Mattermorphosis

Thomas Heine
TU Dresden , Germany
thomas.heine@tu-dresden.de

The properties of a material are defined by their composition and structure. This principle of chemistry is well-known for decades and the basis for the development of molecules and materials. In my talk, I will show some factors that define materials properties beyond their intrinsic characteristics: In the first part, I will show how the edge structure in graphene nanoribbons determines the band gap (including metallic state!) and electronic topology of these all-carbon materials. In the second, I will discuss superlattice states in transition metal dichalcogenide bilayers, which can form flat bands, Dirac or kagome features depending on the twist angle. In the final part, I will discuss how the underlying lattice topology can define the properties of a 2D framework material, such as a 2D polymer, covalent-organic framework or metal-organic framework.
Some of the introductory literature are given below (if you don't have access, they are also available on arXiv or chemRXiv.

References

[1] Structure-Imposed Electronic Topology in Cove-Edged Graphene Nanoribbons. F. M. Arnold, T.-J. Liu, A. Kuc, T. Heine, Phys. Rev. Lett. 129 (2022) 216401
[2] Topological two-dimensional polymers. M. A. Springer, T.-J. Liu, A. Kuc, T. Heine, Chem. Soc. Rev. 49 (2020) 2007-2019
[3] 2D Conjugated Polymers: Exploiting Topological Properties for the Rational Design of Metal-Free Photocatalysts. Y. Jing, X. Zhu, S. Maier, T. Heine, Trends Chem. 4 (9) (2022) 792-806