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Topological insulators are a class of materials that have robust conducting states at the boundary but are insulating in the bulk. They have very promising applications in spintronics and novel electronics devices. The previous research of topological insulators focus on 2D or 3D systems, however, topological phase can also exist in one-dimensional system. Graphene nanoribbons, as a 1D carbon nanostructure, has been reported to host topological phase as well[1-3], which is manifested as localized end states or junction states. The topological phase in carbon nanostructures can be used to build quantum spin chain, spin qubit, or to realize Majorana fermions[1-2]. The previous research on topological phase in graphene nanoribbons focused on the long ribbon limit. However, the localized states exist also in nanographene molecules. Here we extended the topological phase calculation to more general structures, and studied the relation between localized state in small-molecule limit and long periodic ribbon limit. These results will be useful in guiding the design of graphene nanostructures for applications in electronics, spintronics, and quantum technologies,

References

- [1] Cao, Ting, Fangzhou Zhao, and Steven G. Louie, Physical review letters, 119.7 (2017): 076401.
- [2] Rizzo, Daniel J., et al., Nature, 560.7717 (2018): 204-208.
- [3] Gröning, Oliver, et al., Nature, 560.7717 (2018): 209-213.

Figures

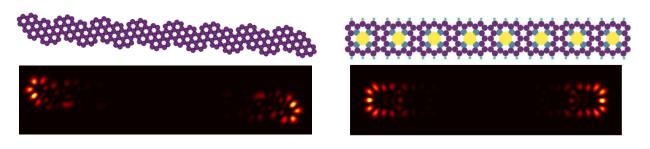


Figure 1: Simulated Local Density of States map of graphene nanoribbon and porphyrin nanoribbon.

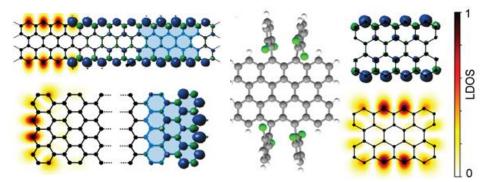


Figure 2: Localized zigzag states in nanographene molecule and long graphene nanoribbons.