chem2Dmat

AUGUST 31 – SEPTEMBER 03, 2021 ● ONLINE

Two-Dimensional Polymers: Playing with Structural Topology

Tsai-Jung Liu[1], Maximilian A. Springer[1,2], Agnieszka Kuc[2], Thomas Heine[1,2]

[1]TU Dresden, Bergstraße 66c, 01069 Dresden, Germany

[2]HZDR, Institute of Resource Ecology, Permoserstraße 15, 04318 Leipzig, Germany

Introduction

In two-dimensional (2D) world, beside graphene's honeycomb structure, there are a large amount of mathematically possible 2D lattices, e.g., square (**sql**), kagome (**kgm**) and hexagonal (**hxl**) lattice. These lattices might be difficult to synthesize as Haeckelites like graphene, but there are possibilities to realize them as conjugated 2D polymers. The electronic properties of these conjugated polymers are determined by structural topology and chemical composition. It has been shown that if 2D polymers can be designed within certain structural topology, similar characteristic bands could be obtained [1]. Hence, it's possible to efficiently look over lattices with different structural topology with tight-binding (TB) model, and then implement them in hypothetical 2D polymers with different fragments and linkers.

Methods

Our TB model Hamiltonian:

$$H = \sum_i \varepsilon_i c_i^\dagger c_i + \sum_{\langle i,j\rangle} t_1 c_i^\dagger c_j + \sum_{\langle\langle i,j\rangle\rangle} t_2 c_i^\dagger c_j + H_{\mathrm{SOC}}$$

contains 1st- (t_1) and 2nd-neighbor (t_2) electron hopping parameters with on-site energies ε_i. Spin-orbit coupling (SOC) are also considered and it can be written in Haldane model form as,

$$H_{\mathrm{SOC}} = \sum_{\langle\langle i,j\rangle\rangle} \lambda e^{-i v_{ij}\phi} c_i^\dagger c_j,$$

or in Kane-Mele model form as,

$$H_{\mathrm{SOC}} = i\lambda \sum_{\langle\langle i,j\rangle\rangle} v_{ij} c_i^\dagger \sigma_z c_j,$$

where ϕ is staggered-flux parameter chosen to be $\frac{\pi}{2}$, λ is spin-orbit coupling constant, σ_z is Pauli matrix, and $v_{ij} = 1 \vee -1$ indicates the orientation path of an electron traveling from vertex i to a 2nd-neighbor vertex j.

TB model + **RCSR database [2]**

A catalog of electronic structrues for 101 different lattices [3]

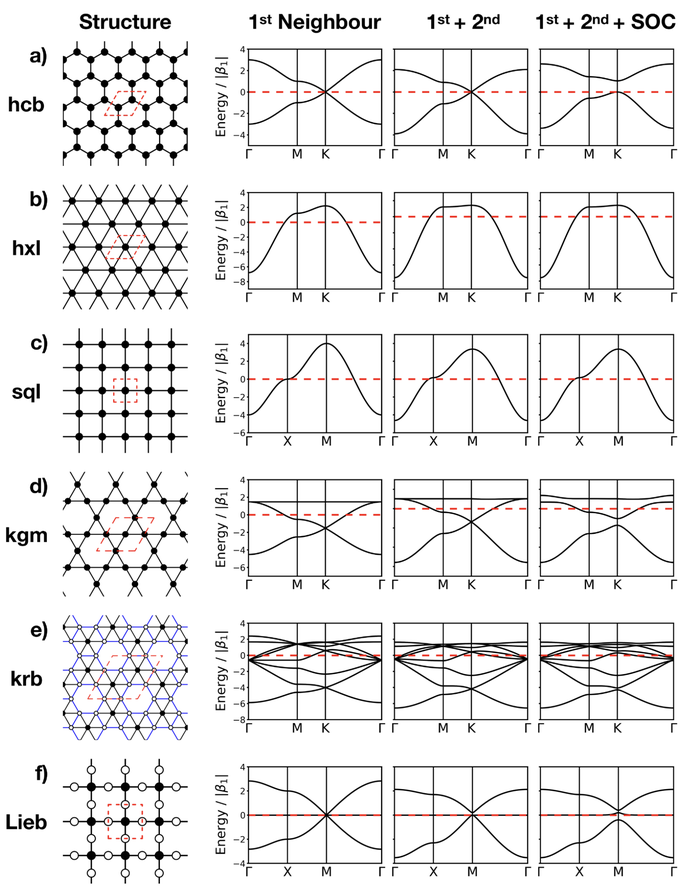

Figure 1: Some of electronic structures for different lattices.

