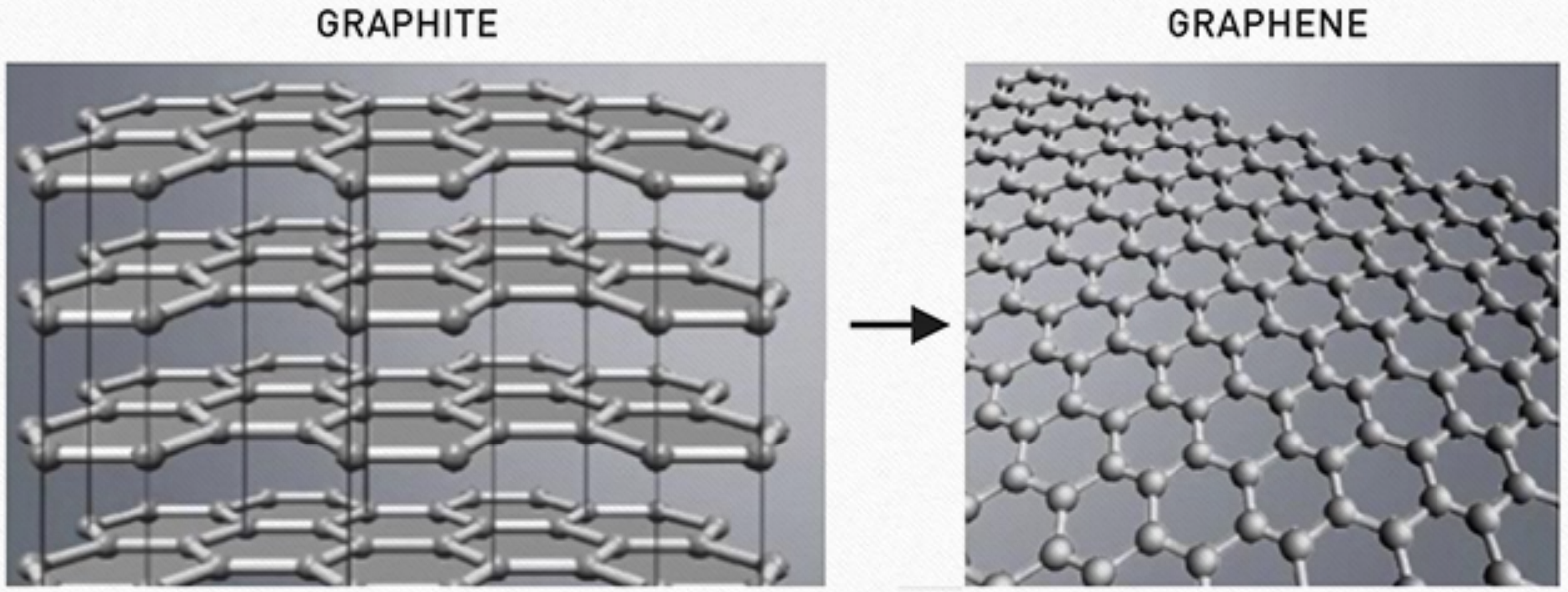


Honeycomb structure





Graphene and graphite band structures



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