High throughput Topological Classification of Graphene Nanoribbons using Machine Learning

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Recent progresses in nanoscale atomic manipulation [1,2] and in the understanding of the topological properties of organic polymers [3,4,5] offer new opportunities for the bottom-up synthesis of topologically-non-trivial artificial lattices, with possible use in quantum sensing and computing. With this regard, the dependence of topological properties on the shape or geometries of the nanostructures formed with these artificial lattices are largely unexplored. In this work, we perform high throughput topological classification of mirror symmetric graphene nanoribbons using machine learning. We use a Monte Carlo based search technique to sample different geometries of GNRs from the huge design space. The topological classification is based on the quantized value of the electronic polarization for the given unit cell. The electronic polarization is obtained from the 1D Hybrid Wannier Charge centers[6] computed by solving the tight-binding Hamiltonian. Such cheap yet reasonably accurate tight-binding model allows us to perform high throughput screening of geometries across the design space to identify topologically non-trivial nanostructures. Furthermore, we train a deep neural network (DNN) on the accumulated data. Our DNN performs the topological classification with more than 90 percent accuracy. Our approach is general and can be easily extended to 2D nanostructures and other lattices beyond graphene.

References:

[1] Gomes et al. “Designer Dirac fermions and topological phases in molecular graphene” Nature 483, 306 (2012)
[2] Slot et al. “p-Band Engineering in Artificial Electronic Lattices”, PHYSICAL REVIEW X 9, 011009 (2019)
[3] Cao et al. “Topological Phases in Graphene Nanoribbons: Junction States, Spin Centers, and Quantum Spin Chains” Phys. Rev. Lett. 119, 076401 (2017)
[4] Gröning et al. “Engineering of robust topological quantum phases in graphene nanoribbons” Nature 560, 209–213 (2018); Rizzo et al. “Topological band engineering of graphene nanoribbons” Nature 560, 204–208 (2018)
[5] Lee et al. “Topological Phases in Cove-Edged and Chevron Graphene Nanoribbons: Geometric Structures, Z2 Invariants, and Junction States” Nano letters 18.11 (2018): 7247-7253
[6] Gresch et al. “Z2 pack: Numerical Implementation of hybrid Wannier centers for identifying topological materials”, Phys. Rev. B 95, 075146 (2017)