hypothetical 2D polymers

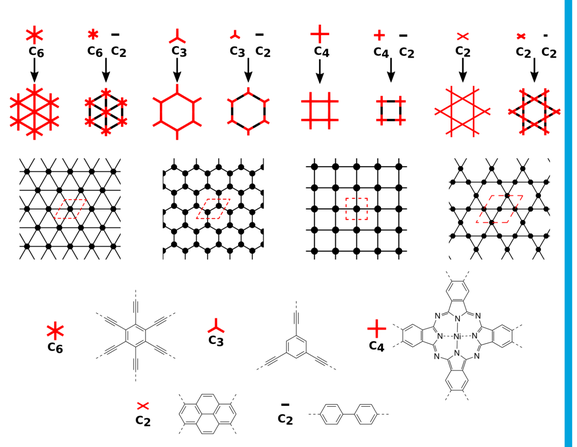

Figure 2: Topology diagram: possible ways to build polymers.

possible method in reality

Tailoring Bands

- By On-site energy ε → Replacing Carbons with Borons or Nitrides
- By Hopping t → Different linkers

Results: fes lattice as an example

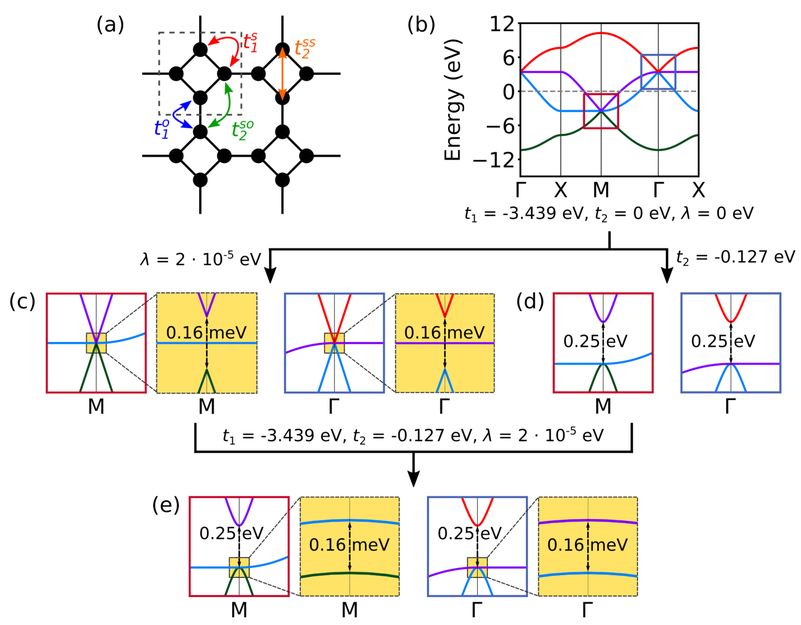

Figure 3: (a) **fes** lattice. (b) Band structure with only 1st-neighbor hoppings ($t_1^o = t_1^s$). (c)-(e) Band structure near originally triply degenerate points (M and Γ) when other interactions are added, i.e., (c) 1st-neighbor hoppings + SOC, (d) 1st- + 2nd-neighbor hoppings, (e) 1st- + 2nd-neighbor hoppings + SOC.