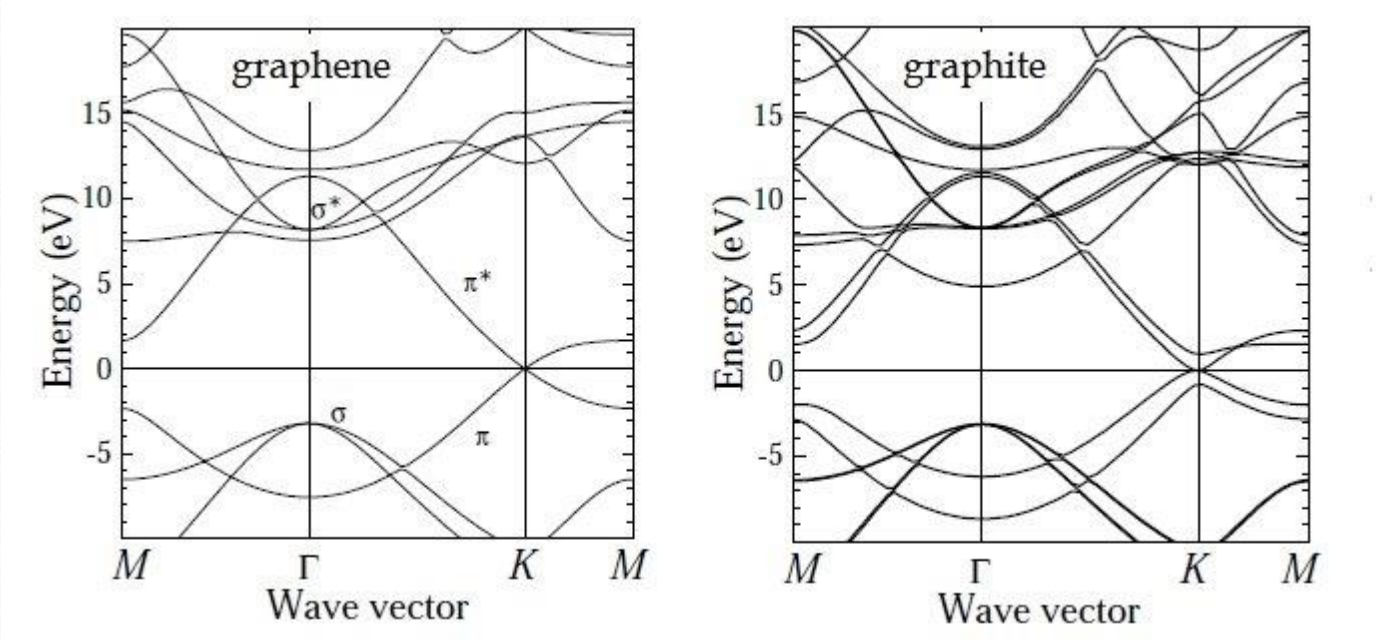

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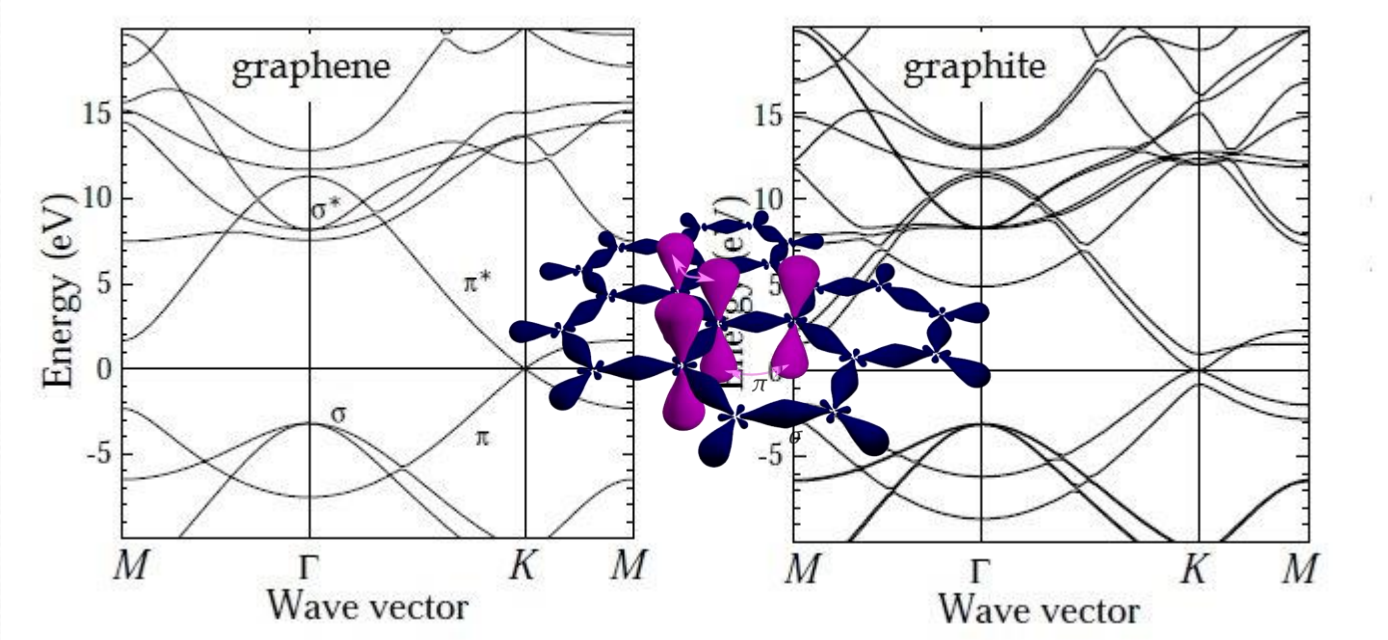

