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Two-Dimensional Polymers: Playing with Structural Topology

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In two-dimensional (2D) world, graphene is one of the most popular material for its intriguing electronic and topological properties. 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]. With the efficiency provided by tight-binding (TB) model with its low computation cost, we ran through Reticular Chemistry Structure Resource (RCSR) database [2], and got electronic band structures for 101 different lattices [3]. We further show that band gaps could be tuned by choosing different 1st- and 2nd-neighbor interactions (Fig. 1) or different on-site energies. And then we also give an example, in which we propose hypothetical 2D polymers with **fes** structure, and implement band tuning by inserting different linkers in these polymers.

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

Figures

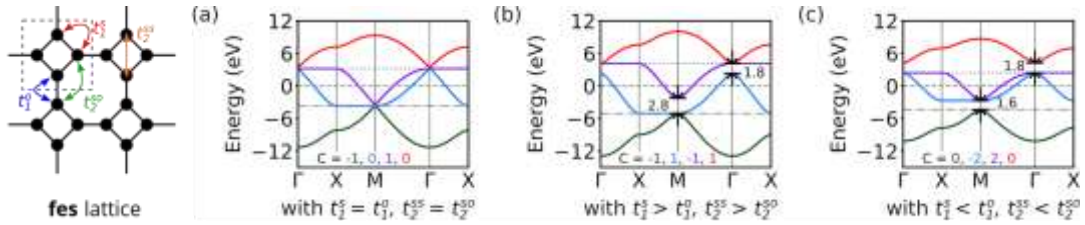

Figure 1: Band structures and the corresponding Chern numbers for each band of **fes** (also known as square-octagon) lattice as representative example. With different 1st- and 2nd-neighbor interactions *t*, gaps can be opened at certain high symmetry points.