Tailoring Bands

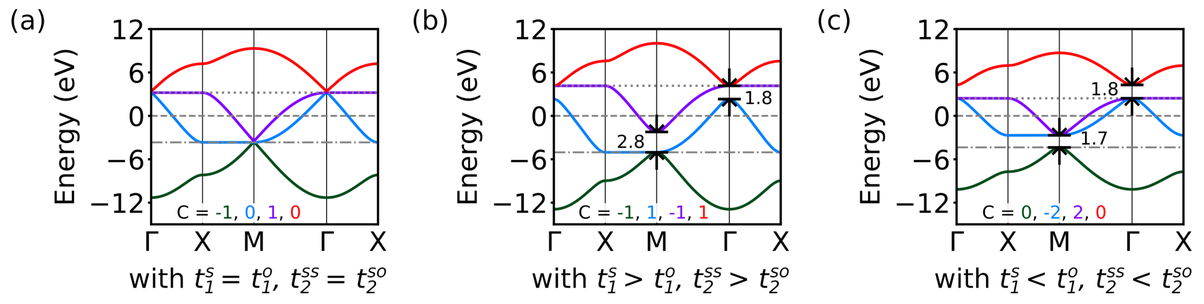

Figure 4: Band structures and corresponding Chern numbers for each band of **fes** lattice. With different 1st- and 2nd-neighbor interactions *t*, gaps can be opened at certain high symmetry points.

Making 2D polymers

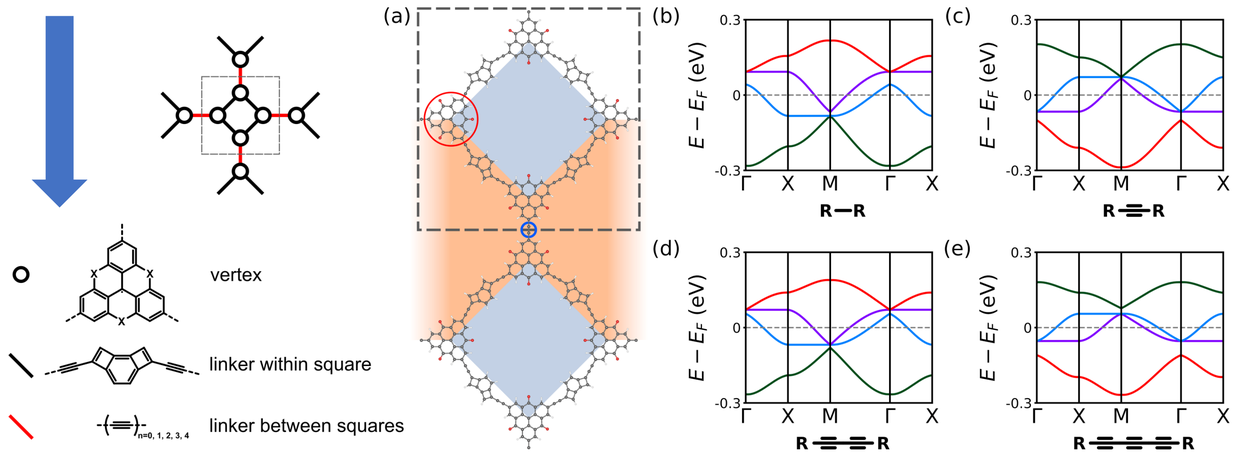

Figure 5: (a) Atomistic structure of a hypothetical 2D polymer with the underlying **fes** net topology and one connecting C_2 unit (blue circle) between triangulene units (red circle). (b-e) Band structures of the hypothetical 2D polymers with different number of C_2 units as linkers connecting the squares. For (b), the electronic effective mass is $m_e^* = 0.01$ (blue band, Γ-point) and for holes is $m_h^* = 0.05$ (purple band, M-point)

Conclusion

- TB model can be used to explore 2D lattices and serves as guidance on building conjugated polymers with same structural topology.
- Example: **fes** lattice → hypothetical 2D polymers
  - Proposed 2D polymers as representative example for implementation → possibility to explore properties via structural modifications (e.g. changing linkers)
  - In this example, SOC-induced band gaps are too small for practical use but low effective masses can be found.

CONTACT PERSON

Tsai-Jung Liu
tsai-jung.liu@tu-dresden.de

REFERENCES

[1] Y. Jing, T. Heine, J. Am. Chem. Soc., 141 (2019), 743−747
[2] http://rcsr.anu.edu.au/
[3] M. A. Springer, T. J. Liu, A. Kuc, T. Heine, Chem. Soc. Rev., 49 (2020), 2007-2019

chem2Dmat
AUGUST 31 – SEPTEMBER 03, 2021 ● ONLINE