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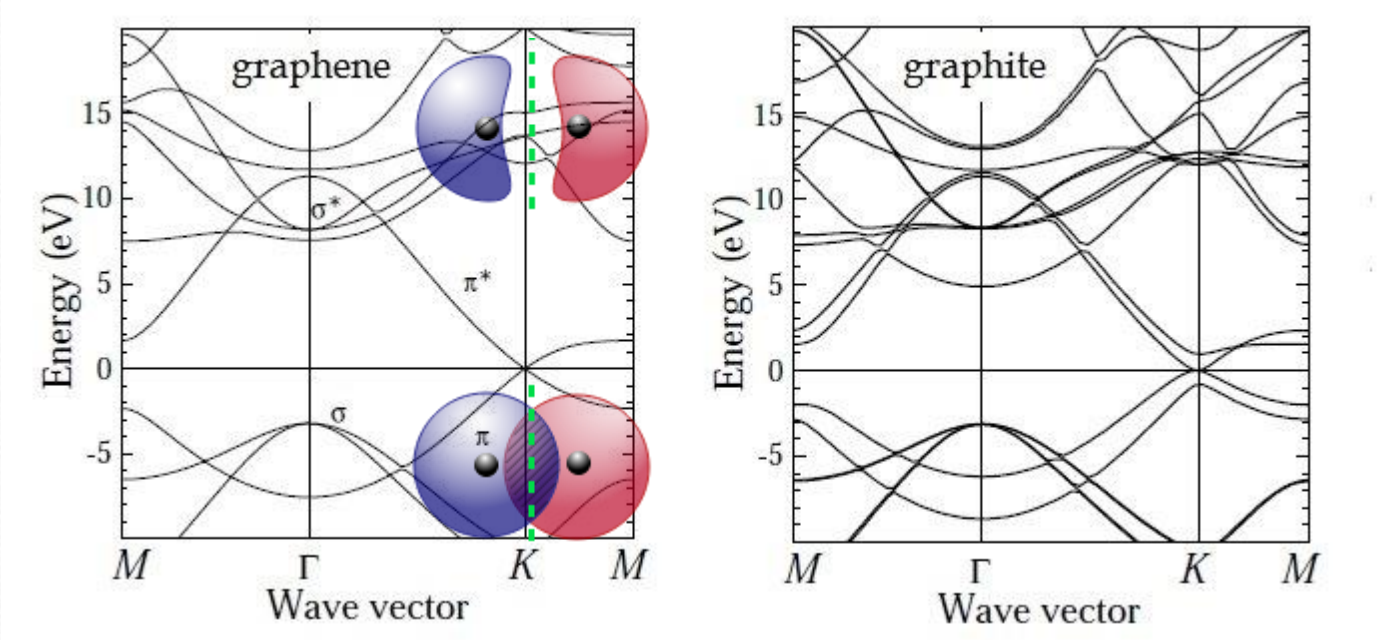
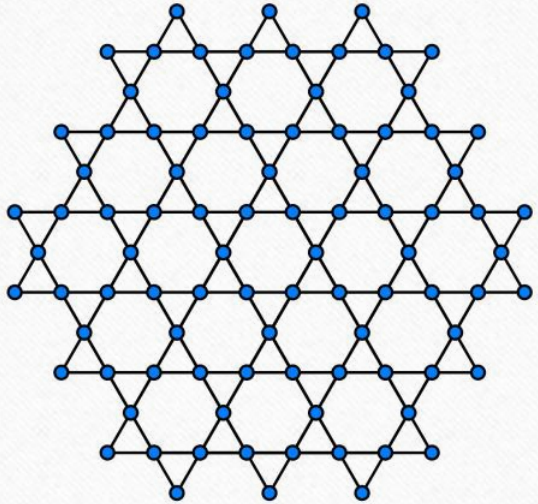
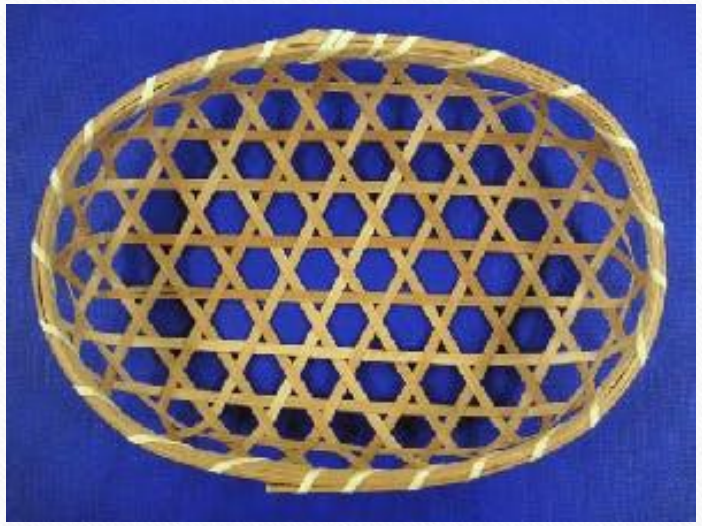
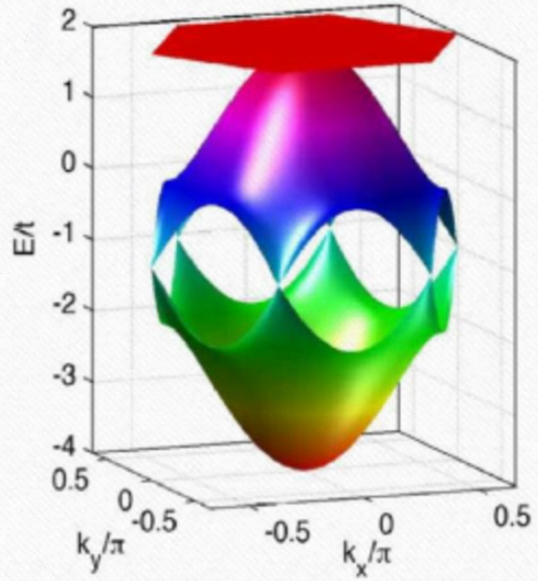


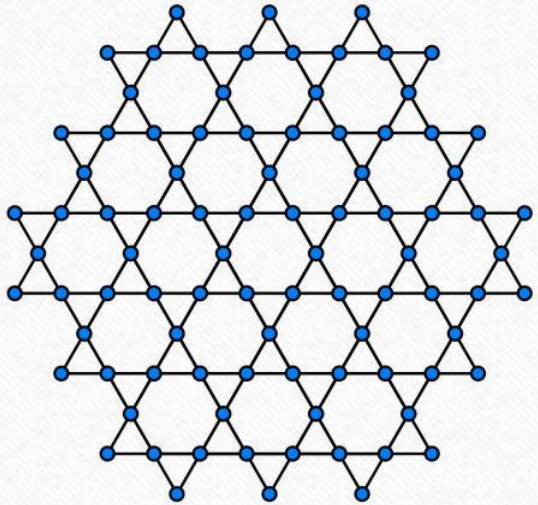
Kagomé structure

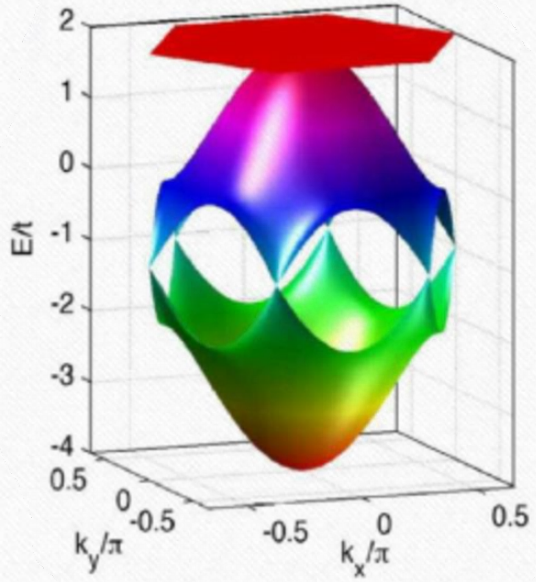




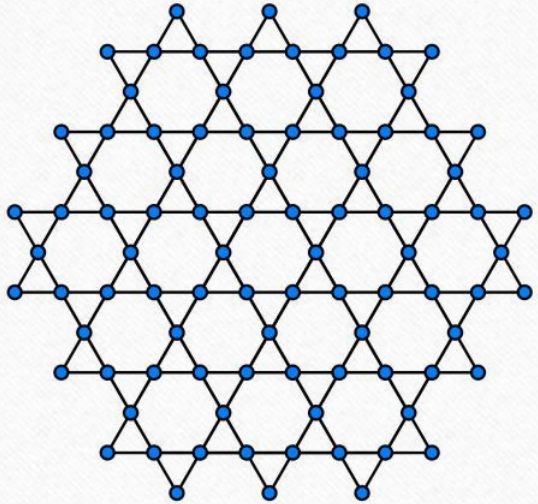


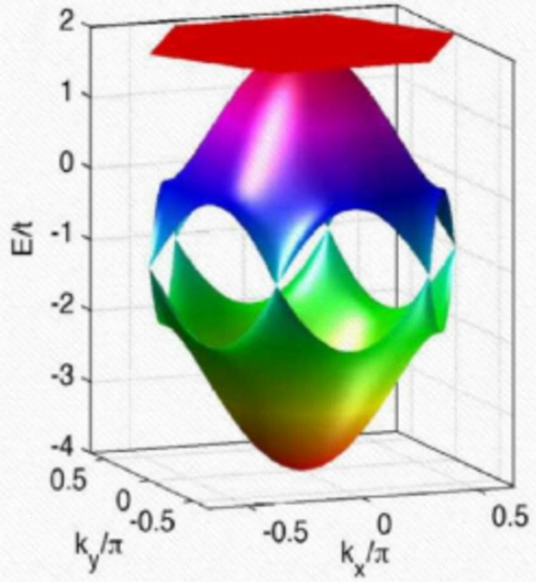
Kagomé/Inuyasha structure





Kagomé/some Japanese juice structure





2D topological insulators

- Property driven by spin-orbit coupling
  - C atoms in graphene are too light to show this effect :/
  - MOFs are potential because of the metal atoms
- "Non-trivial" gap is opened within the linear dispersion
  - Treating the reciprocal space as a topological object
  - The "whole" would be the Berry curvature
  - Topologically protected edge states reside inside the gap

$$H = \left(\frac{p^2}{2m} + V\right) - \frac{p^4}{8m^3c^3} + \frac{e^2}{2m^2c^2r^3}\vec{S}\cdot\vec{L} + \frac{\hbar^2}{4m^2c^2}\nabla^2 V,$$

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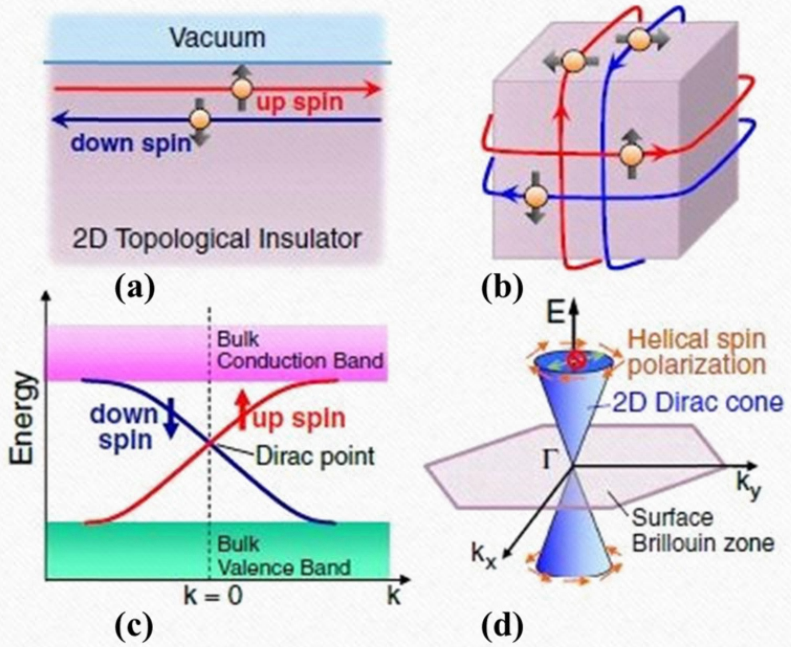
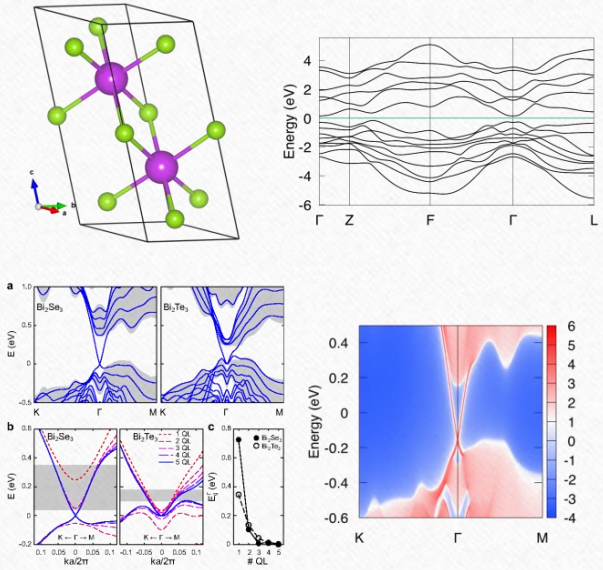


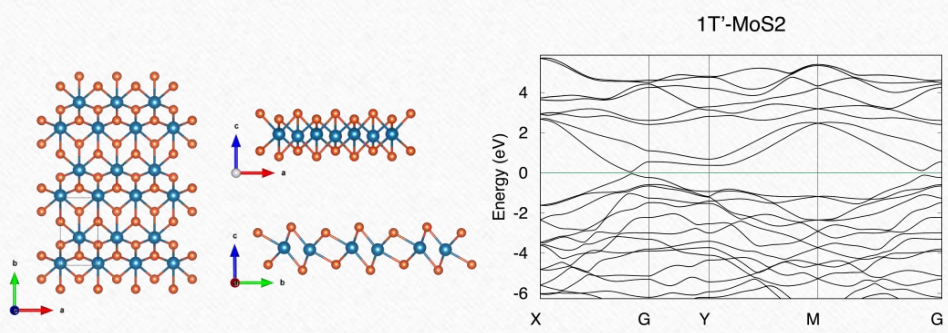
What can we do with DFT?
3D ➞ 2D and 2D ➞ 1D connections

- 3D usually is "easier" to deal with
- Layered materials with vdW forces (not always the case though)
- No dangling bonds when vdW
- We have to converge the band structure with the number of stacking surfaces
- Usually the convergence is easy (not many layers are necessary)
- Even when they are not vdW structures, full DFT calculations are feasible

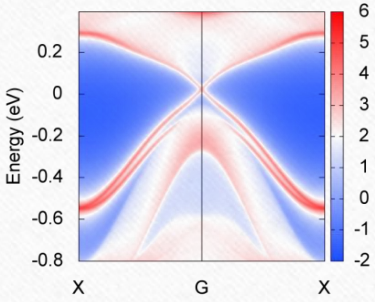
Bi_2Se_3 and Bi_2Te_3
3D topological insulators



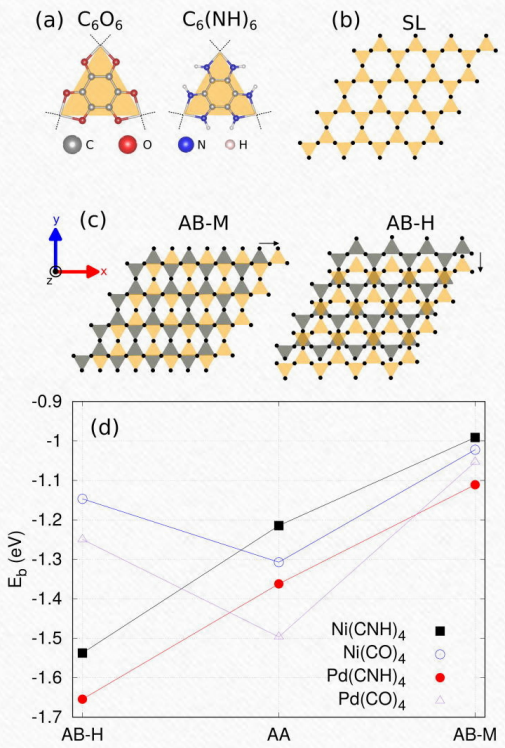
1T' MoS_2 2D Topological insulator

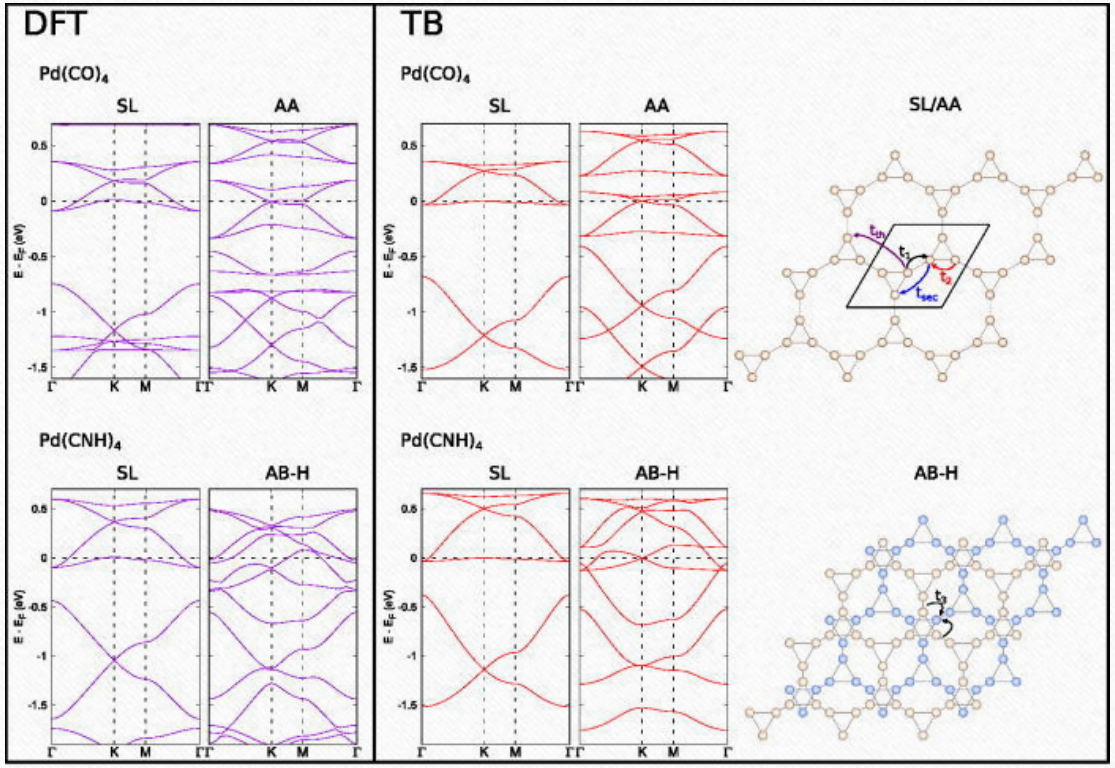


- Things get nasty in 2D
- Lots of dangling bonds when cutting the layers
- H passivation in calculations, but what about real world?)
- Very large strips usually is necessary
- Most predictions were made by "cheating"
- Substrate effects?



My contribution to the ocean of 2D topological insulators





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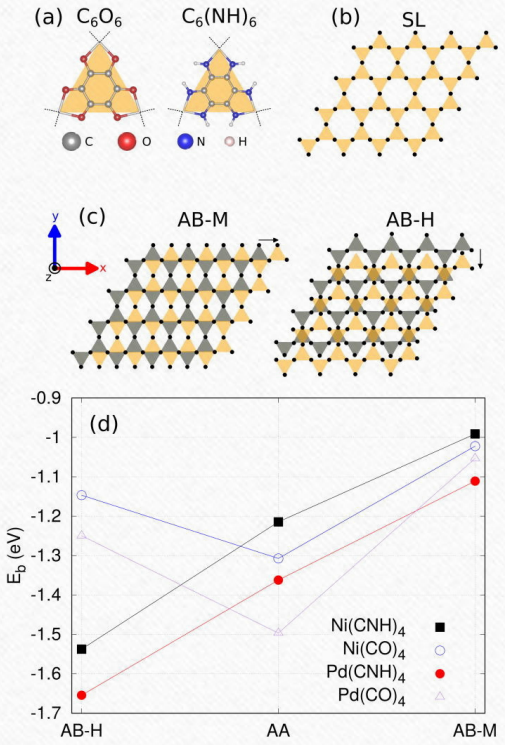

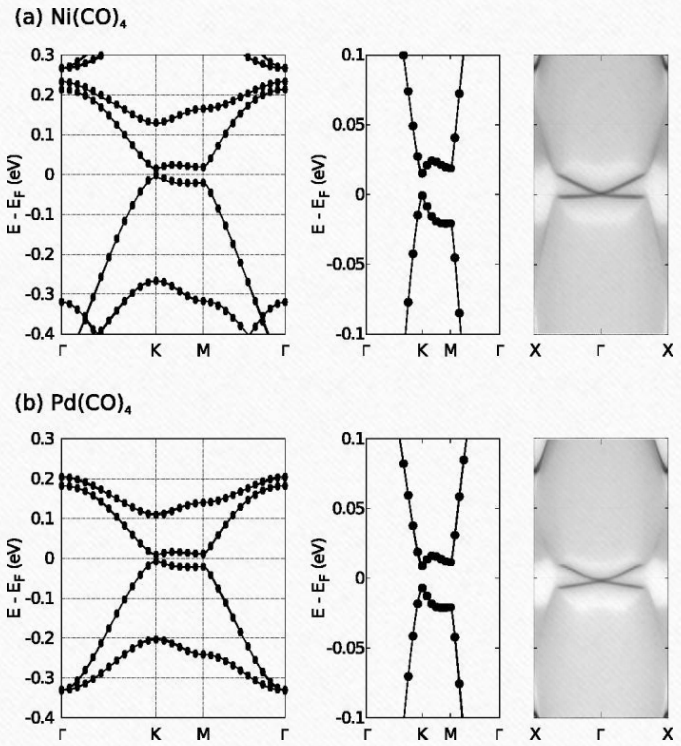

- Transition from metal to "semi metal" phase
  - Monolayer is metallic and AA bilayer is a semi metal
- AB-H is more favorable in the DFT but AA observed in the experiment
  - Metallic substrate
- Spin-orbit coupling splits the bands in K and K' points
- Band gaps of ~ 10 meV (record for 2D ~ 25 meV)


Thanks for the attention!